South Asia Ferroelectric Symposium Bengaluru, India

IEEE

SAFS 2025

5th-8th August, 2025

ABSTRACT BOOKLET

DAY 0

5TH AUGUST 2025

PRE-CONFERENCE TUTORIAL

Day 0		
Tutorials		
8.00-9.30	***Breakfast and registration***	
9:30-11:00	T01	Andrew Bell Title: Fundamental of Piezoelectrics
11.00-11:30	***Tea break***	
11.30-13.00	T02	Andrei Kholkine Title:Piezoforce Microscopy for Ferroelectrics
13:00-14:30	***Lunch break***	
14:30-15:30	T03	Bhagwati Prasad Title: Ferroelectric and mutliferroic devices: device physics (Device 1)
15:30-15:45	***Tea Break***	
15:45-16:45	T04	Veeresh Deshpande Title: Ferroelectric devices and technology integration

SCHEDULE AT A GLANCE...

Schedule at a glance

Day 1	
7.30-8.30	Breakfast and registration
8.30-9.00	**Opening remarks and Inauguration (Main Hall)**
Plenary Session 1 (Main Hall) **Chair: Dragan Damnjanovic (President UFFC-s officers)**	
9.00-9.40	P1: Andrew Bell (Title: Inside Piezoelectricity: why we need both hard and soft interatomic bonds to maximise energy conversion)
9.40-9.45	Mini break
9.45-10.35	**Parallel sessions 1, 2 (Main Hall, Hall A)**
10.35-11.00	**Tea break**
11.00-13.00	**Parallel sessions 3, 4 (Main Hall, Hall A)**
12.55-14.10	**Lunch break**
Plenary Session 2 (Main Hall) **Chair: Florencio Sanchez (ICMAB, Spain)**	
14.10-14.50	P2-Uwe Schroeder (Title: Ferroelectric Doped HfO2-based Devices: Recent progress and future challenges)
14.50-14.55	Mini break
14.55-15.45	**Parallel sessions-5, 6 (Main Hall, Hall A)**
15.45-16.05	**Tea break**
16.05 - 18.00	**Parallel sessions-7, 8 (Main Hall, Hall A)**
18.00 - 19.30	**Poster session-1 (Tea)**
19.30 onwards	Dinner

Day 2	
7.30-9.00	Breakfast and registration
Plenary Session 3 (Main Hall) **Chair: Saswata Bhattacharya (IIT Hyderabad)**	
9.00-9.40	P3: Umesh Waghmere (Title: Polar Half-Metal and Triferroic Insulator based on PbMnO3: First-principles Theory)
9.40-9.45	Mini break
9.45-10.35	**Parallel sessions 9,10 (Main Hall, Hall A)**
10.35-11.00	**Tea break**
11.00-13.00	**Parallel sessions 11, 12 (Main Hall, Hall A)**
12.50-14.00	
Plenary Session 4 (Main Hall) **Chair: Vasant Sathe (UGC-DAE-CSR Indore)**	
14.00-14.40	P4-Andrei Leonidovitch Kholkine (Title: Magnetoelectric nanostructures: synthesis, properties and applications)
14.40-14.45	Mini break
14.45-15.35	**Parallel sessions-13, 14 (Main Hall, Hall A)**
15.35-16.00	**Tea break**
16.00 - 18.10	**Parallel sessions-15, 16 (Main Hall, Hall A)**
18.10 - 19.30	**Poster session-2 (Tea)**
19.30 onwards	Conference Dinner

Day 3	
7.30-9.00	Breakfast and registration
Plenary Session 5 (Main Hall) **Chair: Bharat Jalan (Univ of Minesotta)**	
9.00-9.40	P5: Lane Martin (Title: Advances in Ferroelectric-, Antiferroelectric-, and Relaxor-based Thin Films and Heterostructures)
9.40-9.45	Mini break
9.45-10.35	**Parallel sessions 17, 18 (Main Hall, Hall A)**
10.35-11.00	**Tea break**
11.00-13.00	**Parallel sessions 19, 20 (Main Hall, Hall A)**
12.55-14.00	**Lunch break**
14.00-15.35	**Parallel sessions 21, 22 (Main Hall, Hall A)**
15.35-16.00	**Tea break**
16.00-17.15	**Session 23 (Main Hall)**
17.30-18.15	**Valedictory (Main Hall)**

DAY 1

6TH AUGUST 2025

Day 1

Main Hall			Hall A		
Session 1 (Thin films and properties)			**Session 2 (Bulk ferroelectrics)**		
Chair: Ranjit Ramadurai (IIT Hyderabad)			**Chair: Kaustuv Datta (HZB)**		
Time	Name	Topic	Time	Name	Topic
9.45-10.10	I1: Murugavel (IIT Madras)	Ferroelectric photovoltaic and flexo-photovoltaic effect in bandgap-engineered ferroelectric system	9.45-10.10	I2: V Raghavendra Reddy (UGC-DAE)	Hyperfine interactions in Pb free BaTiO3 based relaxors
10.10-10.35	I3: Vasant Sathe (UGC-DAE)	Optical control of ferroelectric domain structure in $BaTiO_3$	10.10-10.35	I4:Boomishankar Ramamoorthy (IISER Pune)	Ferroelectric Materials Based on Hybrid Metal-Isothiocyantes
10.35-11.00	**Tea break**		10.35-11.00	**Tea break**	
Session 3 (Membranes and 2D ferroelectrics)			**Session 4 (Bulk ferroelectrics)**		
Chair: P. Murugavel (IIT Madras)			**Chair: Saket Asthana (IIT Hyderabad)**		
11.00-11.25	I5: Ying Hao Chu (NTHU, Taiwan)	MICAtronics for flexible ferroelectric memory, piezoelectric actuator, and pyroelectric sensing	11.00-11.25	I6: Kaustuv Datta (Helmholtz Zentrum, Berlin)	Decoding structure-property connections in perovskite ferroelectric oxides via total scattering method
11.25-11.45	Y1: Varun Harbola (MPI, Stuttgart)	Heterostructure and interface design beyond epitaxy	11.25-11.45	Y2: Digvijay Singh (IISc Bengaluru)	From Delusion to Reality: The Isosymmetric Transition in $BiFeO_3$-$PbTiO_3$ and Its Complex Phase Diagram
11.45-12.00	O1: Shubham Parate (IISc Bengaluru)	Operando characterization of temperature assisted ferroelectric to paraelectric phase transitions in In2Se3	11.45-12.00	O2: Saujatya Mandal (IISc Bengaluru)	Micromechanical Insights into Texture and Stress-Driven Electromechanical Behavior in Ferroelectric PZT
12.00-12.15	O3: Soumyaranjan Sahoo (IIT Madras)	Freestanding Ferroelectric Oxide Membranes Designed by Epitaxy for Device Applications	12.00-12.15	O4: Gudeta Jafo (IISc Bengaluru)	Simultaneous increase of d33 and Cuire point of PZT: the phenomenon and mechanism
12.15-12.40	I7: Daisuke Kan (Osaka University, Japan)	Ultrathin Freestanding Membranes of Ferroelectric Hafnia	12.15-12.40	I8: Saurabh Tripathi (IIT BHU)	Impact of Local Structural Ordering on the Thermal Expansion of Relaxor Ferroelectrics
12.40-12.55	O5: Harshita Seksaria (INST Mohali)	Origin of strain tunability in flat valence band and ultrahigh shear piezoelectricity in superflexible non–van der Waals graphitic ScX monolayers (X = P, As, Sb)	12.40-12.55	O6: Pooja Punetha (IISc Bengaluru)	Short range structural correlations and property anomalies in non-MPB compositions of the Pb-free piezoelectric Na0.5Bi0.5TiO3-K0.5Bi0.5TiO3
12.55-14.00	**Lunch Break**		**12.55-14.00**	**Lunch Break**	
Session 5 (Ferroelectric films and device performance)			**Session 6 (Bulk ferroelectrics)**		
Chair: Ying Hao Chu (NTHU)			**Chair: Dillip Kumar Pradhan (NIT Rourkela)**		
14.55-15.20	I9: James Raju (University of Hyderabad)	Ferroelectric thin films for microwave devices: material, measurement, processes and devices	14.55-15.20	I10: Saket Asthana (IIT Hyderabad)	Advancing Ecofriendly Ferroelectrics for Next-Generation Energy Storage and flexible electronics
15.20-15.45	I11: Jayakant Ravichandran (University of Southern California)	Limits to Reliability of Ferroelectric Capacitors	15.20-15.45	I12: Akhilesh Kumar Singh (IIT BHU)	Crystallographic Analysis of Phase Coexistence in Piezoelectric MPB Ceramics by Rietveld Structure Refinement
15.45-16.05	**Tea break**		15.45-16.05	**Tea break**	
Session 7 (Heterostructures and characterization)			**Session 8 (Bulk ferroelectrics)**		
Chair: Jayakant Ravichandran (USC)			**Chair: VRK Murthy (VIT A.P.)**		
16.05-16.30	I13: Srimanta Middey (IISc Bengaluru)	Emergent phases in incipient ferroelectrics upon dilute electron doping	16.05-16.30	I14: Debraj Choudary (IIT Kgp)	Towards realization of metastable ferroelectric phase in orthorhombic rare-earth chromates
16.30-16.50	Y3: Somnath Kale (CEA Saclay, France)	Ferroelectric Size Effects on Statics and Dynamics of Domain Wall	16.30-16.50	Y4: Gobinda Das Adhikary	Large longitudinal electrostrain and electrobending deformation in polycrystalline piezoelectrics
16.50-17.05	O7: Naveen Negi (IISc Bengaluru)	Investigation of Electrical and Multifunctional Properties in High-Entropy BFO–BTO–STO Perovskites	16.50-17.05	O8: Abhinav Kumar (IIT Hyderabad)	Analysis of the comparative scaling behaviour between slanted and square-type polarisation loops in Nb^{5} /Ho^{3} co-substituted NBT systems for enhanced energy storage performance
17.05-17.20	O9: Yeswant Pattipati (IISc Bengaluru)	Epitaxial in-plane ferroelectric BaTiO3 integrated onto Si through a single MgO buffer layer for electrooptic applications	17.05-17.20	O10: Ananda Babu (SSN Univeristy)	Structural, relaxor behaviour, dielectric and energy storage properties of lead-free (1−x)Ba0.95La0.05TiO3–xBi(Zn2/3Ta1/3)O3 ferroelectrics
17.20-17.45	I15: Anju Ahlawat (SAGE university)	Light modulated Magnetization in Ferromagnetic/PMN- PT Heterostructures	17.20-17.45	I16: Dillip Pradhan (NIT Rourkela)	Structural phase transitions and enhancement of physical properties in Li and Ta modified K0.5Na0.5NbO3 system
17.45-18.00	O11: Dipankar Sarkar (IACS, Kolkata)	Antiferroelectric to Ferroelectric Phase Transition and Electrocaloric Effect in Epitaxial $PbZrO_3$ Thin Films	17.45-18.00	O12: SK Upadhyay (HNB Garhwal University)	Re-entrant-like behavior in modified BaTiO3 with pinched hysteresis loop

DAY 2

7TH AUGUST 2025

Day 2

Main Hall			Hall A		
Session 9 (Epitaxial thin films and local polarziation measurements)			**Session 10 (Solution processed ferroelectric devices)**		
Chair: Srimanta Middey (IISc Bengaluru)			**Chair: Pavan Pujar (IIT BHU)**		
Time	Name	Topic	Time	Name	Topic
9.45-10.10	I17: Jieun Kim (KAIST, South Korea)	Understanding Polarization Rotation in Relaxor Ferroelectrics Using Epitaxial Thin Films	9.45-10.10	I18: Subho Das Gupta (IISc) Bengaluru	Fully Printed Negative-Capacitance Field-Effect Transistors with Ultralow Subthreshold Swing and High Inverter Signal Gain
10.10-10.35	I19: César Magén (INMA, CSIC, Zaragosa, Spain)	Probing polar distortions in ferroic oxide films with atomic resolution electron microscopy	10.10-10.35	I20: Bholanath Pal (IIT BHU)	Ferroelectric thin film for memory and neuromorphic device application
10.35-11.00	**Tea break**		10.35-11.00	**Tea break**	
Session 11 (Unconventional ferroelectrics: Hafnia)			**Session 12 (Piezoelectric devices and MEMS)**		
Chair: Jordan Bouaziz (EC Lyon)			**Chair: James Raju (Univ. of Hyderabad)**		
11.00-11.25	I21: Pavan Pujar (IIT BHU)	Solution-Processed Doped-Hafnia Ferroelectrics on Silicon: A Pathway to Commercial Integration	11.00-11.25	I22: Gayathri Pillai (IISc Bengaluru)	Exploring Temperature and Bias-Dependent Switchability and Tuneability of BST based LKu Band MEMS Resonators
11.25-11.45	Y5: Jalaja M (IISc, Bengaluru)	Proximity induced phase transitions in solution processed La doped Hafnia	11.25-11.45	Y6: Shiuan Wu (NTHU, Taiwan)	Gelatin Exfoliation Process: Enhance The Potential of Ferroelectric Component in Electronic Skin Applications
11.45-12.00	O13: Anjana Thomas (Ecole Centrale Lyon)	Enhancing Polarization and Reliability in HZO-Based FTJs Using WOx Electrodes and Interfacial Layers	11.45-12.05	Y7: Sandeep Kongbrailatpam (IISc Bengaluru)	Observation of Akhiezer and Landua-Rumer Regimes in the Temperature Dependence of Longitudinal Wave in BST on Sapphire BAW Resonator
12.00-12.25	I23: Florencio Sanchez (ICMAB, Spain)	Strategies for maximizing polarization in ferroelectric HfO2	12.05-12.30	I24: Siddhartha Ghosh (Northeastern University)	Design and Fabrication of Phononic Integrated Circuits in Scandium Aluminum Nitride
12.25-12.40	O14: Soumyajyoti Mondal (IISc Bengaluru)	Tailoring Ferroelectric HfO_2 Thin Films: A Comprehensive Study of Deposition Parameters, Thermal Treatment, and Electrode Effects	12.30-12.50	Y8: Praveen Kumar (IISc Bengaluru)	Generation of Phononic Frequency Combs via Nonlinear Mode Coupling in Curved Circular Piezoelectric MEMS Resonators
12.40-14.00	**Lunch Break**		**12.50-14.00**	**Lunch Break**	
Session 13 (Epitaxial films and characterization)			**Session 14 (Ferroelectric thin films and topology)**		
Chair: César Magén (INMA, CSIC, Zaragosa, Spain)			**Chair: Ram Janay Chaudary (UGC-DAE)**		
14.45-15.10	I25: Ranjith Ramadurai (IIT Hyderabad)	Polarization Orientation Mapping in Polycrystalline and Epitaxially Grown BCZT Thin Films using Piezoresponse Force Microscope	14.45-15.10	I26: Sudhansu Mandal (IIT Kgp)	Polar Skyrmions in Planes of Strained Ferroelectric Systems
15.10-15.35	I27: John Heron (University of Michigan, USA)	Material-Limited Switching in Nanoscale Ferroelectrics	15.10-15.35	I28: Sujit Das (IISc Bengaluru)	Harnessing the polar vortex motion and tunable skyrmion liquid phase in oxide heterostructures
15.35-16.00	**Tea break**		15.35-16.00	**Tea break**	
Session 15 (Epitaxial thin films and emergent order)			**Session 16 (Ferroelectric/piezoelectric thin films: performance and applications)**		
Chair: John Heron (Univ. Michigan)			**Chair: Gayathri Pillai (IISc Bengaluru)**		
16.00-16.25	I29: Bharat Jalan (University of Minnesota)	Emerging Polar Altermagnetic Metallic States in Epitaxially Strained RuO2 Films	16.00-16.25	I30: Soma Dutta (NAL Bengaluru)	Real time Applications of Piezoelectric and Ferroelectric Materials: A perspective of Material Response to Device Qualification
16.25-16.50	I31: Ram Janay Choudary (UGC-DAE)	Room Temperature Giant Inverse Magnetoelectric Effect in Topotactic Phase Transition Material SrCoO2.5	16.25-16.45	Y9: Antony Jeyaseelan (IISc Bengaluru)	Different textured PZT films grown on Si/Pt substrate
16.50-17.05	O15: Mohit Tanwani (IISc, Bengaluru)	Tuneable skyrmion liquid phase in polar skyrmions	16.45-17.10	I32: Dipankar Mandal (INST Mohali	Initiatives in Piezoelectric Voiceprint for Biometric Healthcare Assessment
17.05-17.20	O16: Kusumpal Yadav (IACS Kolkata)	Ferroelectricity induced giant topological Hall effect in epitaxial multiferroic thin film heterostructures	17.10-17.25	O17: Khadeer Pasha (VIT, A.P.)	Flexible and Wearable Polyvinyl Alcohol/Chitosan/$Ti_3C_2T_x$ MXene-Based Piezoelectric Hydrogels
17.20-17.45	I33: Sayantika Bhowal (IIT Bombay)	Emergent Surface Multiferroicity	17.25-17.50	I34: Abhijit Sangle (IIT Bombay)	Growth of Lead-free Heteroepitaxial Thin Films of (Na0.8K0.2)0.5Bi0.5TiO3 Ferroelectrics by Nd:YAG Laser Pulsed Laser Deposition
17.45-18.10	I42: Saswata Bhattacharya (IIT Hyderabad)	From Constraints to Complexity: Thermodynamic Pathways to Domain Formation in Ferroelectrics	17.50-18.10	Y10: Subhajit Pal (Queens Mary, London)	Photoinduced properties in ferroelectric oxides

DAY 3

8TH AUGUST 2025

Day 3

Main Hall			Hall A		
Session 17 (Ferroelectric/piezoelectric investigation: new measurement approaches)			**Session 18 (Multifunctional ferrroelectrics)**		
Chair: Bhagwati Prasad (IISc Bengaluru)			**Chair: Akhilesh Kumar (IIT BHU)**		
Time	Name	Topic	Time	Name	Topic
9.45-10.10	I35: Saurabh Chandorkar (IISc Bengaluru)	Superharmonic resonant response measurement: a new method to measure spontaneous polarization	9.45-10.10	I36: Devajyoti Mukherjee (IACS Kolkata)	Exploiting giant electrocaloric effects in epitaxial thin films of ferroelectric and antiferroelectric perovskite oxides
10.10-10.35	I37: Pavan Nukala (IISc Bengaluru)	Visualizing solid-state amorphization in 2D ferroelectrics	10.10-10.35	I38: Anirban Chowdhury (IIT Patna)	Giant Electrostriction in La2Ce2O7 Ceramic: Is Texture Always Helpful for Functional Properties?
10.35-11.00	**Tea break**		10.35-11.00	**Tea break**	
Session 19 (Multiferroics, sensing and novel experimental approaches)			**Session 20 (Theoretical tools and multiferroics)**		
Chair: Saurabh Chandorkar (IISc Bengaluru)			**Chair: Sudhansu Sekhar Mandal (IIT Kgp)**		
11.00-11.20	Y11: Binoy De (UGC-DAE/IISc Bengaluru)	A new approach to measure ferroelectric ionic displacement using polarized Raman spectroscopy	11.00-11.25	I39: Ravi Kashikar (IITRAM, Gujarat)	Tunable spin polarization in ferroelectric hybrid organic inorganic perovskites
11.20-11.45	I40: Tuhin Maity (IISER Trivendrum)	Crossing the limits by interface engineering in nano-scale multiferroics	11.25-11.45	Y12: Urmimala Dey (LIST)	Insights into Multifunctional Properties of Ferroelectrics from Atomistic Simulation
11.45-12.05	I41: Maheswaran Shanmugam (IIT Bombay)	Unlocking Single-Phase Magneto-Electric Materials Through Discrete Molecular Architectures	11.45-12.00	O18: Riya Pathak (IISER Tvm)	Curie-Weiss cross-over and quantum spin liquid behavior in multiferroic TbInO3 thin films
12.05-12.30	I43: Arockia Rajan (IIT Madras)	Magnetoelectric Performance of Epoxy-Modulated Ni/PZT/FeGa Composites for Pressure and Displacement Sensing Applications	12.00-12.25	I44: Sobhit Singh (Rochester, USA)	Phase Transitions and Elastic Anomalies in Ferroelectric Hafnia Under Pressure
12.30-12.50	Y13: Ajay Kumar (IISc Bengaluru/INST Mohali)	Nanoconfinement driven mechanical and thermal properties of ferroelectric molecular complex	12.25-12.45	Y14: Subhadeep Bandyopadhyay (CNR Spin, Italy)	Latent electronic (anti-) ferroelectricity in BiNiO3
12.55-14.00	**Lunch Break**		**12.55-14.00**		
Session 21 (Ferroelectric devices and applications)			**Session 22 (Energy harvesting and piezoelectric devices)**		
Chair: Jieun Kim (KAIST, South Korea)			**Chair: Dipankar Mandal (INST Mohali)**		
14.00-14.25	I45: Shankar Selvaraja (IISc Bengaluru)	Highly Oriented PZT Platform for Polarization-Independent Photonic Integrated Circuit and Enhanced Efficiency Electro-Optic Modulation	14.00-14.25	IT1: Abhay Kochar (Optorun)	Piezoelectric Resonators: Powering the Next Wave of RF Communication
14.25-14.40	O19: Md Hanif Ali (IIT Bombay)	Way to achieve Highly Improved State-of-the-Art Ferroelectric Properties in Hf0.5Zr0.5O2 at Low Processing Temperature	14.25-14.40	O20: Sruti Muralikrishnan (IIT Hyderabad)	Microstructure and piezoresponse force microscopy studies on neodymium titanate thin film - a high temperature ferroelectric
14.40-15.05	I46: Jordan Bouaziz (Ecole Centrale Lyon)	State-of-the-Art Research on Hf-ZrO_2 Ferroelectric and Antiferroelectric capacitors	**14.40-14.55**	O21: Nilotpal Deka (IISER Pune)	A Highly Electrostrictive A2BX4-type Hybrid 2D Perovskite Ferroelectric and The Utility of its Composite Piezoelectric Nanogenerator in Wireless Mat-Sensor Technology
15.05-15.30	I47: Veeresh Deshpande (IIT Bombay)	CMOS back-end-of-line compatible Hf0.5Zr0.5O2 ferroelectric devices	**14.55-15.10**	O22: Parvathy Ravindranath (INST Mohali)	Two-Phase Energy Harvesting via Magneto-Pyroelectric Coupling
15.30-16.00	**Tea break**		15.10-15.25	O23: Rajashi Halder (IIT Bombay)	Energizing Tomorrow: Biocompatible Ferroelectric Cu(II) Complexes for Sustainable Energy Harvesting
Session 23 (Devices for memory and neuromorphic applications)					
Chair: Veeresh Deshpande (IIT Bombay)					
16.00-16.20	Y15: Anouk Goussens (CNRS Thales)	Towards room-temperature ferroelectric-spin-orbit (FESO) devices based on perovskite ferroelectrics			
16.20-16.45	I48: Bhaswar Chakraborty (IIT Madras)	Reliability of doped hafnium oxide FeFETs: challenges and mitigation strategies			
16.45-17.10	I49: Arvind Ajoy (IIT Palakkad)	Harnessing the Double-Well potential of Ferroelectrics for Enhanced Sensing and Electromechanical Actuation			
17.10-17.35	IT2: Rohini Kitture (Wiley)	Mastering Research Publishing: Insights from Editor's Desk			

INDEX

FOR

TALKS & POSTERS

Tutorials

No.	Tutor	Title	Page No.
T1	Andrew Bell	Fundamentals of Piezoelectrics	2
T2	Andrei Kholkine	Piezoforce Microscopy for Ferroelectrics	3
T3	Bhagwati Prasad	Ferroelectric and multiferroic devices: Device Physics (Device 1)	4
T4	Veeresh Deshpande	Ferroelectric devices and technology integration	5

Plenary Talks

No.	Presenter	Title	Page No.
P1	Andrew Bell	Inside Piezoelectricity: why we need both hard and soft interatomic bonds to maximise energy conversion	7
P2	Uwe Schroeder	Ferroelectric Doped HfO_2-based Devices: Recent progress and future challenges	8
P3	Umesh Waghmare	Polar Half-Metal and Triferroic Insulator based on $PbMnO_3$: First-principles Theory	9
P4	Andrei Leonidovitch Kholkine	Magnetoelectric nanostructures: synthesis, properties and applications	10
P5	Lane Martin	Advances in Ferroelectric-, Antiferroelectric-, and Relaxor-based Thin Films and Heterostructures	11

Invited Talks

No.	Presenter	Title	Page No.
I1	Murugavel	Ferroelectric photovoltaic and flexo-photovoltaic effect in bandgap-engineered ferroelectric system	13
I2	V Raghavendra Reddy	Hyperfine interactions in Pb free $BaTiO_3$ based relaxors	14
I3	Vasant Sathe	Optical control of ferroelectric domain structure in $BaTiO_3$	15

I4	Boomi Shankar Rammurthy	Ferroelectric Materials Based on Hybrid Metal-Isothiocyantes	16
I5	Ying Hao Chu	MICAtronics for flexible ferroelectric memory, piezoelectric actuator, and pyroelectric sensing	17
I6	Kaustuv Datta	Decoding structure-property connections in perovskite ferroelectric oxides via total scattering method	18
I7	Daisuke Kan	Ultrathin Freestanding Membranes of Ferroelectric Hafnia	19
I8	Saurabh Tripathi	Impact of Local Structural Ordering on the Thermal Expansion of Relaxor Ferroelectrics	20
I9	James Raju	Ferroelectric thin films for microwave devices: material, measurement, processes and devices	21
I10	Saket Asthana	Advancing Ecofriendly Ferroelectrics for Next-Generation Energy Storage and flexible electronics	22
I11	Jayakant Ravichandran	Limits to Reliability of Ferroelectric Capacitors	24
I12	Akhilesh Kumar Singh	Crystallographic Analysis of Phase Coexistence in Piezoelectric MPB Ceramics by Rietveld Structure Refinement	25
I13	Srimanta Middey	Emergent phases in incipient ferroelectrics upon dilute electron doping	26
I14	Debraj Choudary	Towards realization of metastable ferroelectric phase in orthorhombic rare-earth chromates	27
I15	Anju Ahlawat	Light modulated Magnetization in Ferromagnetic/PMN-PT Heterostructures	28
I16	Dillip Pradhan	Structural phase transitions and enhancement of physical properties in Li and Ta modified $K_{0.5}Na_{0.5}NbO_3$ system	29
I17	Jieun Kim	Understanding Polarization Rotation in Relaxor Ferroelectrics Using Epitaxial Thin Films	30
I18	Subho Das Gupta	Fully Printed Negative-Capacitance Field-Effect Transistors with Ultralow Subthreshold Swing and High Inverter Signal Gain	31
I19	César Magén	Probing polar distortions in ferroic oxide films with atomic resolution electron microscopy	32
I20	Bholanath Pal	Ferroelectric thin film for memory and neuromorphic device application	33

I21	Pavan Pujar	Solution-Processed Doped-Hafnia Ferroelectrics on Silicon: A Pathway to Commercial Integration	34
I22	Gayathri Pillai	Exploring Temperature and Bias-Dependent Switchability and Tuneability of BST based LKu Band MEMS Resonators	35
I23	Florencio Sanchez	Strategies for maximizing polarization in ferroelectric HfO_2	36
I24	Siddhartha Ghosh	Design and Fabrication of Phononic Integrated Circuits in Scandium Aluminum Nitride	37
I25	Ranjith Ramadurai	Polarization Orientation Mapping in Polycrystalline and Epitaxially Grown BCZT Thin Films using Piezoresponse Force Microscope	38
I26	Sudhansu Mandal	Polar Skyrmions in Planes of Strained Ferroelectric Systems	39
I27	John Heron	Material-Limited Switching in Nanoscale Ferroelectrics	40
I28	Sujit Das	Harnessing the polar vortex motion and tunable skyrmion liquid phase in oxide heterostructures	41
I29	Bharat Jalan	Emerging Polar Altermagnetic Metallic States in Epitaxially Strained RuO_2 Films	42
I30	Soma Dutta	Real time Applications of Piezoelectric and Ferroelectric Materials: A perspective of Material Response to Device Qualification	43
I31	Ram Janay Choudary	Room Temperature Giant Inverse Magnetoelectric Effect in Topotactic Phase Transition Material $SrCoO_{2.5}$	44
I32	Dipankar Mandal	Initiatives in Piezoelectric Voiceprint for Biometric Healthcare Assessment	45
I33	Sayantika Bhowal	Emergent Surface Multiferroicity	46
I34	Abhijit Sangle	Growth of Lead-free Heteroepitaxial Thin Films of $(Na_{0.8}K_{0.2})_{0.5}Bi_{0.5}TiO_3$ Ferroelectrics by Nd:YAG Laser Pulsed Laser Deposition	47
I35	Saurabh Chandorkar	Superharmonic resonant response measurement: a new method to measure spontaneous polarization	48
I36	Devajyoti Mukherjee	Exploiting giant electrocaloric effects in epitaxial thin films of ferroelectric and antiferroelectric perovskite oxides	49

I37	Pavan Nukala	Visualizing solid-state amorphization in 2D ferroelectrics	50
I38	Anirban Chowdhury	Giant Electrostriction in $La_2Ce_2O_7$ Ceramic: Is Texture Always Helpful for Functional Properties?	51
I39	Ravi Kashikar	Tunable spin polarization in ferroelectric hybrid organic inorganic perovskites	52
I40	Tuhin Maity	Crossing the limits by interface engineering in nano-scale multiferroics	53
I41	Maheswaran Shanmugam	Unlocking single-phase Magneto-Electric Materials through Discrete Molecular Architectures	55
I42	Saswata Bhattacharya	From Constraints to Complexity: Thermodynamic Pathways to Domain Formation in Ferroelectrics	56
I43	Arockia Rajan	Magnetoelectric Performance of Epoxy-Modulated Ni/PZT/FeGa Composites for Pressure and Displacement Sensing Applications	57
I44	Sobhit Singh	Phase Transitions and Elastic Anomalies in Ferroelectric Hafnia Under Pressure	58
I45	Shankar Selvaraja	Highly Oriented PZT Platform for Polarization-Independent Photonic Integrated Circuit and Enhanced Efficiency Electro-Optic Modulation	59
I46	Jordan Bouaziz	State-of-the-Art Research on Hf-ZrO_2 Ferroelectric and Antiferroelectric capacitors	60
I47	Veeresh Deshpande	CMOS back-end-of-line compatible $Hf_{0.5}Zr_{0.5}O_2$ ferroelectric devices	61
I48	Bhaswar Chakraborty	Reliability of doped hafnium oxide FeFETs: challenges and mitigation strategies	62
I49	Arvind Ajoy	Harnessing the Double-Well potential of Ferroelectrics for Enhanced Sensing and Electromechanical Actuation	63

Oral Presentations

No.	Presenter	Title	
O1	Shubham Parate	Operando characterization of temperature assisted ferroelectric to paraelectric phase transitions in In_2Se_3	65
O2	Saujatya Mandal	Micromechanical insights into texture and stress-driven electromechanical behavior in ferroelectric PZT	67

O3	Soumyaranjan Sahoo	Freestanding ferroelectric oxide membranes designed by epitaxy for device applications	68
O4	Gudeta Jafo	Simultaneous increase of d_{33} and Curie point of PZT: the phenomenon and mechanism	69
O5	Harshita Seksaria	Origin of strain tunability in flat valence band and ultrahigh shear piezoelectricity in superflexible non–van der Waals graphitic ScX monolayers (X = P, As, Sb)	70
O6	Pooja Punetha	Short range structural correlations and property anomalies in non-MPB compositions of Pb-free piezoelectric $Na_{0.5}Bi_{0.5}TiO_3$–$K_{0.5}Bi_{0.5}TiO_3$	71
O7	Naveen Negi	Investigation of electrical and multifunctional properties in high-entropy BFO–BTO–STO perovskites	72
O8	Abhinav Kumar	Analysis of the comparative scaling behaviour between slanted and square-type polarisation loops in Nb^{5+}/Ho^{3+} co-substituted NBT systems for enhanced energy storage performance	73
O9	Yeswant Pattipati	Epitaxial in-plane ferroelectric $BaTiO_3$ integrated onto Si through a single MgO buffer for electrooptic applications	75
O10	Ananda Babu	Structural, relaxor behaviour, dielectric and energy storage properties of lead-free $(1-x)Ba_{0.95}La_{0.05}TiO_3$–$xBi(Zn_{2/3}Ta_{1/3})O_3$ ferroelectrics	76
O11	Dipankar Sarkar	Antiferroelectric to ferroelectric phase transition and electrocaloric effect in epitaxial $PbZrO_3$ thin films	77
O12	S. K. Upadhyay	Re-entrant-like behavior in modified $BaTiO_3$ with pinched hysteresis loop	78
O13	Anjana Thomas	Enhancing polarization and reliability in HZO-based FTJs using WO_x electrodes and interfacial layers	79
O14	Soumyajyoti Mondal	Tailoring ferroelectric HfO_2 thin films: a comprehensive study of deposition parameters, thermal treatment, and electrode effects	80
O15	Mohit Tanwani	Tuneable skyrmion liquid phase in polar skyrmions	81
O16	Kusumpal Yadav	Ferroelectricity induced giant topological Hall effect in epitaxial multiferroic thin film heterostructure	82
O17	Khadeer Pasha	Flexible and Wearable Polyvinyl Alcohol/Chitosan/$Ti_3C_2T_x$ MXene-Based Piezoelectric Hydrogels	83

O18	Riya Pathak	Curie-Weiss cross-over and quantum spin liquid behavior in multiferroic $TbInO_3$ thin films	84
O19	Md Hanif Ali	Way to achieve highly improved state-of-the-art ferroelectric properties in $Hf_{0.5}Zr_{0.5}O_2$ at low processing temperature	85
O20	Sruti Muralikrishnan	Microstructure and piezoresponse force microscopy of neodymium titanate films—high-temperature ferroelectric	86
O21	Nilotpal Deka	A highly electrostrictive A_2BX_4-type hybrid 2D perovskite ferroelectric and the utility of its composite piezoelectric nanogenerator in wireless applications	87
O22	Parvathy Ravindranath	Two-phase energy harvesting via magneto-pyroelectric coupling	88
O23	Rajashi Halder	Energizing Tomorrow: Biocompatible Ferroelectric Cu(II) Complexes for Sustainable Energy Harvesting	89

Young Researcher Talks

No.	Presenter	Title	
Y1	Varun Harbola	Heterostructure and interface design beyond epitaxy	91
Y2	Digvijay Singh	From Delusion to Reality: The Isosymmetric Transition in $BiFeO_3$-$PbTiO_3$ and Its Complex Phase Diagram	92
Y3	Somnath Kale	Ferroelectric Size Effects on Statics and Dynamics of Domain Wall	93
Y4	Gobinda Das Adhikary	Large longitudinal electrostrain and electrobending deformation in polycrystalline piezoelectrics	94
Y5	Jalaja M	Proximity induced phase transitions in solution processed La doped Hafnia	95
Y6	Shiuan Wu	Gelatin Exfoliation Process: Enhance The Potential of Ferroelectric Component in Electronic Skin Applications	96
Y7	Sandeep Kongbrailatpam	Observation of Akhiezer and Landua-Rumer Regimes in the Temperature Dependence of Longitudinal Wave in BST on Sapphire BAW Resonator	97
Y8	Praveen Kumar	Generation of Phononic Frequency Combs via Nonlinear Mode Coupling in Curved Circular Piezoelectric MEMS Resonators	98
Y9	Antony Jayaseelan	Different textured PZT films grown on Si/Pt substrate	99

Y10	Subhajit Pal	Photoinduced properties in ferroelectric oxides: From fundamentals to application	100
Y11	Binoy De	A new approach to measure ferroelectric ionic displacement using polarized Raman spectroscopy	101
Y12	Urmimala Dey	Insights into Multifunctional Properties of Ferroelectrics from Atomistic Simulation	102
Y13	Ajay Kumar	Nanoconfinement driven mechanical and thermal properties of ferroelectric molecular complex	103
Y14	Subhadeep Bandyopadhyay	Latent electronic (anti-) ferroelectricity in $BiNiO_3$	104
Y15	Anouk Goussens	Towards room-temperature ferroelectric-spin-orbit (FESO) devices based on perovskite ferroelectrics	105

Industry Talks

Code	Presenter	Affiliation	Title
IT1	Abhay Kochar	Optorun	Piezoelectric Resonators: Powering the Next Wave of RF Communication

Poster Presentation

S. No	Name	Abstract title	Category
1	Akhil Raman T. S.	Crystallization of Ferroelectric Thin Films on Polymer Microwave Substrates for Tunable Microwave Device Applications	Thin films/ Devices
2	Ganga S Kumar	Dependence of Transient Negative Capacitance on Domain Switching Kinetics in La-doped Pb(Zr0.4Ti0.6)O3 Ferroelectric Capacitor	Thin films/ Devices
3	Jishnu Ghosh	Coexistence of Negative Differential Resistance and Resistive Switching mediated by Phase change in a FeSFET Device	Thin films/ Devices
4	Kaushal	CMOS-Compatible HfxZr1-xO2 Ferroelectrics for Tunable Band-Pass Filters in Space Applications	Thin films/ Devices
5	kaushiga chandrasekaran	Enhanced Energy Storage Density in Lead-Free Ba0.7Sr0.3TiO3/Ba0.6Sr0.4TiO3 Multilayer Thin Films	Thin films/ Devices
6	Lalit Jena	Energy Storage and Harvesting Potential of Eco-friendly Ca-substituted Ba0.8Sr0.2TiO3/PVDF Ferro-Flexible Composite Films	Thin films/ Devices
7	P Sadanand	Emotion-Responsive Neuromorphic Behavior in SrTiO3/Nb:SrTiO3 Heterostructures	Thin films/ Devices
8	Sandeep Moprathi	Strategies for Optimization of Negative Output Conductance and Gate-Induced Drain Lowering in Ferroelectric Negative Capacitance FET	Thin films/ Devices
9	Vivek Dey	Sub-Coercive Field Switching in Ferroelectric PZT Capacitors via Stochastic Resonance	Thin films/ Devices
10	Harshvardhan	C-axis Oriented AlN Thin Films for High-Frequency Acoustic Resonator Applications	Thin films/MEMS
11	Linet Thomas C	A HYBRID MEMS - COMBINING PIEZOELECTRIC AND FERROELECTRIC THIN-FILM FUNCTIONALITIES	Thin films/MEMS
12	Chhavi Rastogi	Unveiling ferrielectric and ferroelectric phases in $PbHfO_3$ thin films	Thin films
13	Dharnesh dexterious	Interfacial Compositional Analysis of Dielectric/Semiconductor Stacks Employing Electronic-Grade Metal Oxides	Thin films
14	Dibyajyoti-Sahoo	Electrical and Mechanical Switching of Ferroelectric Polarization in BaTiO3 Ultrathin Films	Thin films
15	Garima Kaura	High Dielectric Tunability in Lead-Free $Ba_{1-x}Sr_xTiO_3$ Thin Films	Thin films

16	Gokul Krishna	Facile Room-Temperature Synthesis of alpha Quartz-like GeO2 from Amorphous GeTe	Thin films
17	Jajjara Sandeep	Sol–Gel Deposition and Rapid Thermal Annealing of Ferroelectric HfO_2 Thin Films on TiN-Coated Silicon Substrates	Thin films
18	Jishnu N K	Heterogeneous Integration of Complex Epitaxial Oxides on to Silicon	Thin films
19	Kartick Biswas	Understanding strain relaxation behaviour in epitaxial neodymium nickelate thin films	Thin films
20	Mahiman Bansal	Understanding the Interface in Transparent Conducting Oxides with Dielectric and Semiconductor Capping Layers	Thin films
21	Meenal Dhanetwal	Temperature and Frequency-Dependent Field Effects on Polar States in BaHf0.6Ti0.4O3 Thin Films	Thin films
22	Neeraj Yadav	Manipulations of multiferroic topology in self-assembled BiFeO3	Thin films
23	Nihal Raut	CMOS Compatible Ferroelectric Devices Featuring Amorphous Oxide Semiconductor Layer	Thin films
24	Niraj kumar	Electric field-driven polarization extension phenomenon in multiferroic oxide	Thin films
25	Phani Shankar	Epitaxial growth of AlN & AlScN on TiN(111) buffered Si (111) by Pulsed Laser Deposition	Thin films
26	Rahul Lakra	Sol-Gel method to synthesize SAO buffer layers on strontium titanate (STO) substrates, focusing on the growth chemistry and characterization of SAO.	Thin films
27	Rahul Tiwari	Precision-Transferred Flaky Hafnia Ferroelectric/High- k Dielectric Heterostructures	Thin films
28	S. Sandeep	Influence of Nitrogen flow on CMOS compatible Sputtered Aluminium Nitride Thin Films for Piezoelectric Applications	Thin films
29	Saikarthikey Bhat	Strain-Engineered Suppression of Meta-Magnetic Transition and Its Effects on Magnetocaloric Effect in Multiferroic Dy2NiMnO6 Thin Films	Thin films
30	Tribhuvan Kushwaha	Understanding the Interface in Transparent Conducting Oxides with Dielectric and Semiconductor Capping Layers	Thin films
31	Uma Ganguly	Structural and Property Correlation in BCT-BZT Piezoelectric Thin Films at the Morphotropic Phase Boundary	Thin films
32	Vaishnavi SM	Strain-Driven Ferroelectric Domain Evolution in Epitaxial BCZT Thin Films near MPB	Thin films
33	Vishal Mankare	Electromechanical response and its dependance on stoichiometry of BaTiO3	Thin films

34	Himansu	Design the Next-Gen, Flexible, Fiber-based Magnetoelectric composite of Zn Doped BCZT-NZFO@PVDF for wireless power transmission application for implantable devices.	Nanostructures/Devices
35	Mou Sarkar	Work Function Engineered, Electrically Poled SnS–PVDF Nanofiber based nanogenerators for Enhanced Piezoelectric-triboelectric Energy Harvesting and Sensing	Nanostructures/Devices
36	Navya Abraham	Effect of higher aspect ratio 2-D platelet filler on the electroactive phase fraction and ferroelectric characteristics of BiT/PVDF nanocomposite	Nanostructures/Devices
37	Nayak Ram	Fiber-based flexible magneto-mechano-electric generators enhanced by UV and IR treatments for sustainable IoT sensors	Nanostructures/Devices
38	Neha Kumari	Piezoelectric Material for Energy Harvesting Application: Enabling Self-Powered Systems	Nanostructures/Devices
39	Shubha raja Chowdhury	3D-Printed Microstuctred Triboelectricity induced Piezoelectric Handwriting Pad Based on MoS_2/PDMS Nanocomposites for AI-Driven Digital Text Conversion	Nanostructures/Devices
40	Utsa Sarkar	1D Monochalcogenide in Nanocomposite Fibers: A Hybrid Approach Toward Flexible Energy-Harvesting and Sensing Applications	Nanostructures/Devices
41	Aryan Keshri	Self-Assembled Ferroelectric Nanodots in Imidazolium Tetrafluoroborate with Multiaxial Polarization	Organic
42	Ashlesha-Goswami	Homochirality induced piezoelectricity in a single component molecular system	Organic
43	Bapan Jana	Co(ii)complex promoted PVDF β-phase crystallization: innovations in pressure sensing and energy harvesting	Organic
44	Chetna sharma	Fabrication of high output performance piezoelectric nanogenerator based on PVDF/BFBT for energy harvesting	Organic
45	Debopam Sarkar	Towards Advanced Multiferroic materials: Interplay Between Magnetism and Ferroelectricity	Organic
46	Ganeshmoorthi B	Harnessing Chirality: Piezoelectric [Mn-Camp-4BPY] Metal–Organic Framework for Nanogenerator Applications	Organic
47	Gifty Godson P	Ferroelectric Polymer Nanocomposite Based Triboelectric Nanogenerators for Efficient Energy Harvesting Applications	Organic
48	K Vignesh	Engineering 3d metal Based Molecular Magnetoelectric Materials and its Applications	Organic
49	K M Shristi	MechanicalManipulation of Ferroelectric Domains in Molecular Ferroelectric	Organic
50	Nimish Trivedi	Spin Polarization in Lead-Free Ferroelectric Hybrid Halide Perovskite	Organic
51	Siva baskar	L-phenylalanine (LPA) -poly-ethylene-oxide (PEO) based piezoelectric electrospun nanofibers for energy harvesting applications.	Organic

52	vinayak Gadgin	Ferroelectricity and Piezoelectric Energy Harvesting of an A3M2X9 type 0D Bromobismuthate Hybrid with Bulky Organic Quaternary Amine	Organic
53	vipu vinayak	Synergistic Effect of Ti_3AlC2 MAX Phase and PEDOT b-PEG on the Dielectric and Electrochemical Behavior of Flexible PVDF Nanocomposites	Organic
54	Dhanranjan Kumar	Lead-Free Piezoelectric Ceramics for Energy Conversion and Packaging Applications	Bulk/Devices
55	Gaurav Gautam	High Entropy Perovskite Ceramics for Capacitive Energy Storage	Bulk/Devices
56	Jumana P J	Tuning the switching dynamics through cation engineering in PbZrO3-based materials for enhanced energy storage and electrostrain characteristics	Bulk/Devices
57	Ranjan Kumar Sahu	Composition optimization for recoverable energy storage density performance, breakdown strength, relaxor nature, and thermal stability in eco-friendly Eu3+ substituted Na0.2K0.3Bi0.5TiO3	Bulk/Devices
58	sumit Chahal	Synergistic Enhancement of Energy Storage Properties in 2D-3D Composites of Graphene and Barium Titanate	Bulk/Devices
59	Sumit kumar	Investigations of energy storage and thermal stability properties in eco-friendly B-site substituted Na0.5Bi0.5TiO3	Bulk/Devices
60	sundarapandian	Improved Relaxor Characteristics in A and B-site Substituted Perovskite BaTiO3 for Energy Storage Applications	Bulk/Devices
61	Twinkle	The prominence of sintering temperature optimization in amelioration of densification and energy storage behavior in KNN based ceramics	Bulk/Devices
62	Abhikshtia Sahu	Phase Transition and Ferroelectric Properties of KNN- BiScO3 Ferroelectric System	Bulk
63	Amit Kumar	Weak ferroelectric response in bulk polycrystalline Y2O3-Hf0.5Zr0.5O2 ceramics	Bulk
64	Amiya Ranjan Sahoo	Polarization Reversibility and Electrothermal Response in lead free Disordered Perovskite 0.9Ba0.6Sr0.4TiO3-0.1Bi0.5Na0.5TiO3 system	Bulk
65	Anil adukkadan	Influence of poling-field strength on the thermal restoration of antiferroelectric order in (Pb, La)(Zr, Sn, Ti)O3 ceramics	Bulk
66	Anagha Baby	Role of A-site volatile Compensation and its influence on the Structural and Functional Properties of high TC $BiScO_3$–$PbTiO_3$ Piezoceramics	Bulk
67	Ankur	Enhanced energy density in the low electric field region via hybrid polarization mechanism in BNT-based relaxors	Bulk
68	Aravindkrishna Talluri	Enhancing the Energy Storage performance in (Ba, Ca)(Zr, Ti)O3 Ceramics via Cerium Oxide Doping	Bulk
69	Deepak Sharma	Influence of Local Polarisation and octahedral tilt on the specific volume of the ferroelectric alloy system SrTiO3-Na0.5B0.5TiO3	Bulk

70	Eliya. Y	Influence of defect engineering on electrocaloric behaviour in non‐stoichiometric lead-free $BaTiO_3$-based system	Bulk
71	Getaw abebe-Tina	Simultaneous enhancement of d33 and depolarization temperature of the morphotropic phase boundary composition of the Pb-free piezoceramic Na1/2Bi1/2TiO3–BaTiO3	Bulk
72	Helga Mary S	Microstructure and ferroelectric studies of aliovalent doped lead-free (K,Na)NbO3 ceramics	Bulk
73	Manoranjan Sahoo	Influence of A-Site Samarium Substitution on the Dielectric Behaviour of $Ba0.6Sr0.4TiO_3$	Bulk
74	Monika	Dimension dependence electrodeformation behavior (K0.5Na0.5)NbO3 -based Pb-free piezoceramics	Bulk
75	Mukul kumar	Superior Piezoelectric Properties in $BiGaO_3$-Modified $BiFeO_3$–$BaTiO_3$ Ceramics: Insights from Phase Stability and Defect Engineering	Bulk
76	Pinki-Yadav	Compositional Control and Phase Evolution in NBT-KBT Single Crystals Near the Morphotropic Phase Boundary	Bulk
77	Prosun Mondal	High-Performance Lead-Free Piezoelectric Ceramics for Sensors and Actuators via Phase Boundary Engineering in KNN-Based	Bulk
78	Shubham Modgil	Rare-Earth-Driven Structural Engineering for enhanced Piezoelectricity and high Curie temperature in MPB based Pb(1-x)Sm(x)(Mg0.05Nb0.1Zr0.43Ti0.42) Ceramics.	Bulk
79	Sumit	Magnetoelectric Performance and Stability of Epoxy-Modulated Ni/PZT Composites: Quasi-Static, Dynamic, and Fatigue Characterization	Bulk
80	Utkarsh Jain	Study of anomalous phase transition in modified barium titanate system via structural, electrical and local analysis	Bulk
81	Varun Kamboj	Grain Boundary Engineering via Microwave Sintering in Lead-Free Na0.5Bi0.5TiO3-based Ceramics for Enhanced Dielectric and Energy Storage Applications	Bulk
82	YAMMALA ELIYA	Influence of defect engineering on electrocaloric behaviour in non‐stoichiometric lead-free $BaTiO_3$-based system	Bulk
83	Aniruddha Ray	Effect of multipoles on the band structure of MnSiN2	Theory
84	Sourabh vairat	Emergence of polar monoclinic phase in ferroelectric CsGeX3 (X = Cl, Br, I)	Theory

ABSTRACTS

For

TUTORIALS

Fundamentals of Piezoelectricity

Andrew J Bell
University of Leeds, Leeds, UK

In this tutorial we will investigate the basic science of the piezoelectric effect and introduce the most technologically relevant families of materials.

The outline is as follows:

1. The piezoelectric effect
    a. Basic phenomena and some example applications
    b. Constitutive equations and tensor representation
2. Intrinsic phenomena
    a. Thermodynamics
    b. Microscopic models
3. Extrinsic phenomena
    a. Phase instability and polarisation rotation
    b. Domain wall contributions
    c. Nanodomain phenomena
4. Piezoelectric Materials
    a. Non-ferroelectrics
    b. Simple perovskites: $BaTiO_3$, $PbTiO_3$, $KNbO_3$
    c. $Pb(Zr, Ti)O_3$ ceramics
    d. $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ single crystals
    e. Lead-free perovskites
        i. $(K, Na)NbO_3$,
        ii. $(Na_{1/2}Bi_{1/2})TiO_3$-$BaTiO_3$
        iii. $(Ba,Ca)(Zr, Ti)O_3$
        iv. $BiFeO_3$-$BaTiO_3$
5. Summary

Piezoforce Microscopy for Ferroelectrics

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Ferroelectric and Multiferroic devices: Device Physics

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This tutorial provides an overview of ferroelectric memory devices—Ferroelectric Tunnel Junctions (FTJs), Ferroelectric Field-Effect Transistors (FeFETs), and Ferroelectric RAM (FeRAM)—focusing on their working principles, device structures, and recent progress in materials like hafnium oxide. It also introduces magnetoelectric and multiferroic devices, which enable electric-field control of magnetic states, offering pathways to ultra-low-power memory technologies such as MeRAM. The tutorial highlights integration challenges and opportunities for implementing these devices in beyond-CMOS computing architectures, aiming to equip participants with foundational insights into emerging non-volatile memory technologies.

Ferroelectric Device and Technology integration

Veeresh Deshpande

The discovery of ferroelectric phases in doped hafnium oxide has revitalized ferroelectric memory technology, overcoming key limitations of traditional perovskite-based ferroelectric random-access memory (FRAM). Hafnia-based ferroelectrics enable ultra-thin ferroelectric films compatible with advanced CMOS technology, supporting device miniaturization and integration benefits that prior materials couldn't achieve due to scaling and material challenges.

In this tutorial, we will discuss various ferroelectric memory device architectures: ferroelectric capacitor, ferroelectric tunnel junction, and ferroelectric field effect transistor. We will discuss their physics of operation, and integration in CMOS technology. We will also look at emerging applications such as neuromorphic computing with ferroelectric devices

ABSTRACTS

For

PLENARY TALKS

Inside Piezoelectricity: why we need both hard and soft interatomic bonds to maximise energy conversion

Andrew J. Bell

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The piezoelectric effect is used throughout electrotechnology to convert mechanical energy to electrical energy and vice versa. Its thousands of applications include medical ultrasound imaging, industrial structural health monitoring, automotive fuel injection, ink-jet printing, micro-positioning, vibration sensing, surface acoustic wave devices and both microphones and speakers for acoustic reproduction. Over the last 75 years, tens of thousands of man-hours have been spent optimising piezoelectric material properties, initially focussing on Pb(Zr, Ti)O_3 (PZT) ceramics and more recently on lead-free materials. The concepts of manipulating morphotropic phase boundaries, promoting polarisation rotation and tailoring ferroelastic domain wall motion are very familiar to those engaged in such research, which almost exclusively centres on perovskite oxides. We might consider these concepts as extrinsic mechanisms of piezoelectricity. However, the intrinsic mechanisms of how stress translates into polarisation or electric field into strain at the atomic level have been rarely considered. With the growing interest in non-perovskite piezoelectrics, particularly organic crystals, it is more important than ever to understand the intrinsic mechanism of piezoelectricity in terms of the dependence of key characteristics on crystal chemistry.

Here we firstly consider the thermodynamics of the direct (stress) and converse (field) piezoelectric effects, which shows that despite their piezoelectric charge coefficients being equal in value, the relationship between polarisation and strain in the two effect is different. This leads to the conclusion that maximal piezoelectric coupling in ferroelectric crystals is achieved not by increasing the total polarisability of the crystal, but by maximizing the difference in the absolute polarizabilities of the cations and anions. This premise is explored and verified for barium titanate from density functional theory. The piezoelectric coefficient in the direct effect is determined from two structure optimizations under different stress states. Evaluation of the force constants of nearest neighbour bonds facilitates calculation of the atomic positions during the converse effect, confirming that the direct and converse effects are manifest through different atomic displacements for the same induced strain. The influence of each of the interatomic bonds on the electromechnical properties is assessed, with results that are consistent with the thermodynamic arguments; optimal properties occur for large piezo-induced displacements of the B-site cation combined with vanishingly small anion displacements. Finally, consideration of a large dataset for perovskite oxides concludes that the rigidity of the oxygen octahedra is as important as the polarisability of the cations in determining the magnitude of piezoelectricity in this family of materials

Ferroelectric Doped HfO_2-based Devices: Recent progress and future challenges

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About twenty years ago, scientists discovered that doped HfO_2 films have ferroelectric properties, even in layers thinner than 5 nm [1][2][3]. This allowed the fabrication of various semiconductor devices, such as high-aspect-ratio ferroelectric capacitors (FeCap) and field-effect transistors (FeFET). Other devices, such as ferroelectric tunnel junctions (FTJ), dynamic random-access memory (DRAM) capacitors, neuromorphic, piezoelectric, and pyroelectric devices, are also being developed [4][5] Technology nodes down to 15 nm can be used to make multiple devices and large memory arrays. The first production-type devices have been reported. These include 32 Gb dual-layer and 64 Gb single-layer non-volatile DRAM [6][7].But there are still challenges that make it demanding to improve reliability and performance. In particular, polarization retention at elevated temperatures and field cycling endurance need to be studied.

When talking about the three main memory devices (FeCap, FeFET, FTJ) and in addition the DRAM capacitor, the FeCap is chosen as an example device to explain how the ferroelectric structural phase forms. This is influenced by the amount of dopant and oxygen, the electrode material, and the strain in the doped HfO_2 layer. Structural characterization during the doped HfO_2 crystallization process reveals the effect of strain on phase transitions. Medium strain values of about 0.5% are favorable for forming the ferroelectric orthorhombic phase [8].

Electrical characterization confirms single grain/domain nucleation-limited switching kinetics with slightly different coercive fields for each single grain [9]. One difference of doped HfO_2 ferroelectric films compared to their perovskite counterparts is the high coercive field of about 1 MV/cm². For commercial semiconductor applications, lower switching voltages are preferable. These can be achieved by scaling the film thickness.

Overall, the fundamentals of ferroelectricity in HfO_2-based films, the latest progress in integrating this material and improvments of its properties in functioning devices are reviewed.

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Title: Polar Half-Metal and Triferroic Insulator based on $PbMnO_3$: First-principles Theory

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Detailed crystal structure, electronic and magnetic properties of $PbMnO_3$, a member of $PbMO_3$ (M=3d transition metal ion) family of perovskites exhibiting a variety of physical properties, are still elusive. We present an in-depth first-principles theoretical analysis of structure, magnetic order, and lattice instabilities of its low energy states, and identify pathways connecting them using symmetry principles. We show that the ground state of $PbMnO_3$ is a half-metallic ferromagnet with orthorhombic *Pnma* crystal structure, which involves condensation of MnO_6 octahedral rotational modes at π/a[110] and π/a[111] points in the cubic perovskite structure.

While the half-metallic ferromagnetic state of $PbMnO_3$ is shown to be quite robust against the epitaxial strain and substitutional doping at the Mn site, we demonstrate a *polar ferromagnetic half-metal* with hybrid improper ferroelectricity in its superlattices with $AMnO_3$ (A=Sr and Ba).

We propose a new type of triferroic insulator with coexisting ferromagnetism, polar structural distortion and Berry curvature dipole as switchable ordering fields and demonstrate its realization in $PbMnO_3$/$PbVO_3$ superlattice.

Our work opens up new types of devices based on polar half-metallicity and electric-field controlled anomalous Hall effects in multiferroic oxides.

Magnetoelectric nanostructures: synthesis, properties and applications

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Magnetoelectric (ME) materials have emerged as promising candidates for a wide range of biomedical applications due to their unique ability to couple and manipulate both magnetic and electric signals. Many applications of ME materials have been proposed, e.g. sensing, brain stimulation, tissue engineering, cancer therapy, drug delivery, theranostics, etc [1]. In particular, core-shell magnetic particles consisting of magnetic core and functional piezoelectric shell have attracted widespread attention in multidisciplinary fields spanning from chemistry, physics, and materials science to biomedicine, and bioengineering due to their excellent ME properties, tunable interfaces and geometry, and the possibility of the composition design [2,3]. In recent decades, various surface engineering strategies have been developed to endow them with desired properties (e.g., surface functionalization, roughness, acidity, target recognition) for efficient applications in catalysis, optical modulation, environmental remediation, biomedical devices, etc. Various compositions including simple metal oxides, silica, graphene/graphene oxide, ferroelectric perovskites and polymers, metal−organic frameworks and ferromagnetic spinels have been proposed to exploit these new functional ME materials. In this presentation, I will overview major synthesis methods, composition strategies, interface engineering, and applications of core-shell magnetoelectric particles, nanodiscs, and nanofibers [1-3]. The fundamental methodologies for controllable synthesis of nanoscale ME structures with diverse organic, inorganic, or hybrid compositions, will be outlined [4,5]. In addition, the local techniques to measure magnetoelectric effect in such structures will be briefly discussed [5]. Several examples of the core-shell and fiber-based ME structures will be given and their applications in biomedicine will be introduced [6-8]. Finally, the remaining challenges, future research directions, and novel biomedical applications of the nanoscale magnetoelectric composites will be briefly given.

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Advances in Ferroelectric-, Antiferroelectric-, and Relaxor-based Thin Films and Heterostructures

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Over the last 30 years, the study of ferroelectric oxides has been revolutionized by the implementation of epitaxial-thin-film-based studies that compliment efforts on bulk versions of such materials. At the same time, the explosion of studies on ferroelectric-based multilayer and superlattice heterostructures has been made possible by the co-development of exacting deposition techniques, new characterization approaches that provide mesoscopic insights into the structure and properties of these complex structures, and ever-advancing theory, modeling, and simulation that allows us to extract ever deeper insights. The ability to delicately balance and tailor different energies (e.g., electric, elastic, gradient, etc.) of ferroelectrics in such low-dimensional forms and nanostructures has made these structures a veritable playground for the observation of exotic effects ranging from unexpected dielectric and ferroelectric properties to emergent dipolar textures, to new types of polar order. As the approaches to study these heterostructures have marched on, researchers have also sought new materials to include in these structures to elicit ever-more interesting effects. There is growing interest in creating multilayers and superlattices that include not just dielectric and ferroelectric materials (wherein the vast majority of work has been done before), but also all-ferroelectric systems and systems including more exotic "polar" materials such as antiferroelectrics and relaxors – offering a nearly infinite design space to produce effects not seen in the bulk.

Here, we will review a few vignettes looking at single-layer, multi-layer, and superlattice structures based on these materials. Beginning with single-layer films, we will explore differences between ferroelectric, antiferroelectric, relaxor ferroelectric, and relaxor antiferroelectric materials in their ultra-thin limit. Such so-called size effects and their implications for response will be probed as we progressively shrink down materials. In turn, we will explore various multilayer and superlattice systems based on the same. From the formation of emergent dipolar textures to creation of artificial relaxors we will probe how combining thoughtful strain engineering and heterostructuring of (anti-)ferroelectric and relaxor materials can beget large changes to dielectric, electromechanical, and electric breakdown strengths. For example, in trilayers of the form $PbZr_{0.2}Ti_{0.8}O_3/0.68PbMg_{1/3}Nb_{2/3}O_3$-$0.32PbTiO_3/PbZr_{0.2}Ti_{0.8}O_3$ it is possible to produce a co-existence of classical c/a and a_1/a_2 domain structures wherein this mixed-phase state exhibits a significant enhancement of the electromechanical response. In these trilayers, the influence of the relaxor middle layer on the domain structure as well as the properties will be explored wherein these structures have been shown to have significantly reduced leakage and enhanced electrical breakdown strength, and thus exhibit larger maximum field-induced strains that outperform many current thin-film piezoelectric materials. Finally, we will explore multilayers based on antiferroelectrics wherein we build upon our observation of large electromechanical response in epitaxial $PbZrO_3$ and $PbHfO_3$ films such that multilayers based on antiferroelectric $PbHfO_3$ and ferroelectric $PbHf_{1-x}Ti_xO_3$ have been shown to overcome substrate clamping to produce large electromechanical strains (>4.5%). By varying the chemistry of the $PbHf_{1-x}Ti_xO_3$ layer (x = 0.3-0.6) it is possible to alter the threshold field for the antiferroelectric-to-ferroelectric phase transition, reducing the field required to induce the onset of large electromechanical response. Furthermore, varying the interface density (from 0.008-3.1 nm^{-1}) enhances the electrical-breakdown field by >450%.

ABSTRACTS

For

INVITED TALKS

Ferroelectric photovoltaic and flexo-photovoltaic effect in bandgap-engineered ferroelectric system

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Abstract

The anomalous photovoltaic (PV) effect in ferroelectric systems has generated significant research interest in tuning the PV characteristics of these systems. However, the large bandgap of most of the ferroelectric oxides makes them unfit to observe the solar spectrum in the visible range. In this work, we have tuned the bandgap of $BaTiO_3$ by chemical doping to bring it around 2 eV. In addition, the role of the flexoelectric effect, induced by the strain gradient, to enhance and extend the PV effect beyond the ferroelectric Curie temperature (T_C) has been investigated in detail. Accordingly, the flexo-photovoltaic effect is demonstrated on the bandgap-tuned $BaTiO_3$-$Bi(Ni_{1/2}Nb_{1/2})O_3$ samples, which are epitaxially deposited under the compressively strained condition on the $SrRuO_3$ buffered $SrTiO_3$(100) substrate by PLD technique. The details will be presented in this talk.

Hyperfine interaction studies in lead-free $BaTiO_3$ based relaxors : signatures of structural modifications across its dielectric maxima

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ABSTRACT

Lead-free relaxors, particularly those based on barium titanate $BaTiO_3$ (BTO), have received a lot of attention due to their nontoxic nature, high dielectric permittivity, several phase transitions, and the possibility of tuning transition temperature close to room temperature. It is noteworthy that doped BTO materials exhibit relaxor behavior even in the absence of charge disorder. This characteristic distinguishes them from traditional lead-based relaxors, such as $PbMg_{1/3}Nb_{2/3}O_3$, which typically display nominal charge disorder. The present talk will deal with unambiguous signatures of structural modifications across the dielectric maxima of iso-valent (Sn^{4+}) substituted BTO realxor, probed with synchrotron based hyperfine interaction measurements, further complimented with Raman spectroscopy, x-ray absorption spectroscopy (XAS) etc [1-3].

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Optical control of ferroelectric domain structure in $BaTiO_3$

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Optical control and switching of domain configuration is an intriguing option to overcome the sluggish time response, hysteresis and Joule heating losses present in conventional methods where resistive contacts are involved. The effective optical control of the domain configuration has remained challenging and far from fully understood. It has been reported earlier that light polarization can be used to control the domain configuration in BaTiO3, however, with an indirect method and without much focus on origin of its mechanism. By combining the experimental techniques that are sensitive to the local and average crystal structure and electric polarization and electronic structure, we detect and demonstrate the optically guided variations in the domain configurations of BaTiO3 and show that the strain field generated through the bulk photovoltaic effect plays a key role in domain reconfiguration. Complete mechanism of reversible domain control via light polarization is discussed. Details of Raman spectroscopy studies and some unresolved issues will also be discussed. The two domain configuration in *a*-domains is detected and optical control in the in-plane domain structure is also presented.

Ferroelectric Materials Based on Hybrid Metal-Isothiocyantes

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The field of ferroelectric materials began a century ago with the discovery of Rochelle salt, but early applications were hindered by instability and fragility. Today, ferroelectrics comprehend a diverse range of systems, including inorganic perovskites, organic polymers, two-dimensional (2D) materials such as α-In_2Se_3, liquid crystals, and organic and organic-inorganic hybrid compounds. Recent developments in quantum theory and polarization models have improved the understanding of ferroelectric mechanisms and enabled better control over their design, dielectric, piezoelectric, and pyroelectric properties, making them vital for sensing, energy storage, and electronic applications. Recent breakthroughs in molecular and hybrid ferroelectrics have demonstrated their potential as excellent alternatives for inorganic materials, while offering unique advantages such as mechanical flexibility, biocompatibility, and tunable properties. One of the key challenges in the design of such organic and hybrid ferroelectric materials is the strict requirement of the noncentrosymmetry of their crystals in the polar point group. Our group focuses on developing ferro- and piezoelectric materials supported by heteroleptic phosphorus and nitrogen-centric scaffolds and their applications as electrical nanogenerators and as ferroelectric memtransistors. we have recently discovered that metal-isothiocyanate complexes are ideal hybrids to exhibit fast polarization reversals, aided by the distortions in the M-N-CS angles from linearity, while rigid heteroleptic cations stabilize the noncentrosymmetric structure in them. Under the electric fields, these distortions, ranging from 140-170º, produce two distinct states, making the $M(NCS)_x$ complexes ideal for molecular switches. We have also studied the FeFET and neuromorphic measurements for one of these derivatives that show a large number of conduction states with high memory and significantly modulated synaptic weights (Figure 1). These results show the promise of ferroelectric metal-NCS systems as potential alternatives for hafnia-based systems.

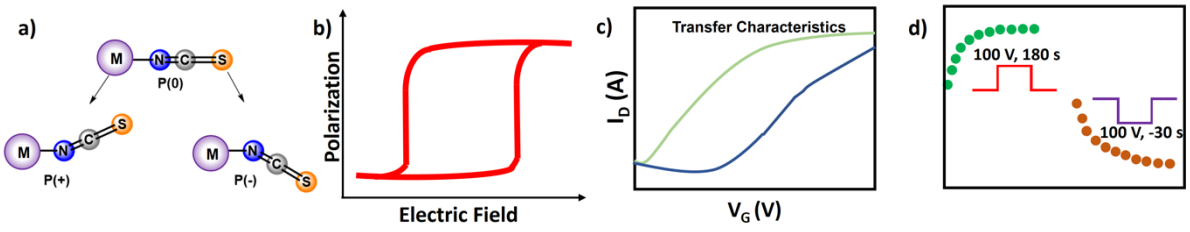

Figure 1: Schematic diagram showing the switching behaviour of metal-isothiocyanate complexes (a) leading to robust ferroelectricity (b) and applications in Fe-FETs (c) and neuromorphic memtransistors (d).

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MICAtronics for flexible ferroelectric memory, piezoelectric actuator, and pyroelectric Sensing

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Muscovite mica, a layered oxide, possesses unique optical transparency and mechanical flexibility characteristics. Due to its layered structure, it can achieve an atomically flat surface through cleavage. Such a surface creates an essential environment for van der Waals epitaxy, enabling the growth of ceramics, conventional semiconductors, 2D materials, and polymers. This methodology can overlook the lattice mismatch effect to deliver superior crystal quality for heteroepitaxy. In this research direction, various flexible applications have been demonstrated. Thus, I named this field "MICAtronics," an inorganic platform for flexible electronics. In this talk, I will emphasize heterostructures, including various polar materials such as PZT, BTO, and PVDF. The verification of heteroepitaxy will be illustrated based on combined results from X-ray diffraction and transmission electron microscopy. P-E loop and PFM measurements will provide proof of polar characteristics, offering macroscopic and microscopic evidence. Finally, I will present device prototypes, including ferroelectric memory, piezoelectric actuators, and pyroelectric sensors. Such demonstrations highlight great potential of MICAtronics for practical applications.

Decoding structure-property connections in perovskite ferroelectric oxides via total scattering method

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Understanding structure-property relationships in complex ferroelectric-piezoelectric oxides has long been a challenging problem because often materials exhibit unusual and unpredicted behaviour driven by their atomic-level dipolar correlations. For example, the structural characteristics giving rise to amplified piezoelectricity at the morphotropic phase boundary of famous PZT or analogous systems, or the nano-scale structural anomalies responsible for relaxor behaviour in well-known PMN-based materials are still topical issues in this field. In this context, we have applied neutron total scattering method to several Pb containing and Pb-free solid solutions to study exclusively the local dipolar correlation functions and its development as functions of compositions and temperature. In general, large atomistic models were refined against the experimental pair distribution functions implementing reverse Monte Carlo method as a function of composition or temperature, which revealed quantitative cation-specific information on order-disorder, distortion and coupling of dipolar displacements from which generic atomistic features can be identified to develop robust structure-property connections of such materials.

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Ultrathin Freestanding Membranes of Ferroelectric Hafnia

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Two-dimensional nanosheets of materials, which can be transferred onto and make interfaces with any material, have attracted attention in the search for functional properties. We fabricated ultrathin hafnia nanosheets having the metastable crystal structures and exhibiting ferroelectric polarizations as large as 13 μC/cm^2 (Figure 1) [1]. We also found that the rhombohedral(-like) phase transforms into another metastable orthorhombic phase without the ferroelectricity deteriorating as the thickness increases. Our results reveal the key role of the meta-stable structural phases (rhombohedral and orthorhombic) in the scale-free ferroelectricity of hafnia. In this talk, I will also present our recent research progress on free standing membranes of hafnia and related oxides, including the fabrication of ZrO_2 membranes with h igh dielectric constant [2] and the formation of Moiré superlattices in $ZrO_2/Hf_{0.5}Zr_{0.5}O_2$ bilayers. This work was done in collaboration with Y. Shen, K. Ooe, L. Xie, K. Shitara, X. Yuan, T. Yamada, S. Kobayashi, M. Haruta, T. Yoshimura, and Y. Shimakawa.

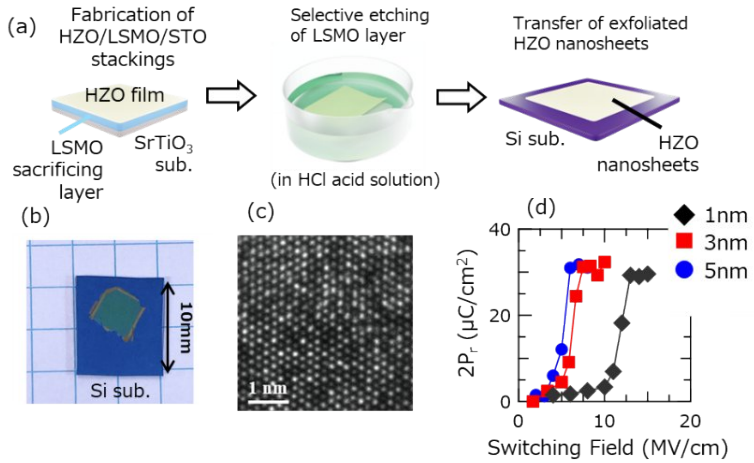

Figure 1: (a) Fabrication processes of HZO nanosheets. (b) Optical image of photoresist-covered 5-nm-thick HZO sheets transferred onto Si substrates. (c) Top-view HAADF-STEM image of a grain in 1nm-thick HZO sheets. (d) PUND measurement results for HZO nanosheets.

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Impact of Local Structural Ordering on the Thermal Expansion of Relaxor Ferroelectrics

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ABSTRACT

Relaxor ferroelectrics are well known for their distinct structure at various length scales (long/short ranges) and associated physical properties. This unique structural configuration of relaxor ferroelectrics plays a crucial role in tuning thermal expansion of dielectric materials. In the present work, Zero Thermal Expansion (ZTE) has been explored for $K_{0.5}Na_{0.5}NbO_3$-based solid solution *viz.,* $(1\text{-}x)(K_{0.5}Na_{0.5}NbO_3)\text{–}x(Ba_{0.9}Sr_{0.1}TiO_3)$ [KBST*x*] for $0.20 \leq x \leq 0.90$. KBST*x* ceramics demonstrate a non-polar cubic structure with $Pm\bar{3}m$ space group. The two end compositions *viz.,* KBST20 and KBST90, exhibit polar monoclinic phase and polar rhombohedral phase at short ranges [1-2]. Both the end compositions demonstrate zero thermal expansion at low temperatures. On the other hand, KBST40 exhibits coexistence of two distinct polar orderings, *viz.,* monoclinic and rhombohedral, at short ranges. A combined analysis of temperature-dependent Raman scattering, Synchrotron X-ray diffraction, and Pair distribution function data demonstrates zero thermal expansion with a very low coefficient of thermal expansion (CTE) for KBST40. Moreover, KBST40 exhibits CTE less than by about 65% and 59% in comparison to KBST20 and KBST90 at 100 K, respectively [3].

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Ferroelectric thin films for microwave devices: Material, Measurement, Processes and Devices

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Physical phenomena exhibited by materials are often exploited to achieve devices with different functionalities. One such material is ferroelectrics and in their paraelectric state they are useful for their voltage dependent dielectric constant, induced piezoelectricity and strain. If we need to access these properties in their bulk form, the voltage that needs to be applied is enormous. Hence, they are made in to thin films where the voltage levels come down to single or double digits. When a capacitor is made with these films in their paraelectric state, their dielectric constant will change with a DC bias voltage. Hence such a capacitor becomes a varactor or variable capacitor. Using inductors and capacitors LC resonators are made at low frequencies. But at microwave frequencies the Q value of these resonators are too low. But cavity resonators got high Q values but are too big at microwave frequencies. A solution is to use the ferroelectric thin film which facilitates electro acoustic conversion through piezoelectric effect. In this process, the rf energy gets converted to acoustic energy. Both of them got the same frequency but the acoustic wave got a velocity that is 5 orders of magnitude lower. This results in that much reduction in wavelength and hence the size of the resonator comes down. There are 2 types of resonators possible with this phenomena. High overtone Bulk Acoustic Resonators (HBAR) and Film Bulk Acoustic Resonators (FBAR), Former is easy to fabricate and gives high Q values but plagued by the presence of large number of closely spaced resonances. However the extra ordinarily high Q values observed has found to be important in coupling cubits used for quantum computing. The HBAR need deep etching but it gives high Q values in minimum space leading to unparalleled miniaturization. These paraelectric films will become a piezoelectric only under DC bias. Hence these resonators got the added advantage that they are switchable.

The processing of these materials into thin films is quite important as the material quality determines the device performance. The temperature of processing is quite important as that determines the substrates and processes to which these films can be integrated. The usage of laser annealing has proved to be interesting in lowering the crystallization temperature of films of (Ba,Sr)TiO3 which is widely being studied for microwave applications. Process integration issues are the primary reason why these films are less exploited for their interesting microwave range properties. The measurement of the microwave range dielectric properties especially tunability is very important for these applications. It is interesting to note that these measurements require a fabricated test structure that satisfies the impedance matching conditions and the limitations of on-wafer probing, especially for broadband measurements.

Once a varactor and resonator are available, it is possible to use these devices in a particular circuit to achieve non reciprocal propagation of microwaves. It is normally done in a ferrite based circulator employing Faraday Effect. But both magnet and ferrite are bulky. Here the ferroelectric thin film based devices come handy to achieve miniaturization. Such magnet free circulators are needed in quantum computing Qubit systems operating at cryogenic temperatures using Josephson junctions to keep them isolated from the microwave electronics kept at ambient temperature so that they will not increase their entropy. Another drive behind developing such circulators is to make the same circuit usable for both the outgoing and returning signals in communication channels, thereby achieving a reduction in circuitry. There are different ways proposed for realizing magnet free circulators and one of the scheme involves the use of multiple high Q resonators and varactors in a Y configuration which are possible to be realized with these films in an integrated manner.

Advancing Ecofriendly Ferroelectrics for Next-Generation Energy Storage and Flexible Electronics

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Over the past several years, our research has been dedicated to the rational design and engineering of advanced functional materials tailored for high-performance energy storage and emerging flexible electronic technologies. Focus has been placed on enhancing relaxor ferroelectric behavior in lead-free systems through compositional tuning and microstructural optimization. Potassium and sodium bismuth titanates (KBT and NBT) were extensively investigated due to their promising dielectric and thermal characteristics. Through strategic doping and processing, significant improvements were achieved in their energy storage capabilities [1]. For instance, compositional engineering of NKBT-based systems resulted in slim P–E loops and enhanced recoverable energy densities. Europium doping played a pivotal role in stabilizing polar nanoregions and lattice structures, achieving energy densities as high as 1.7 J/cm³ with efficiencies exceeding 80% [2]. Similarly, rubidium incorporation led to grain size refinement and improved mechanical robustness, supporting applications in biocompatible systems [3] . Niobium doping further refined the electromechanical response, enhancing piezoelectric coefficients and dielectric breakdown strength. The synergy of these modifications has enabled the development of materials with excellent thermal stability, high mechanical integrity, and superior electrical properties, making them suitable candidates for capacitive energy storage devices, actuators, and bio-implantable systems[4]. Additionally, the integration of optimized ceramic compositions with polymeric matrices such as PVDF has led to the fabrication of efficient nanogenerators for use in wearable and flexible electronic applications[5].

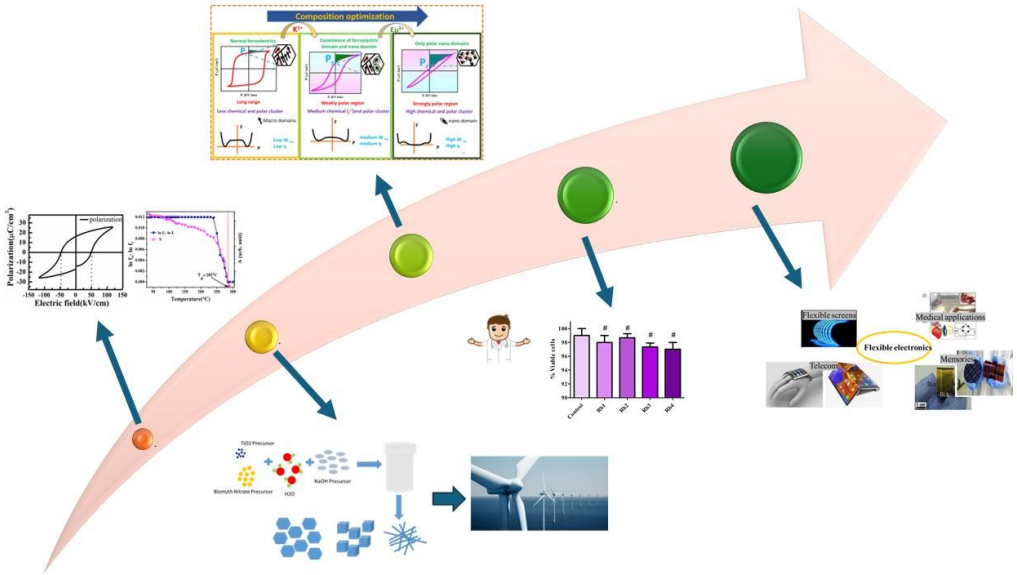

Fig.1. Progress of research in the recent years.

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Limits to Reliability of Ferroelectric Capacitors

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The growing interest in low-voltage electronic switches has renewed the attention to ferroelectrics as a functional unit of semiconductor devices. Among the candidate materials, $BaTiO_3$, a prototypical ferroelectric material, presents significant promise due to its low coercive field with appreciable remnant polarization. Despite years of research, several outstanding challenges in the growth and fabrication of ultrathin epitaxial $BaTiO_3$ capacitor heterostructures remain. Recent demonstration of ultralow switching in $BaTiO_3$ ferroelectric capacitors (coercive voltage < 100 mV) has piqued the interest of the community and presents the basis for low-voltage electronic switches. Despite this impressive tuning of the coercive field, important parameters such as retention and endurance of these capacitors remain poor. In this talk, I will outline the advances achieved in my group and co-workers to address these challenges. Specifically, we show that by controlling both the interfacial and bulk perfection of $SrRuO_3/BaTiO_3/SrRuO_3$ heterostructure ferroelectric capacitors, we show endurance $>10^{11}$ cycles and retention $>10^4$ s. Next, we show that high temperature (upto ~250°C) accelerated testing shows a record high ratio of breakdown to coercive voltage ratio, high dielectric constant with wake-up and fatigue free operation. I will also briefly discuss some of the fabrication advances achieved in my group to enable the use of $BaTiO_3$ for electronic applications.

Crystallographic Analysis of Phase Coexistence in Piezoelectric MPB Ceramics by Rietveld Structure Refinement

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Piezoelectric materials convert mechanical energy into electrical energy and vice versa, which makes them very important for smart sensors, transducers and actuator applications. Crystal structure and crystallographic phase coexistence is the key for high piezoelectric response in these materials. Our research group has investigated several Bi-based piezoelectric solid solutions with reduced Pb-concentration such as (1-x)$Bi(Mg_{1/2}Zr_{1/2})O_3$-x$PbTiO_3$, (1-x)$Bi(Ni_{1/2}Ti_{1/2})O_3$-x$PbTiO_3$, (1-x)$Bi(Mg_{1/2}Ti_{1/2})O_3$-x$PbTiO_3$, (1-x)$Bi(Mg_{1/2}Zr_{1/2})O_3$-x$BaTiO_3$, (1-x)$Ba(Cu_{1/3}Nb_{2/3})O_3$-x$PbTiO_3$ etc. for developing better alternative of widely used piezoelectric ceramics, due to growing concern about toxicity of lead. Many applications under non ambient conditions, require high Curie Temperature (T_C) such as actuators and transducers for automotive industries, space technology etc. for which Bi-based morphotropic phase boundary [MPB] ceramics have shown considerable promise. Tuning the optimum composition and electric field induced phase transitions in these materials are the main focus of researchers for developing good piezoelectric ceramics. In this seminar, I will present the results of Rietveld structural investigations on the crystal structure of the coexisting phases and phase transitions in several piezoelectric ceramic solid solutions developed in my group. I will discuss the resutls of structural investigations on electric field poled piezoceramic compositions across morphotropic phase boundary that reveals significant modifications in the crystal structure. I will also discuss phase coexistence and phase transitions in some newly investigated piezoelectric solid solutions. A novel Pb-free solid solution system (1-x)$Bi(Mg_{1/2}Zr_{1/2})O_3$-x$BaTiO_3$ is explored which exhibit monoclinic crystal structure and phase coexistence. We have recently investigated room temperature crystal structures of a new solid solution (1-x)$Ba(Cu_{1/3}Nb_{2/3})O_3$-(x)$PbTiO_3$ in the entire composition span. Despite both the end components, $Ba(Cu_{1/3}Nb_{2/3})O_3$ and $PbTiO_3$, having tetragonal (*P*4*mm*) symmetry, new cubic and monoclinic phases have been discovered for the intermediate compositions with multiple phase boundaries. Results of our investigation on unusual crystal structure evolution, phase coexistence and multiple phase boundaries in this system will also be discussed in the presentation.

Emergent phases in incipient ferroelectrics upon dilute electron doping

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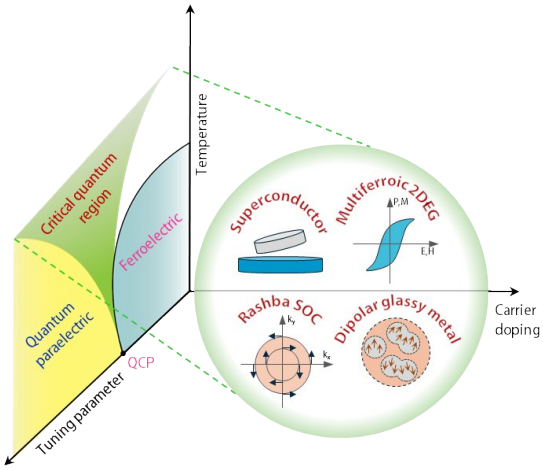
Incipient ferroelectric materials are a unique class of electronic systems that exhibit a paraelectric phase even though they possess an inherent ferroelectric instability. Two prominent examples, $SrTiO_3$ and $KTaO_3$, are also referred to as quantum paraelectrics. Their high dielectric constant value yields metallic behavior upon very dilute electron doping, aligning with the Mott's criterion of metal-insulator transition. In this talk, I'll share our latest discoveries of some really intriguing new electronic phases we've found in these materials. By carefully combining electron doping, cationic vacancies, and interface engineering, we've been able to create phenomena such as dipolar glassy metal phases, polar metals, and even two-dimensional superconductivity.



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Towards realization of metastable ferroelectric phase in orthorhombic rare-earth chromates

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Rare-earth chromates present a functional class of multiferroic compounds which exhibit antiferromagnetic ordering either around room-temperature ($LaCrO_3$: T_N =290 K) or below room-temperature (as in $GdCrO_3$: T_N=150 K). Some of these compounds were earlier reported to undergo ferroelectric ordering concomitant with the antiferromagnetic ordering or at temperatures slightly above the magnetic ordering temperature, raising questions on the driving force behind the ferroelectric ordering. It has been reported in literature, using first principles calculations, that some of the rare-earth chromates, which were found to be paraelectric or quantum paraelectric, also inherently possess ferroelectric instabilities which can be tuned through external perturbations, like strain. Kinetic stabilization of metastable ferroelectric structures often can lead to disruptive technologies, as in the case of HfO_2/ ZrO_2 based materials. Our initial results, which will be discussed here, seem to suggest that using a kinetically-driven synthetic technique, we have been able to stabilize a metastable ferroelectric phase at room-temperature in at least three representative members of the $RCrO_3$ family of compounds.

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Light modulated Magnetization in Ferromagnetic/PMN- PT Heterostructures

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The discovery of optically driven magnetization control has revolutionized spintronics, introducing a groundbreaking scientific paradigm that harnesses light-induced strain to manipulate magnetic order. This contactless and energy-efficient approach utilizes photostriction light-induced strain generated in ferroelectric materials through the combined effects of the bulk photovoltaic response and inverse piezoelectricity. The light-driven ferroelectric manipulation stands out as a promising yet underexplored avenue. Recently, $PbTiO_3$-based compounds, particularly PMN-PT ($Pb(Mg_{1/3}Nb_{2/3})O_3$–$PbTiO_3$), have gained attention due to their exceptional piezoelectric and electromechanical properties. PMN-PT exhibits photo-strictive behavior, making it a promising candidate for optically controlled domain engineering. Figure 1 shows photo induced strain in the PMN-PT lattice via X-ray diffraction.

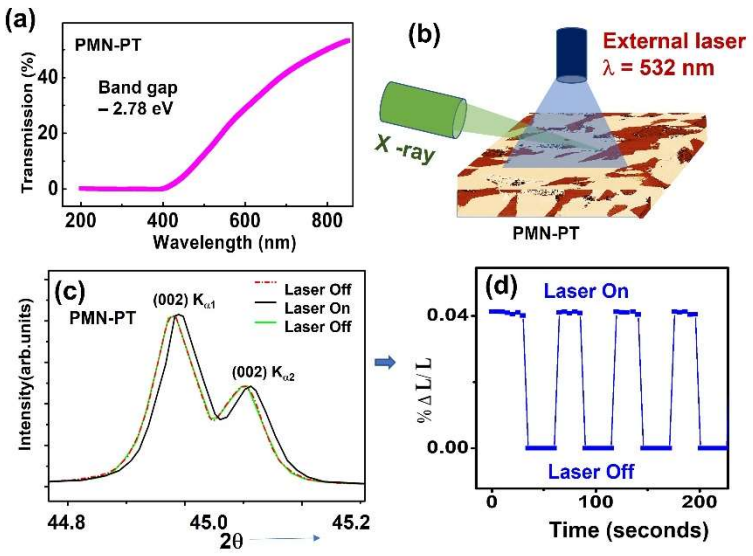

Fig 1. *(a) Optical absorption spectrum of PMN-PT, showing increasing transmission with wavelength. (b) Schematic of the experimental setup, where a 532 nm laser and X-ray (λ = 0.154 nm) are used to probe structural changes due to laser illumination. (c) XRD patterns of PMN-PT (002) under laser illumination, showing a shift in peak positions. (d) Time-dependent strain response (% ΔL/L) of PMN-PT (002) under laser ON/OFF cycles.*

In FM/PMN-PT heterostructures, light illumination induces non-thermal strain in PMN-PT, which is mechanically transferred to the adjacent FM magneto strictive layer (e.g., Fe, Ni, or Co), resulting in modulation of magnetic anisotropy, domain configuration, or net magnetization. As research advances, FM/PMN-PT heterostructures are emerging as versatile platforms for optically tunable magnetoelectric devices, with significant potential in low-power spintronics, adaptive logic, and high-speed optomagnetic memory systems.

Structural phase transitions and enhancement of physical properties in Li and Ta modified $K_{0.5}Na_{0.5}NbO_3$ system

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Perovskite-based ferroelectric materials have strong potential to be utilized in numerous electrical and electronic devices due to their high piezoelectric coefficients, excellent dielectric and ferroelectric properties, and strong electromechanical coupling. The physical properties of the ferroelectric materials and the theory of phase transition have been studied using wide experimental investigations as well as theoretical considerations. The structural phase transition in the ferroelectric materials are accompanied by a change in the symmetry due to the external stimuli like chemical substitution, temperature, pressure, electric field, and also with swift heavy ions (SHI). Among the various lead-free ferroelectrics, sodium potassium niobate, $(K_{0.5}Na_{0.5})NbO_3$ (KNN)) has gained notable attention due to its interesting physical properties such as high Curie temperature (T_C ~ 420°C), high remanent polarization (P_r = 33 μC/cm^2) and moderate electromechanical coupling. At room temperature, KNN crystallizes into an orthorhombic structure (SG: *Amm2*) and undergoes a sequence of phase transitions similar to the phase transitions observed in $BaTiO_3$. With decreasing temperature, the cubic paraelectric phase (SG: Pm-3m) transforms to ferroelectric tetragonal structure (SG: *P4mm*) at 420 °C. Further cooling below 200 °C (T_{O-T}), it transforms to orthorhombic structure (SG: *Amm2*), and finally, it transforms to *R3m* symmetry with rhombohedral crystal structure also having ferroelectricity below -150 °C (T_{O-R}). In order to overcome the inherent problems associated with KNN systems, we have investigated the composition-driven structural phase transition and their correlation with the physical properties of Li and Ta co-substituted KNN ceramics. Various reports are available on the enhancement of the physical properties of the KNN system due to the existence of morphotropic phase boundary (MPB), which are attributed to the existence of different crystallographic phases. The improvement in the physical properties in KNN-based systems also reported due to the shifting of the polymorphic phase boundary (PPB i.e., T_{OT}) close to RT rather than the existence of a MPB. Hence, it is imperative to understand the microscopic origin of enhancement of the physical properties of Li and Ta co-substituted KNN system.

In view of the above, Lead-free $(K_{0.48}Na_{0.48}Li_{0.04})(Nb_{1-x}Ta_x)O_3$ (KNLNT-*x*) ceramics were synthesized using the conventional solid-state synthesis route. XRD analysis revealed composition-driven structural phase transitions, which was further supported by Raman spectroscopic studies. The phase transitions behavior was further analyzed using temperature-dependent dielectric properties at different frequencies. The dielectric, ferroelectric and piezoelectric properties shows maximum values at a specific composition, particularly within the phase coexistence region. To develop a clear understanding of the phase transition phenomena across various compositions and temperatures, phase diagrams were constructed using the room temperature XRD, Raman, and temperature-dependent dielectric data. Finally, the enhancement in functional properties was correlated with the crystal structure as interpreted through the phase diagram. The details of our result will be discussed during the time of presentation.

Understanding Polarization Rotation in Relaxor Ferroelectrics Using Epitaxial Thin Films

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In this talk, I will present a series of recent investigations on the structure-property relationships in epitaxial thin films made of the prototypical relaxor ferroelectric $0.68PbMg_{1/3}Nb_{2/3}O_3$-$0.32PbTiO_3$ (PMN-PT). First, I will present the work on the epitaxial strain dependence of domain structures and dielectric and ferroelectric properties in PMN-PT thin films. Next, I will present the work on the relationship between polarization rotation and polar nanodomains using a multi-scale approach that probes the structural evolution in both the average unit-cells and polar nanodomains. We observed that the boundary between (pseudo-)rhombohedral and (pseudo-)tetragonal crystal structures of unit-cells is located in the same region of the strain-electric-field diagram as the boundary between ellipsoidal and cylindrical polar nanodomains, which are elongated along the <011> and [001], respectively, which implies that structural transitions between polar nanodomain configuration underpins the polarization rotation and large electromechanical coupling of relaxors.

Keywords: Relaxor ferroelectrics, polarization rotation, epitaxial strain, polar nanodomain

Fully Printed Negative-Capacitance Field-Effect Transistors with Ultralow Subthreshold Swing and High Inverter Signal Gain

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The switching of conventional field-effect transistors (FETs) is limited by the Boltzmann barrier of thermionic emission, which prevents the realization of low-power electronics. In order to overcome this limitation, among others, unconventional device geometry with a ferroelectric/ dielectric insulator stack has been proposed to demonstrate stable negative-capacitance behavior. Here, the switching of the ferroelectric layer offers a step-up amplifier like behavior within the device, which results in a body factor less than 1. This implies a larger change in the semiconductor surface potential can be achieved compared to the applied gate voltage variation. Transistors with such ferroelectric/ dielectric stack are known as negative-capacitance field-effect transistors (nc-FETs), and they can demonstrate a subthreshold slope lower than the Boltzmann's limit at room temperature (60 mV/decade).

While nc-FETs have typically been realized with high-vacuum-deposition processes, here we show fully printed nc-FETs, at first with amorphous indium–gallium-zinc oxide (a-IGZO) as the semiconductor material, Al_2O_3 as the dielectric, and poly(vinylidene fluoride-trifluoroethylene) (PVDF-TrFE) as the polymer ferroelectric. These printed nc-FETs demonstrate an extremely low subthreshold slope of ~2.3 mV/decade at room temperature, which remains below Boltzmann's limit for over 5 orders of magnitude of drain currents. Furthermore, the unipolar pseudo-CMOS depletion-load-type inverters fabricated using *n*-type nc-FETs are found to demonstrate an extraordinary signal gain of 2691.

In the next step, all organic insulator fully printed nc-FETs are demonstrated, which can be fabricated at or near room temperature on inexpensive flexible substrates, such as photopaper or polyethylene terephthalate (PET). In this case, polyvinyl alcohol (PVA) and PVDF-TrFE are used as the dielectric and ferroelectric material, respectively, and a subthreshold slope of 20.3 mV/dec has been demonstrated. The unipolar, pseudo-CMOS depletion-load inverters fabricated using these nc-FETs have exhibited signal gain of 1967, at the supply voltage (V_{DD}) as high as 16 V. It is believed that these fully printed and low temperature processed nc-FETs would be able to find huge application potential in printed low power (power-on-chip) sensor patches, where the interface electronics made of nc-FETs would be able to magnify low intensity and noisy analog signal of a temperature, toxic gas, chemical or biosensor.

Probing polar distortions in ferroic oxide films with atomic resolution electron microscopy

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Polar distortions play a pivotal role in defining the functional properties of ferroelectrics and multiferroics. These atomic displacements of non-centrosymmetric crystals give rise to electrical polarization that, depending on their response to external electric fields and coupling with additional order parameters, gives rise to ferroelectricity and multiferroicity, respectively. In ferroic oxide thin films, subtle modifications in crystal symmetry or stoichiometry can induce or modify their polar nature, and consequently their their macroscopic properties [1] In the pursuit of understanding and tailoring the ferroic properties of ferroic oxide materials, quantitative atomic-scale scanning transmission electron microscopy (STEM) has provided unique capabilities to understand key polar-driven phenomena, such as flexoelectricity [2], polar textures [3], or domain wall conductivity [5]. In this lecture, we review our recent atomic-scale STEM investigation of polar oxide thin films, focusing on two exciting systems. Firstly, we will evidence the possibility of tailoring polarization orientation in epitaxially strained multiferroic $Sr_{1-x}Ba_xMnO_3$ thin films. We have demonstrated that non-centrosymmetric polar distortions can be induced in strained ultrathin films, and that these distortions can be tuned by a combination of epitaxial strain and tailoring stoichiometry [4]. Second, we will present the atomic-scale investigation of the conductive nature of nominally neutral 180° domain walls (DWs), artificially created in an epitaxial $PbZr_{0.1}Ti_{0.9}O_3$ thin film. Our results show that the 180° DW conductivity is associated with the emergence of polar discontinuities, including the formation of tail-to-tail charged segments, which has been further confirmed by electron energy loss spectroscopy [5].

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Ferroelectric thin film for memory and neuromorphic device application

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Ferroelectric insulating thin film can be used as a gate dielectric of a memory transistor that can control the On or Off state of the channel conduction even after removing gate bias due to the spontaneous polarization of the ferroelectric thin film. However, duration of this On or Off state of the transistor depends on the depolarization field that operates on the ferroelectric film due to the imbalanced electric polarization of the interface across the ferroelectric gate dielectric. Therefore, we proposed to sandwich this ferroelectric thin film in between two ion-conducting dielectrics or in alternating stacked structure. Using these two different configurations, it is possible to fully 'compensate' the depolarization field that greatly enhances the memory retention time of the transistor. Beside, these memory transistors are used as neuromorphic devices. Again, by using a thin layer of ion-conducting dielectric in-between two ferroelectric insulating thin film, we fabricated a multilevel resistive switching device which can show largely enhanced memory retention with cyclic stability, also can be used as neuromorphic device.

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Brief Biodata: Dr. Bhola Nath Pal is a professor of School of Material Science and Technology, IIT(BHU). He did his B. Sc. and M. Sc. (in Physics) from University of Calcutta and PhD from Indian Association for the Cultivation of Science (2005). He was post-doctoral fellow at Johns Hopkins University, Los Alamos National Laboratory and at University of Queensland before he joined in IIT(BHU) in 2014. He has published more than 100 papers in peer reviewed international journals and has three US and 10 Indian patents. His research area is on solution processed thin films for electronics, optoelectronics, energy applications.

Invited Talk

Solution-Processed Doped-Hafnia Ferroelectrics on Silicon: A Pathway to Commercial Integration

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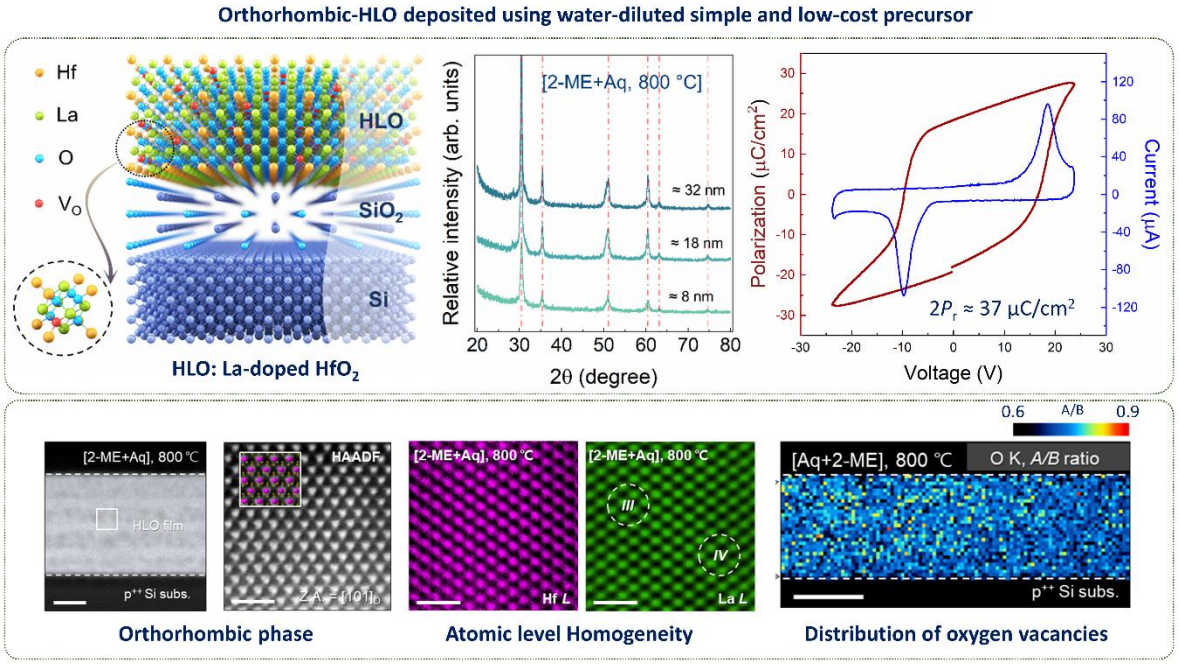
Abstract

Solution-processed thin films face challenges such as poor film quality, reproducibility issues, and high operational costs due to volatile solvents and moisture-sensitive precursors. Achieving high-quality films often requires multilayered deposition with prolonged processing cycles, limiting their commercial viability. However, hafnia-based ferroelectrics offer a promising alternative, as they exhibit ferroelectricity even at low thicknesses, reducing deposition complexity. Unlike oxide semiconductors, they do not have stringent film-quality or charge transport requirements, making solution-processed doped-hafnia ferroelectrics a viable option for next-generation electronics. To address these challenges, we developed lanthanum-doped hafnium oxide (HLO) thin films using a water-based precursor with excellent shelf life. Unlike conventional methods that rely on nanocrystalline morphology and carbonaceous impurities for o-phase stabilization, our approach enables large-grained (>100 nm) HLO films on silicon via engineered precursors with minimal carbon content. The well-distributed La dopant generates oxygen vacancies, stabilizing the o-phase without requiring oxygen-scavenging electrodes. These films exhibit a high remnant polarization of 37.6 μC/cm² ($2P_r$), withstand large fields (>6.2 MV/cm), and enable improved MOSFET switching through the negative capacitance effect. By eliminating the need for nanostructuring, capping stresses, or reactive electrodes, our solution-processed HLO films provide a scalable, wake-up-free ferroelectric platform for advanced electronic applications.



Exploring Temperature and Bias-Dependent Switchability and Tuneability of BST based L-Ku Band MEMS Resonators

Kongbrailatpam Sandeep Sharma[1]; Akhil Raman T.S[2]; Chandrashekar L. N[1]; James Raju K. C[2]; ***Gayathri Pillai***[1]

The capability of HBAR in providing a high Q multimode response across a wide microwave frequency range translates well for applications in material characterization, RF filters and microwave sources [1] [2]. Recent developments in the field of hybrid quantum acousto dynamic (QAD) circuits, HBARs has proved to be a viable candidate for utilisation as a phonon source [1] [3]. [1] uses an epitaxial thin film (GaN) and reports the highest Q is in the order of 106 and for sputtered thin film (AlN) based HBAR in [3], the Q is in the order of 10^5.

At the core for the pursuit in achieving ever higher *Q* (and $f \times Q$), lies the motivation of using the high *Q* resonator in tandem with microwave or optical components which will complete the hybrid systems such as QAD circuits. In particular, the lack of micromachining or ease in fabricating an HBAR compared to other MEMS resonators is overwhelmed by the complexities and challenges one encounters during the resonator characterization because of the overabundance of high *Q* modes in a wide frequency spectrum. Overestimating the *Q* could lead to inability to couple or inefficient coupling with other subsystems in complex systems like QAD or acousto-optic modulators. Due to this reason, in the work reported here, considerable effort has been put forth during the measurement set-up, data processing and data interpretations to accurately estimate the *Q* factor of the resonator.

In this work, we report the excitation of extremely high-quality factor (Q) bulk acoustic wave modes with a degree of switchability and tuneability achievable by utilizing the electric field-induced piezoelectric effect in the transducing barium strontium titanate (BST) thin film of a high overtone bulk acoustic resonator (HBAR). The HBAR exhibits Qs in the order of 10^5 over multiple resonant modes around 5 GHz measured at 50 K temperature and with a DC electric field applied across the transducer stack. The diversion from the conventional piezoelectric material route as a transducer material in such HBAR can facilitate additional functionality such as reconfigurability with competitive values of quality factors compared to traditional piezoelectric-based HBARs. The work demonstrates the highest recorded Q for a polycrystalline ferroelectric thin film based Bulk Acoustic Wave (BAW) resonator.

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Strategies for maximizing polarization in ferroelectric HfO_2

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Ferroelectric HfO_2, a CMOS compatible material, holds great promise for new memory and energy devices. Ferroelectric HfO_2 films are mostly studied in their polycrystalline form. The mixture of polar and nonpolar phases with different orientations challenges the understanding of ferroelectric properties and impedes fine tuning of the ferroelectric orthorhombic phase stabilization. The orthorhombic phase of hafnia is ferroelectric, but this phase is metastable and its stabilization is usually achieved only in ultrathin films where the contribution of surface energy is relevant. In addition, other factors can be important. Doping optimal concentration is particularly relevant, and also interfaces, point defects like oxygen vacancies and lattice strain can affect the formation energy of competing polymorphs. Understanding the role of these factors is important to achieve further control over the stabilized phases and thereby improve ferroelectric polarization and stabilize the ferroelectric phase in thicker films. Epitaxial layers are well suited to increase our understanding of ferroelectricity in these oxides. To gain insight into the role of defects and stress at interfaces, we compare series of $Hf_{0.5}Zr_{0.5}O_2$ and Y-doped HfO_2 epitaxial films of various thicknesses. The films were grown on (001) and (110) oriented $SrTiO_3$ substrates to impose different symmetry at the interface. We also investigate the impact of redox conditions during growth, by comparing films deposited in a pure O_2 or mixed O_2/Ar atmosphere. We find that interface symmetry and redox conditions are critical, and they can be cooperatively optimized to maximize the ferroelectric polarization. In contrast, lattice strain is not a relevant factor. We also show that Y is a more efficient dopant than other atoms more commonly used, which allows the stabilization of the ferroelectric phase in epitaxial films thicker than 100 nm.

Design and Fabrication of Phononic Integrated Circuits in Scandium Aluminum Nitride

Abstract:

Acoustic waves are well-suited for a variety of signal processing applications including RF filtering and optical modulation. Advances in material and fabrication capabilities have enabled the demonstration of chip-scale subsystems in which phonons can exhibit strong interactions with a variety of other physical domains. To this end, the guidance and control of acoustic waves in phononic integrated circuits (PnICs) enables numerous opportunities. This talk focuses on the development of such guided surface acoustic wave components in suspended as well as solidly mounted 30% scandium-doped aluminum nitride (ScAlN). Numerical modeling, coupled with experimental results, showcases the characteristics of focusing interdigitated transducers (FIDTs) for injecting acoustic energy into piezoelectric etch-defined acoustic waveguides and highlights their advantages over conventional uniform aperture transducers. We also demonstrate the behavior of 90-degree bends, low-loss Y-junctions as splitters/combiners, directional couplers and traveling wave racetrack resonators to enable phononic integrated circuit applications in slow-on-fast piezoelectric platforms.

Bio:

Siddhartha Ghosh is an Assistant Professor in the Department of Electrical and Computer Engineering at Northeastern University. He received the B.S. degree in from Cornell University in 2007, the M.S.E. degree from the University of Pennsylvania in 2011 and the Ph.D. degree from Carnegie Mellon University in 2015, all in electrical engineering. From 2015-2020 he was a member of the Technical Staff at MIT Lincoln Laboratory. He is the co-author of over 40 journal and conference publications and co-inventor on 3 US patents. Dr. Ghosh received the DARPA Young Faculty Award in 2023 and the NSF CAREER Award in 2024. His research interests include piezoelectric MEMS, optomechanical resonators, oscillator-based computing and acousto-electronic devices.

Mapping of Polarization Orientation Microstructure in Polycrystalline and Epitaxially Grown BCZT Thin Films using Piezoresponse Force Microscope

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Abstract

The presence of significant strain-polarization coupling that exists in ferroelectric materials, facilitates tuning the strain conditions and serves as an effective strategy for tailoring the ferroelectric properties in thin films. In this talk the major focus would be on the lead-free (1-x)(Ba,Ca)TiO3-xBZrTiO3 (BCZT)solid solution, in the morphotropic phase boundary (MPB)composition. The Polarization components would be derived from the electrical signal and polarization vector mapping of the piezo response force microscope (PFM) and the respective domains in both epitaxial and polycrystalline layers of BCZT will be discussed. The polarization orientation map highlights the role of strain relaxation in the epitaxial thin films and in the case of polycrystalline thin films, it facilitates the observation of polarization under externally induced strain gradient using a novel 3 point bending stage under the scanning probe microscope. The results pertaining to strain gradient induced structural transformation in MPB phases of BCZT thin films will also be presented.

Keywords: Ferroelectrics, PFM, lead-free piezoelectric, BCZT & Structural transformations

Polar Skyrmions in Planes of Strained Ferroelectric Systems

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Superlattice of ferroelectric perovskite material (PbTiO$_3$)$_n$/(SrTiO$_3$)$_n$ hosts exotic topological structures such as polar skyrmion bubbles at room temperatures [1]. Despite the absence of analogous to Dzyloshinskii-Moriya type interaction, stabilization of these non-collinear polarization structures is mystifying. We identify [2] that the electrostriction energy term, which couples electric polarization vector and elastic strain, is responsible for any such possible non-collinear structures because it provides, upon integration by parts, quintessential gradient in polarization. We have formulated the coupled Euler equations of the polarization vector and the elastic displacement vector and have found skyrmion solution with a unique topological number in each layer of the superlattice for a range of electric field applied perpendicular to the plane. The types of skyrmions vary from Neel to Bloch depending upon the position of the layer, in agreement with the n-layer structure within the bubble structure reported in the experiments [1]. The lower and upper limits of the electric field for which the skyrmions are stabilized, have been estimated, and these bounds possibly explain why skyrmion bubbles are obtained for a specific range of n. These bounds together with the scaling in the parameter regime are exploited to find a phase diagram for stabilizing skyrmions in the electric field-temperature plane. This is consistent with the previous phase-field simulation result [3].

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Material-Limited Switching in Nanoscale Ferroelectrics

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The ferroelectric switching speed, a critical metric behind the operations per second or latency possible in a non-volatile memory, has been experimentally obfuscated by the interaction between the measurement circuit and the ferroelectric switching itself. Here I will discuss our investigation of this interaction in a suite of popular ferroelectric thin films particularly as the diameter is decreased from micro- to nano-scales. We simulate the interaction using nucleation and growth models embedded in a circuit model. The results well simulate the results. At the nanoscale, we observe some of the fastest switching times reported for any ferroelectric. Further, for polycrystalline $Hf_{0.5}Zr_{0.5}O_2$ capacitors, a fundamental switching limit of ~210 ps is observed. I will also discuss the scaling behavior of material parameters and related technological figures of merit. Lastly, a criterion for reaching the material-limited regime will be provided. This regime enables observation of intrinsic material properties and favorable scaling trends for high-performance computing.

Harnessing the polar vortex motion and tunable skyrmion liquid phase in oxide heterostructures

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Abstract

Polar topological structures such as vortices and skyrmions offer promising pathways toward low-power, high-density, and CMOS-compatible nanoelectronic devices due to their intrinsic stability, ultrasmall dimensions, and rich functional properties.[1-2] However, their practical application remains limited by challenges in controlled manipulation and post-synthesis tunability. In this study, we demonstrate real-time control of polar vortices and skyrmions in $PbTiO_3/SrTiO_3$ superlattices using localized electric fields and thermal stimuli. Piezoresponse force microscopy (PFM) and scanning transmission electron microscopy (STEM), complemented by phase-field simulations, reveal reversible motion, reshaping, and annihilation of vortex structures, along with electric-field and temperature-dependent evolution of skyrmion phases. Correlation function analysis confirms a liquid-like skyrmion state, enabling tunable phase behavior. These findings establish a framework for dynamic control of polar topologies, advancing their integration into reconfigurable and energy-efficient topological devices.

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Emerging Polar Altermagnetic Metallic States in Epitaxially Strained RuO_2 Films

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RuO_2, a rutile 4d-transition metal oxide, exhibits a unique crystal structure with both edge- and corner-sharing octahedra. This intrinsic anisotropy, when combined with strain engineering, provides a powerful avenue for tuning anisotropic electronic and optical properties. However, from a synthesis perspective, challenges such as variable Ru valence states, Ru/O stoichiometry control, anisotropic strain states, and structural defects can make it difficult to distinguish intrinsic properties from extrinsic effects in RuO_2 thin films—a classic trick in the pursuit of novel functionalities in quantum materials.

In this talk, I will highlight our group's efforts in overcoming these synthesis challenges while demonstrating metallicity in epitaxial RuO_2 films down to the unit cell scale. Through a combination of advanced X-ray scattering, X-ray absorption spectroscopy, transmission electron microscopy, temperature-dependent transport, magneto-optical measurements, and density functional theory (DFT) calculations, we uncover robust magnetism in epitaxially strained RuO_2, consistent with an altermagnetic metallic phase [1-3]. Additionally, we reveal a novel polar phase in strained films with significant implications for electrical transport—an unexpected treat in the realm of functional oxides. I will discuss these findings in detail, emphasizing their sensitivity to material defects and structure—key ingredients that are often overlooked but crucial in determining emergent quantum phenomena.

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Real time Applications of Piezoelectric and Ferroelectric Materials: A perspective of Material Response to Device Qualification

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Piezoelectric materials offer exceptional precision, high response, and versatility, making them indispensable in advanced engineering systems spanning aerospace, automotive, healthcare, and consumer electronics. Their inherent attributes—compactness, low weight, durability, and rapid electromechanical conversion—enable integration into miniaturized, high-performance components. The effectiveness of these materials in real-world applications is governed by key parameters such as the piezoelectric coefficient and resistance to depolarization across wide frequency and temperature ranges.

In aerospace systems, piezoelectric accelerometers are utilized for critical tasks including vibration and shock monitoring, structural health diagnostics, modal analysis, and flight data acquisition. Acousto-ultrasonic transceivers facilitate localized damage detection and real-time structural integrity scanning, as well as fluid pulsation analysis in pipe networks. In the context of Piezoelectric actuators and their applications in the aerospace, they may play multiple roles, starting from controlling aerodynamic flutter to imitating insect flight dynamics for Micro Aerial Vehicles (MAVs), while also performing precision valve operations and targeted force application.

On the other hand, ferroelectric materials are emerging as pivotal components in modern energy storage solutions, thanks to their remarkable polarization properties coupled with naturally high dielectric constant. Ferroelectrics are especially promising for use in capacitors, where efficient storage and release of energy is essential. The practical implications are vast. Ferroelectric capacitors are now commonly integrated into electronic systems that demand rapid energy discharge or stable energy retention. Their utility spans a wide spectrum of applications—from pulsed power and advanced electromagnetic systems to life-saving medical equipment. As demand for smarter, more efficient energy solutions rises, ferroelectric materials stand out not only for their performance, but also for their potential to revolutionize how energy is managed in both everyday gadgets and cutting-edge technologies.

This talk highlights the multifaceted nature of product formulation, emphasizing not only the adaptability of underlying processes but also the critical role played by intrinsic material properties and rigorous qualification standards. Successful demonstrations in targeted scenarios demand a calibrated alignment of technical precision, operational robustness, and contextual relevance. By examining specific cases, we unveil how excellence in design and execution elevates product validation from a mere technical formality to a strategic enabler of innovation and credibility.

Room Temperature Giant Inverse Magnetoelectric Effect in Topotactic Phase Transition Material SrCoO2.5

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The topotactic phase transition in $SrCoO_x$ (x = 2.5 and x = 3) end members promotes these materials prospects for various applications, such as solid oxide fuel cell, neuromorphic computation, mottronics, memory devices, etc. The correlated structural, electronic and magnetic properties of SrCoO2.5 (SCO2.5) offer tunable electrical and magnetic phases via strain in thin film form. It is shown that the strained SrCoO2.5 film is ferromagnetic, while the relaxed SrCoO2.5 is antiferromagnetic and SrCoO3 is ferromagnetic. In a hetero-structure of SrRuO3/SrCoO2.5/Nb doped SrTiO3, we exhibit a room temperature giant change in magnetization ~200% at a miniscule electric voltage of 2V, akin to inverse magnetoelectric effect (ME). We term it as volto-magnetic (VM) effect. The observed volto-magnetic effect arises due to electric field tuneable structural and magnetic phase of SrCoOx.

Initiatives in Piezoelectric Voiceprint for Biometric Healthcare Assessment

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In this talk, we explore the exciting possibilities of programmable piezoelectric interfaces, where the realms of nanotechnology converge with smart wearable technology.[1-3] We delve into the fabrication of advanced sensors harnessing the power of piezoelectricity, enabling us to unlock new dimensions in human-machine interaction. These sensors pave the way for a myriad of applications, from voice biometrics to the recognition of different emotions, and non-invasive disease detection.[3-5] Join us on a journey through the innovative landscape where materials and technology harmonize to shape the future of wearable devices with limitless possibilities.

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Emergent Surface Multiferroicity

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In my talk, I will present our recent findings on the emergence of multiferroicity at the surface of centrosymmetric, collinear, and compensated antiferromagnets that host ferroically ordered magnetic octupoles in the bulk. Unlike the bulk, which is nonpolar, magnetically compensated, and lacks a linear magnetoelectric response, the surface exhibits all key signatures of multiferroicity: a net electric dipole moment, net magnetization, and a linear magnetoelectric effect. Particularly intriguing is the case of nonrelativistic *d*-wave spin-split antiferromagnets, where both bulk octupoles and surface multiferroicity arise even in the absence of spin-orbit interaction. I will illustrate these results using FeF_2, as a model system. Our work highlights the role of bulk-boundary correspondence and demonstrates how bulk multipoles can be used to engineer surface multiferroicity in otherwise non-multiferroic materials.

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Growth of Lead-free Heteroepitaxial Thin Films of (Na0.8K0.2)0.5Bi0.5TiO3 Ferroelectrics by Nd:YAG Laser Pulsed Laser Deposition

Abstract:

Heteroepitaxial thin films of (Na0.8K0.2)0.5Bi0.5TiO3 (NKBT) ferroelectrics were grown by Nd:YAG laser coupled pulsed laser deposition. Compared to conventional excimer-laser based PLD, Nd:YAG laser provides several advantages including low capital costs, low operational costs and small foot-print, without compromising significantly on the performance. High quality heteroepitaxial thin films of NKBT were shown to be useful for capacitive energy storage (energy density ~ 26.4 J/cm3 and energy storage efficiency ~ 60.3%) and piezoelectric actuators (d33 ~ 160 pm/V) with high breakdown strength (>1.9 MV/cm). The study provides a cost-effective way of producing high quality ferroelectric films compared to traditional excimer-laser based PLD.

Superharmonic Resonant Response Measurement: A novel method for measuring spontaneous polarisation in pyroelectric thin films

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We introduce a new method, called Superharmonic Resonant Response Measurement (SRRM), for measuring the spontaneous polarization (Ps) in pyroelectric thin films. Crucially, this method does not rely on polarization switching and, therefore, can be used for measurements of materials such as AlN, GaN, etc., which do not exhibit switching of spontaneous polarization. We first validate our technique using a PZT-based PMUT device. This allows us to independently measure the spontaneous polarization for PZT, thereby verifying our results. Next, we use this method to measure the spontaneous polarization of AlN films. The technique yields a measured spontaneous polarization value of 0.05-0.15 C/m2 for MOCVD AlN films. Additionally, we demonstrate that the spontaneous polarization (Ps) of materials with a high coefficient of nonlinear dependence of the dielectric constant on the electric field depends on this nonlinear coefficient. This obviates the need for even a PUND measurement.

Exploiting giant electrocaloric effects in epitaxial thin films of ferroelectric and anti-ferroelectric perovskite oxides

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Giant electrocaloric effects are large thermal changes that occur in ferro- and anti-ferroelectric materials in response to external electric fields [1]. Electrocaloric materials offer a promising alternative approach to energy-efficient and environment-friendly solid-state cooling technologies [2]. In recent times, breakthroughs in thin film fabrication have revealed that giant electrocaloric effects can exist at the nanoscale thus giving hope to tangible microelectronic cooling applications. We will address some of the outstanding challenges for the fundamental understanding and practical implementation of electrocaloric effects. We will highlight on the role of interfaces in epitaxial ferroelectric BCZT and antiferroelectric $PbZrO_3$ thin film heterostructures for achieving giant electrocaloric effects [3]. Electrocaloric effects are typically estimated from the thermodynamic analyses of polarization and field in ferroelectric materials, which implies that higher field application gives larger temperature changes. However, this may not be always true. In this direction, using both indirect and direct methods, we will discuss an anomalous effect where larger thermal changes occur by applications of lower fields in multi-domain ferroelectric $BaTiO_3$ single crystals. We attribute this counterintuitive effect to the interplay of the *c*- and *a*-domains in the $BaTiO_3$ (001) single crystals under the influence of temperature and field changes [4]. This work provides a fundamental understanding of the complex role of domains in governing the electrocaloric response of ferroelectric materials which is often overlooked but critical for their practical applications.

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Visualizing solid-state amorphization in ferroelectric In_2Se_3 through in situ electron microscopy

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In2Se3 is a van der Waals material, displaying rich polymorphism, with some phases being polar. In any polar In2Se3, we show that application of electrical bias parallel to the van der Waals layers slides the layers, creating sliding (and domain) boundaries through electromechanical coupling. When these domain boundaries start interacting with each other they emit Barkhausen's noise, which replicate the sliding defects and their interaction in longer range. Defect intersection also leads to local amorphization, which also replicates with the mechanical shocks described above. All in all, when the amorphous regions percolate, they undergo a percolative low resistance to high resistance state transition at powers that are a billion times less than what is needed to amorphized the same material through melt-quench process.

We show that such layer sliding, rotations and associated phase transitions are also very common in real devices such as ferroelectric semiconducting field effect transistors, and play a crucial role in designing novel neuromorphic devices.

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Giant Electrostriction in $La_2Ce_2O_7$ Ceramic: Is Texture Always Helpful for Functional Properties?

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Traditionally, heavily Lantha doping in ceria have been reported for issues involving dopant segregations, poor sinterability, etc. The reason for the same was attributed to high (~15%) mismatch in ionic radii between La^{3+} and Ce^{4+} ions that eventually created problems in high temperature diffusion pathways. Heavily La_2O_3 doped ceria compositions (e.g., $La_2Ce_2O_7$) is also known for their ultralow (0.5 W/m.K) thermal conductivity [1,2] values, thus, making the issues further complicated for making dense, bulk sintered $La_2Ce_2O_7$ ceramic. For the last ten years, our laboratory at IIT Patna has made dedicated efforts to make highly (111) textured dense $La_2Ce_2O_7$ ceramic (Lotegerring factor- 0.97) via innovative synthesis and processing modifications [3-5]. The current work focuses on the role of texture and sintering parameters of a dense $La_2Ce_2O_7$ ceramic on its dielectric and electrostriction properties.

Texture has generally accepted as a convenient tool to enhance various functional properties particularly dielectric of numerous ceramic systems. However, in this work, we show its selective dependence on specific functional properties. While ionic conductivity (driven by oxygen vacancies) [6], thermal conductivity (a majorly phonon driven phenomenon for ceramic systems) [7] showed no influence of texture, an order of magnitude improvement in dielectric losses [8] was noted for textured $La_2Ce_2O_7$ ceramic. Both the textured and nontextured ceramic depicted promising electrostriction values. A remarkable electrostrictive coefficient [$M_{33} \approx 10^{-18}$ $(m/V)^2$, exceeding conventional electrostrictive materials], coupled with a high effective piezoelectric response (d_{33}^{eff}= 40 pm/V at E= 100 kV/cm) was obtained [8]. The combination of electromechanical and dielectric properties creates conditions for high energy-harvesting performance, comparable to lead-containing ceramics and far superior to lead-free alternatives.

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Tunable spin polarization in ferroelectric hybrid organic-inorganic perovskites

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Hybrid organic-inorganic perovskites (HOIPs) of the form ABX_3 (A: organic molecule or element, B: divalent cation, X= monovalent anion) have emerged as suitable optoelectronic materials and have certain advantages over oxide counterparts because of semiconducting, flexible nature and need low processing temperatures. However, these perovskites have yet to reach their maximum potential in their applications. Using first principle methods, we investigated the electronic properties of both hybrid ferroelectrics and Ge-based halide perovskites. In the first part, we examined the electronic structure of new hybrid organic-inorganic perovskites $MHyPbX_3$, where MHy is methylhydrazinium(MHy) molecule $CH_3NH_2NH_2$ and X is Br or Cl, have been experimentally synthesized. First-principles simulations predict giant spin splitting in methylhydrazinium lead halide hybrid organic-inorganic perovskites. The values can reach 408.0 meV at zero Kelvin and 281.6 meV at room temperature. Moreover, SOC leads to the development of persistent spin textures in the momentum space, which are known to enhance spin relaxation time significantly.

Hybrid formate perovskites with the chemical formula $AB(HCOO)_3$ are another set of hybrid perovskites exhibiting coupled degrees of freedom between magnetic and ferroelectric ordering. Many exhibit AFM ordering and undergo phase transitions into polar space groups above room temperature. The first-principle simulations in hydrogenium Co-Formate predict SOC-induced spin splitting that exists already in the prototype of the centrosymmetric phase of the material and even in the time-reversal invariant momenta points of the Brillouin zone. The phase transition from the centrosymmetric to the polar phase of the material results in a dramatic change in the spin-splitting landscape in the Brillouin zone, thus offering additional tunability by the electric field or temperature. .

Halide-based hybrid perovskites exhibit spin-polarized bands in their polar phase, whereas AFM-ordered formate one exhibit in their non-polar phase. The strength of spin-splitting varies with entities at A and B sites and the type of temperature, pressure, and magnetic orientation. In nonmagnetic lead-based perovskites, spin-splitting reaches 400 meV and exhibits persistent spin-texture. In the case of Co-based magnetic formate, the spin-splitting originates from AFM ordering in both centrosymmetric and polar phases. Our investigation unravels the origin and manipulation of spin-splitting in hybrid perovskites, which find applications in spintronics.

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Crossing the limits by interface engineering in nano-scale multiferroics

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Keywords: Spintronics, Magnetism, Magnetoelectrics, Ferroelectricity

Interfaces of 3d transition-metal oxides are promising for atomic-scale interactions such as charge transfers, spin dynamics, structural deformations, orbital reconstructions and new ferroic properties. These atomic scale interactions in multiferroics could lead to novel physical phenomena such as magnetoelectric coupling, unconventional exchange bias coupling, or even ultrathin ferroelectricity. Such new phenomena hold significant importance for the development of advanced, ultra-fast, small and energy-efficient logic and memory devices. However, investigating atomic scale interactions is challenging due to factors including interface roughness, altered atomic interactions, and dead layers.

Here, we investigate how interface physics within the $La_{0.7}Sr_{0.3}MnO_3$ (LSMO)-$BaTiO_3$ (BTO) system can influence the properties of either LSMO or BTO or both, leading to novel functionalities. We discuss in detail the emergence of unconventional exchange bias in bilayer thin films without the presence of an antiferromagnetic material and the persistence of ferroelectricity down to a single-unit cell in superlattices of $La_{0.7}Sr_{0.3}MnO_3$-$BaTiO_3$. We observe an exchange bias (~42-50 Oe) arising from induced antiferromagnetism at the LSMO interface due to the ferroelectric properties of BTO. Thicknesses of BTO and LSMO are optimized to achieve the maximum exchange bias. We make use of piezoresponse force microscopy and second harmonic generation to study the ferroelectricity in different thicknesses of BTO. Further, we find using density functional theory calculations that the structural distortions and orbital reconstructions at the interface of epitaxially strained ferromagnet-ferroelectric thin films creates an exchange bias coupling in the LSMO-BTO system. Additionally, we engineer switchable polarization in BTO without any critical thickness in carefully designed coherently strained superlattice structures of LSMO-BTO. We confirm the presence of polarization in BTO down to a single unit cell by piezoresponse force microscopy and second harmonic generation techniques. By density functional theory calculations, we confirm that the polarization in any ferroelectric or paraelectric system can be sustained by sandwiching it between a material consisting of interface charges such as $La_{0.7}Sr_{0.3}MnO_3$. These innovative nanoscale material systems exhibit exotic functionalities with potential applications in low-energy, high-density electronic devices.

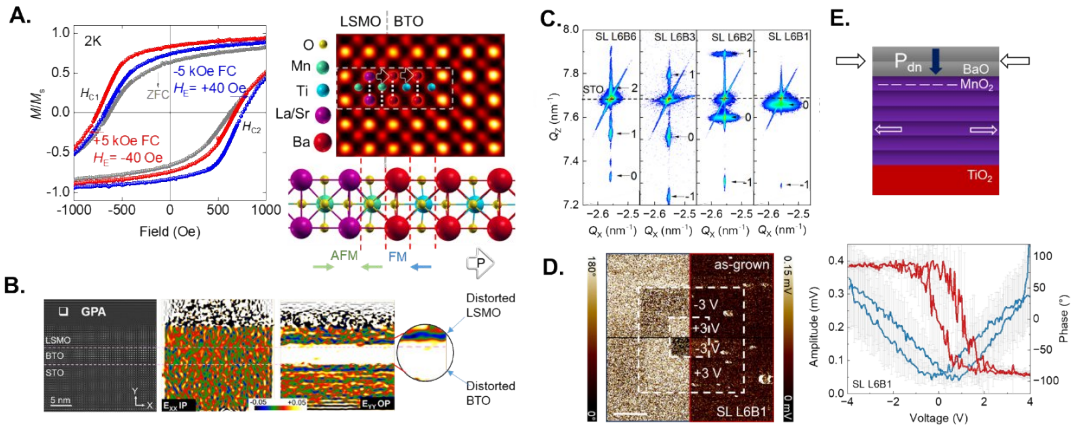

Fig.1: (A) (Left) Exchange bias (~42 Oe) for the LSMO-BTO bilayer. (Right) Crystal structure from STEM and DFT. (B) Geometric phase analysis of the LSMO-BTO bilayer. (C) Reciprocal space mapping of the series of superlattices. (D) Piezoresponse Force Microscopy of the superlattice with BTO 1 u.c. (E) Schematic showing the mechanism to achieve unit cell level ferroelectricity.

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Unlocking Single-Phase Magneto-Electric Materials Through Discrete Molecular Architectures

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Tuning electrical (or magnetic) properties using a magnetic (or electric) field is a highly active area of research, owing to its potential applications in energy-efficient storage devices, spintronics, sensors, actuators, and more.[1] Achieving a strong coupling between electric and magnetic orders, referred to as magnetoelectric (ME) coupling (α), in bulk oxide systems such as perovskites and ceramics remains a significant challenge. This difficulty stems from the inherent complexity of realizing simultaneous ferroelectric and ferromagnetic ordering within a single-phase material. Although alternative strategies have been explored for bulk oxides, the resulting ME coupling is typically very weak. Discrete molecular complexes have emerged as promising alternatives, where enhancing ME coupling is comparatively more feasible. In our work, we demonstrated that a heteronuclear [Co_3Dy] complex exhibits an ME coupling coefficient (α) of 250 mV/Oe/cm^{-1}, currently the highest reported value among known discrete molecular systems (Figure 1).[2] The device based on the [Co_3Dy] complex not only provides direct evidence of magnetoelectric (ME) coupling through its ability to convert stray magnetic fields into electrical signals, but also demonstrates potential for harvesting other forms of ambient waste energy.[2-8] Besides, a plausible mechanism underlying the ME coupling observed in these systems will be discussed.

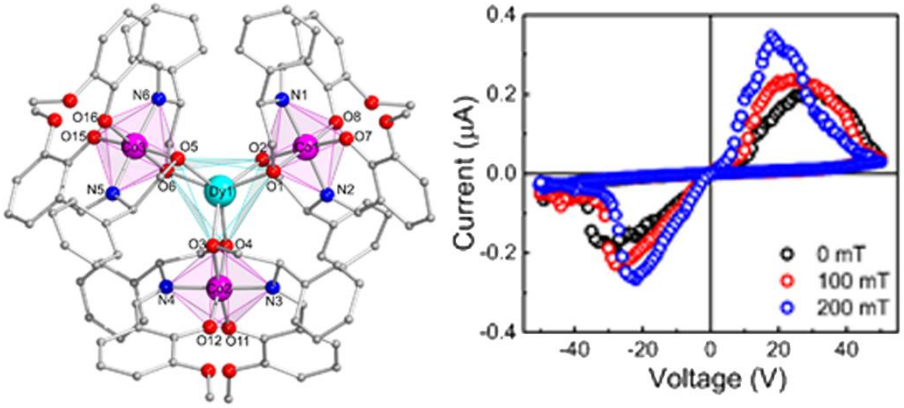

Figure 1. Crystal structure of heteronuclear Co_3Dy complex (left panel). The right panel shows the switchable electrical polarization can be modulated through the external magnetic field.

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From Constraints to Complexity: Thermodynamic Pathways to Domain Formation in Ferroelectrics

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The formation of domain structures in ferroelectric materials is governed by a balance between electrostatic interactions, elastic fields, and domain wall energy. These internal fields are strongly influenced by mechanical and electrical boundary conditions, which act as constraints that reshape the system's thermodynamic landscape. In this talk, I will present a series of phase-field simulations and thermodynamic analyses that examine how mechanical constraint—imposed through epitaxial strain, clamping, or internal lattice mismatch—affects domain evolution. In thin films, tensile strain promotes in-plane polarization, while compressive strain favors out-of-plane variants. Clamped conditions often lead to local phase coexistence and fine-scale domain patterns that minimize elastic energy despite increasing wall area. We also observe that such constraints can alter phase stability even in bulk-like systems, leading to different transformation pathways on heating and cooling. These results demonstrate that domain morphologies are not solely determined by material properties, but also by the imposed constraints that redirect thermodynamic driving forces. By examining these effects across multiple systems, we highlight how mechanical constraints can be systematically

Magnetoelectric Performance of Epoxy-Modulated Ni/PZT/FeGa Composites for Pressure and Displacement Sensing Applications

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Magnetoelectric (ME) composites have garnered considerable attention for advanced sensing applications due to their multifunctional response to magnetic, electric, and mechanical stimuli. Epoxy-modulated Ni/PZT/FeGa magnetoelectric (ME) composites were developed and systematically evaluated for high-performance pressure and displacement sensing applications. The composites were fabricated using a vacuum bagging technique and featured various structural configurations, including square and octagonal nickel geometries combined with ring-shaped PZT and disc-shaped FeGa layers. ME performance was first assessed under quasi-static and dynamic magnetic fields. Among the tested configurations, the octagonal four-ring design with 0° orientation demonstrated the highest quasi-static ME coefficient (~1945 mV/cm·Oe), marking a ~20% improvement over the single-ring and a ~95% increase compared to the dual-ring design. Although the single-ring structure exhibited the peak dynamic ME output (~2983 mV/cm·Oe), octagonal designs retained over 70% of that performance, offering improved design flexibility. All configurations exhibited a self-biased ME effect, with the octagonal 0° structure achieving a 26% higher coefficient than the dual-ring variant. Reliability testing under 10^5 DC magnetic field cycles at both room and elevated temperatures confirmed the long-term stability of these composites. For sensing applications, the single-ring composite showed the highest pressure sensitivity (11.58 $mV \cdot cm^{-1} \cdot Oe^{-1}/MPa$), outperforming the dual- and four-ring designs by 84% and 65%, respectively. Displacement sensing showed similar trends, with the octagonal 0° orientation offering over 40% higher sensitivity than the dual-ring counterpart. These results clearly demonstrate that structural design significantly influences ME behavior and sensing efficiency. The epoxy-modulated Ni/PZT/FeGa composites presented here offer promising potential for robust, next-generation pressure and displacement sensors in smart systems, industrial monitoring, and multifunctional device integration.

Phase Transitions and Elastic Anomalies in Ferroelectric Hafnia Under Pressure

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Materials Science Program, University of Rochester, Rochester, New York, USA

Ferroelectric hafnia (HfO_2) is a promising material for next-generation nanoelectronics and non-volatile memory devices, owing to its robust polarization, scalability, and CMOS compatibility. However, its complex phase behavior under external stimuli, such as pressure, remains an open question. In this talk, I will present our recent works on the structural phase transitions and elastic response of ferroelectric hafnia under hydrostatic pressure. We uncover a cascade of pressure-driven phase transitions involving polar and nonpolar monoclinic, orthorhombic, and tetragonal phases. Notably, we observe distinct elastic anomalies that emerge with increasing pressure, serving as precursors to structural transitions. These anomalies highlight strong coupling between mechanical strain and ferroelectric order. Overall, our findings provide a comprehensive understanding of pressure-tunable ferroic behavior in hafnia and establish a foundation for strain-engineered device applications leveraging its multifunctional properties.

*** Abstract for 2025 IEEE-South Asia Ferroelectric Symposium, IISc Bangaluru, India*
https://2025.ieee-safs.org/

Sputtered PZT as a platform for the development of Si-based photonic devices

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Indian institute of Science, Bangalore

We demonstrate, for the first time, sputtered PZT as a platform for the development of Si-based photonic devices such as rings, MZI, and electro-optic modulators. We report the optimization of PZT on MgO(002) substrate to obtain highly oriented PZT film oriented towards the (100) plane with a surface roughness of 2 nm. Si gratings were simulated for TE and TM mode with an efficiency of -2.2 dB/coupler -3 dB/coupler respectively with a polarization insensitive efficiency of 50% for both TE and TM mode. Si grating with an efficiency of around -10 dB/coupler and a 6 dB bandwidth of 30 nm was fabricated. DC Electro-optic characterization for MZI yielded a spectrum shift of 71 pm/V at the c-band.

State-of-the-Art Research on Hf-ZrO_2 Ferroelectric and Antiferroelectric Capacitors

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In 2011, NamLab reported ferroelectricity in Si-doped HfO_2 [1], sparking widespread interest due to its CMOS compatibility. Since then, HfO_2-based materials have been investigated for various applications, mainly in memory devices (FeRAM, FeFET, FTJ), but also in energy storage, IR detection, electrocaloric cooling devices, and pyroelectric/piezoelectric systems.

This presentation reviews the development of ferroelectric and antiferroelectric capacitors (FeCaps and AFeCaps) at Institut des Nanotechnologies de Lyon (INL). We describe the fabrication of $Hf_{1-x}Zr_xO_2$ (HZO)-based capacitors by reactive sputtering using metallic [2] and ceramic [3] targets, and more recently by ALD [4]. Structural characterization and electrical performance—endurance (via DHM, PUND, DLCC), retention, leakage, and imprint—will be discussed. For FeCaps, the orthorhombic phase associated with ferroelectricity is observed, with $2P_r$ exceeding 40 µC/cm² using both sputtering and ALD. Endurance strongly depends on the cycling protocol. In AFeCaps, a tetragonal phase is identified [5]. Recent advances in understanding antiferroelectricity in HZO will be discussed.

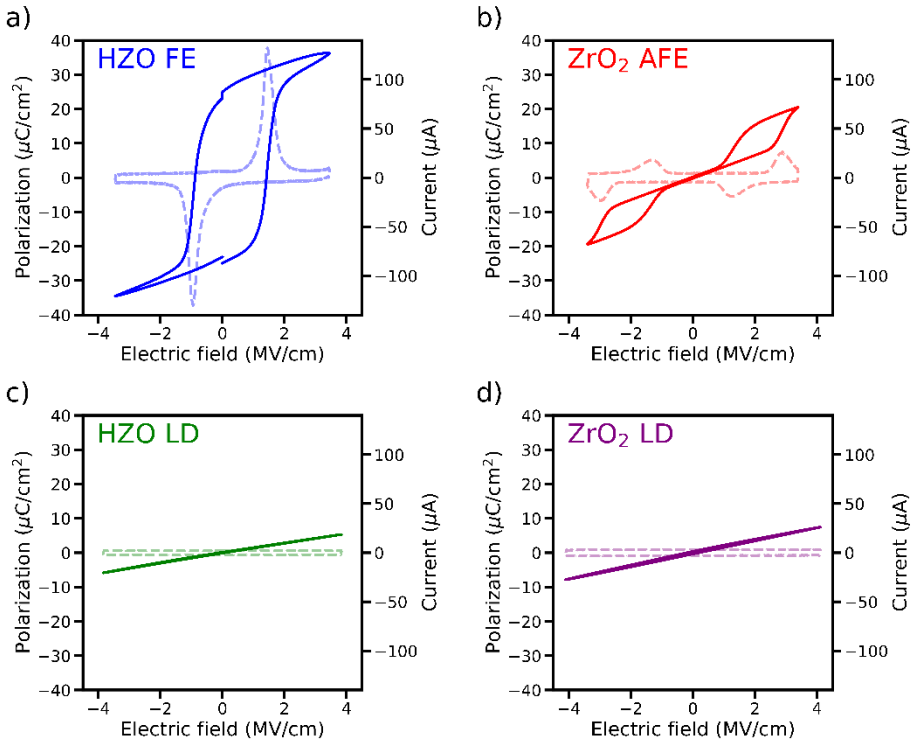

Figure 1. *Polarization vs electrical field (straight lines) and current vs voltage (dashed lines) after 10^3 cycles for (a) a ferroelectric HZO, (b) an antiferroelectric ZrO_2, (c) a linear dielectric HZO, and (d) a linear dielectric ZrO_2.*

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CMOS back-end-of-line compatible $Hf_{0.5}Zr_{0.5}O_2$ ferroelectric devices

The demand for power efficient computing technology to cater to mobile applications such as Internet-of-Things and autonomous vehicles has led to significant interest in the development of edge-computing hardware. It will be necessary to implement non-Von Neumann architecture such as 'neuromorphic computing' to achieve ultra-low power consumption at the edge. Emerging non-volatile memory (NVM) devices are well suited to implement synaptic and neuron functionalities in such systems. Among the emerging NVM, ferroelectric memory devices show promise for ultra-low power consumption owing low switching energy. In this context, development of $Hf_{0.5}Zr_{0.5}O_2$ (HZO) based ferroelectric devices: a) Ferroelectric capacitor for FeRAM; b) Ferroelectric tunnel junction (FTJ) memristors and Ferroelectric FET for CMOS back-end-of-line (BEOL) will be presented. The optimization of device design, role of interfaces and process sequence on the operation of the various devices will be discussed. As HZO exhibits 'wake-up' effect, its impact on devices applications and it's optimization for circuit design parameters will be explored. Finally, integration of ferroelectric devices on the BEOL of CMOS chips will be presented.

Reliability of doped Hafnium Oxide FeFETs: challenges and mitigation strategies

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Indian Institute of Technology Madras

Abstract: The discovery of ferroelectricity in doped Hafnium Oxide (HfO_2) films is considered by many to be a turning point for ferroelectric technologies. The HfO_2-based Ferroelectric Field-Effect Transistor (FeFET) has gained popularity as an emerging non-volatile memory due to its compatibility with advanced technology nodes, multi-bit storage and low write-energy. Despite these attributes, the technology is far from commercialization, mainly due to reliability issues. This talk will focus on some of these challenges, such as variability, long-term endurance and retention degradation. We will discuss the reliability trends and the potential impacts in different application space. We will then discuss some of the possible origins of reliability degradation, and focus on the impact of interfacial (N_{it}) and near-interfacial oxide (N_{ox}) traps. Extraction of these parameters in Si-doped HfO_2 (HSO) FeFETs using the charge-pumping technique will follow. We will show that an endurance-aware pulse programming scheme can partially recover the memory window, but material stack optimizations will be necessary for further enhancement of performance.

Harnessing the Double-Well potential of Ferroelectrics for Enhanced Sensing and Electromechanical Actuation

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We present two possible applications resulting from harnessing the inherent double-well potential of a ferroelectric capacitor.

The first application deals with a ferroelectric-electrostatic MEMS hybrid actuator. This envisages a ferroelectric capacitor exhibiting negative capacitance, connected in series with the MEMS actuator. We show via simulations that the static and dynamic (step input) pull-in voltages of the hybrid actuator can be reduced as compared to the standalone electrostatic MEMS actuator. We predict a reduction in the energy consumption during dynamic pull-in in the hybrid actuator as compared to the standalone actuator, even in the presence of damping.

The pull-in instability restricts the maximum distance traveled by the movable electrode before it is pulled-in, to a fraction of the air-gap. We propose the elimination of pull-in instability accompanied by low-voltage operation, in the hybrid actuator by adding a nonlinear spring (with cubic nonlinearity) to it. Based on the value of the cubic spring constant, we show that the hybrid actuator can work in three distinct modes: (i) monostable (ii) bistable and (iii) always-stable. We also estimate the threshold values of the cubic spring constant that demarcate the aforementioned modes. We show that the pull-in free and low-voltage operation can be achieved when the hybrid actuator operates in the always-stable mode.

The second application describes the possibility of Stochastic Resonance (SR) in a ferroelectric system. A system is said to demonstrate SR when the addition of an appropriate amount of noise leads to the improvement of some figure-of-merit. SR was first proposed in the early 1980's to describe the periodicity of ice ages. In systems whose dynamics can be described by a double-well potential, noise can help the system overcome energy barriers, leading to a more pronounced response to a weak signal. We describe a simulation and modeling framework to understand the phenomenon of SR in thin-film ferroelectrics. We show how the first-passage time (referred to as Kramers time) can provide an intuitive description of SR. Finally, we suggest that linear-response theory to be a useful way of quantitatively capturing SR in ferroelectrics, even though the ferroelectric capacitor is inherently non-linear.

ABSTRACTS

For

ORALS

Unconventional amorphization in ferroelectric *β''*-In_2Se_3 nanowire

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ABSTRACT

Electrically induced amorphization is uncommon and has so far been realized by pulsed electrical current in only a few material systems, which are mostly based on the melt–quench process [1]. However, if the melting step can be avoided and solid-state amorphization can be realized electrically, it opens up the possibility for low-power device applications [2–5]. Here we report an energy-efficient, unconventional long-range solid-state amorphization in a new ferroic β″-phase of indium selenide nanowires through the application of a direct-current bias rather than a pulsed electrical stimulus. The complex interplay of the applied electric field perpendicular to the polarization, current flow parallel to the van der Waals layer and piezoelectric stress results in the formation of interlayer sliding defects and coupled disorder induced by in-plane polarization rotation in this layered material. On reaching a critical limit of the electrically induced disorder, the structure becomes frustrated and locally collapses into an amorphous phase [6], and this phenomenon is replicated over a much larger microscopic-length scale through acoustic jerks [7,8]. Our work uncovers previously unknown multimodal coupling mechanisms of the ferroic order in materials to the externally applied electric field, current and internally generated stress, and can be useful to design new materials and devices for low-power electronic and photonic applications.

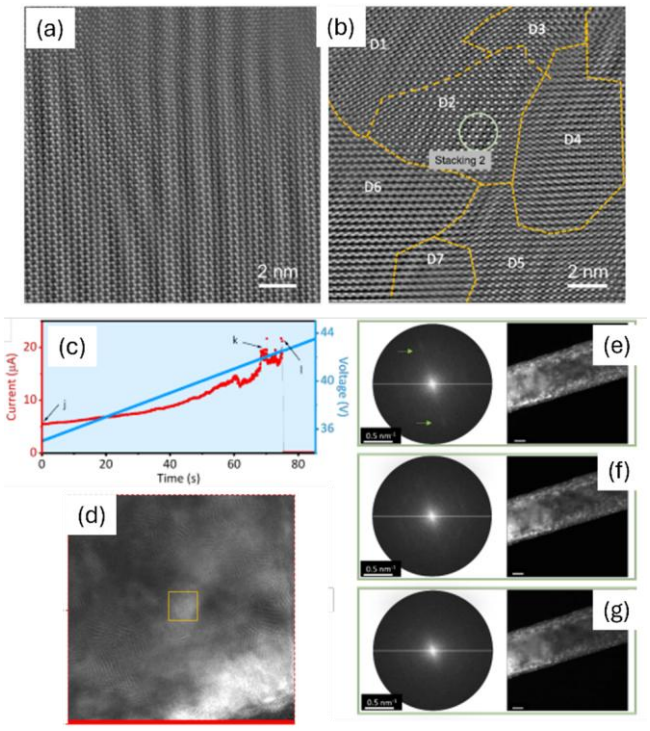

Fig: (a) Bands intersecting to form superlattice dislocation corresponding to the noisy spiking current that we see in IV plot. (b) several microscopic domains form as a resulting of 2D layer intersecting by sliding, rotation and fractional translation (c) shows IV characteristics (d) shows intersecting defects forming amorphous disorder region (e-g) shows the FFT and their DFTEM image corresponding to points (j-l) in (c, IV plot)

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Micromechanical Insights into Texture and Stress-Driven Electromechanical Behavior in Ferroelectric PZT

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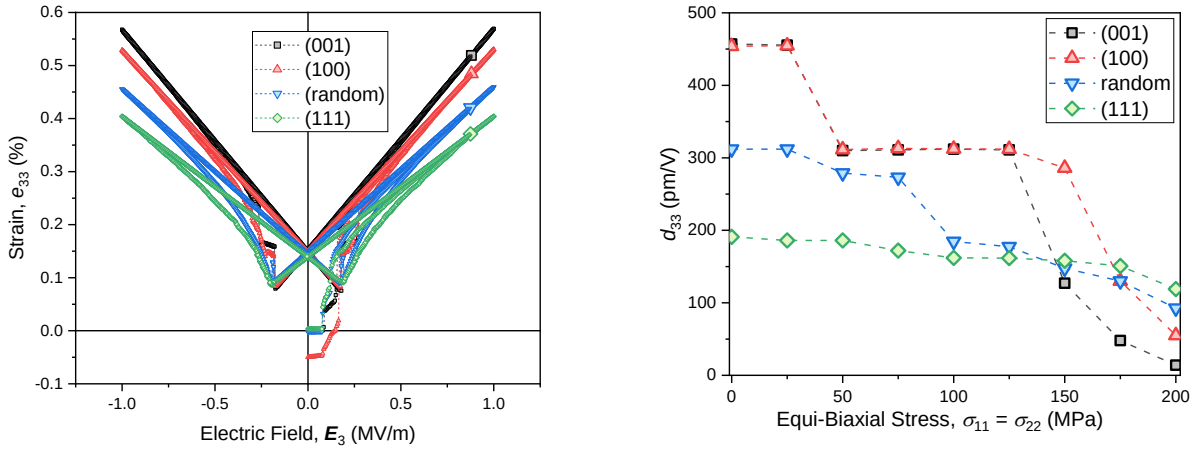
Abstract

Ferroelectric ceramics such as lead zirconate titanate ($PbZr_{0.52}Ti_{0.48}O_3$) are widely used in sensors, actuators, energy harvesters, RF switches, inkjet printer heads, and Micro-Electromechanical Systems (MEMS). The electromechanical behavior of PZT near the morphotropic phase boundary (MPB) is governed by crystallographic texture and residual stress, both of which modulate domain switching. Yet, their combined influence remains poorly understood. In this study [1], we introduce a micromechanical model that captures the coupled effects of residual stress and electric field on polarization switching in textured PZT near the MPB. Built on the framework of Hwang *et al*. [2], the model accounts for tetragonal and rhombohedral switching as well as interphase transformations, enabling simulation of nonlinear electromechanical behavior. It reproduces key experimental observations, including enhanced response in (001)-textured ceramics and degradation under in-plane tension. Notably, the model predicts a linear increase in the ratio $d_{31(001)}/d_{31(111)}$ with (001) texture fraction, in close agreement with experimental data [3]. By linking microstructural alignment and stress state to macroscopic electromechanical response—and offering open-source MATLAB code—this work provides a practical tool for designing next-generation piezoelectric materials.



(a) **(b)**

Figure 1. (a) Strain (e_{33}) vs. electric field (E_3) butterfly loops for various textures illustrating that (001)-textured crystallites exhibit the highest strain response and slope (d_{33}), followed by (100), random, and (111) orientations. **(b)** Decrease in piezoelectric coefficient d_{33} with increasing equi-biaxial tension for various textures.

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Freestanding Ferroelectric Oxide Membranes Designed by Epitaxy for Device Applications

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Abstract

Epitaxial oxide thin films have gained significant attention due to their emergent phenomenon and tunable properties. The epitaxial growth of oxide thin films with a perovskite structure on a flexible substrate provides a promising path to incorporate various electronic and optoelectronic functionalities into cost-efficient flexible electronic devices. However, fabricating flexible epitaxial oxide films remains challenging, primarily due to the substrate clamping effect. The exceptional flexibility and elasticity of freestanding single-crystalline ferroelectric oxide membranes have recently drawn significant attention, as they overcome substrate constraints, enabling advanced strain engineering in ferroelectric thin films and seamless integration into next-generation flexible devices. In this work, we explore the fabrication of Sn-modified $BaTiO_3$ (BSTO) thin films using the pulsed laser deposition (PLD) technique with a KrF (248 nm) excimer laser. The films were epitaxially grown on $SrTiO_3$ (001) (STO) substrates with $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) sacrificial buffer layers to facilitate strain engineering and subsequent detachment to get a freestanding BSTO membrane. Structural characterization was performed via X-ray diffraction (XRD), while ferroelectric properties were studied through P-E hysteresis loop measurements. A wet-chemical etching-based epitaxial lift-off process was employed to dissolve the sacrificial layers, facilitating the fabrication of freestanding membranes. These membranes were subsequently transferred onto alternative substrates, offering a way for flexible device integration. Detailed findings on the structural and ferroelectric properties, along with the fabrication methodology, are presented.

Keywords: Ferroelectrics, Oxide thin film, Freestanding membrane, Pulsed laser deposition

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Simultaneous increase of d33 and Cuire point of PZT: the phenomenon and mechanism

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Abstract

Ever since the discovery of large electromechanical response at the morphotropic phase boundary of the classical piezoceramics system $PbZr_yTi_{1-y}O_3$ (PZT) more than six decades ago, different variants of PZT are in use in wide-ranging applications. Stability of electromechanical performance of piezoelectric devices against inadvertent temperature increase requires use of piezoceramics with high Curie point. In general, chemical modifications which significantly improve the piezoelectric response lowers the Cuire point. In contrast to this general trend, here we report a phenomenon wherein slight Eu modification of PZT, not only increase its piezoelectric charge coefficient (d_{33}) remarkably from 204 pC/N to 415 pC/N, but also increased the Cuire point notably from 373 ℃ to 389 ℃. We report here this phenomenon and the underlying mechanism by investigating the structures at the local and global length scales using a combination of tools like Eu^{3+} photoluminescence, Raman spectroscopy and X-ray powder diffraction. We found that while the increase in Cuire points is caused by Eu-doping pushing the system from a two-phase (rhombohedral + tetragonal) state to a single-phase tetragonal state with increased tetragonality, the remarkable increase in the d_{33} is associated with Eu increasing the structural heterogeneity of the system by limiting the field driven tetragonal → rhombohedral transformation on the local scale. We reproduce the same phenomenon by doping PZT with dilute concentration of Sm and La, thereby demonstrating the generality associated with the remarkable effect of dilute doping notably increasing the electromechanical properties while also improving the Curie point in piezoelectric system.

Keywords: PZT, electromechanical behaviour, Cuire point, Crystal structure.

Origin of strain tunability in flat valence band and ultrahigh shear piezoelectricity in superflexible non–van der Waals graphitic ScX monolayers (X = P, As, Sb)

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Keywords: non-vdW, flat band, strain, shear piezoelectricity

ABSTARCT:

Research on non-van der Waals (n-vdW) 2D materials has garnered significant growth in recent years, owing to their potential for diverse applications and the development of new synthesis techniques. This study stabilizes one-atom-thick ScX (X=P, As, Sb) monolayers drawn from their non-vdW bulk counterpart in the wurtzite phase by applying a minimal tensile strain of 1-2%. The resulting high flexibility, owing to the extremely small in-plane elastic constants (6-43 N/m) and *Y*oung's modulus (6-20 N/m), suits them ideally for extensive strain engineering on a large scale. Complex mixing of acoustic and optic phonon modes for higher strains ensures a large shear-piezoelectric coefficient of up to d_{16} = -228.08 pm/V, -469.87 pm/V, and -397.52 pm/V for ScP, ScAs and ScSb respectively. This coefficient notably surpasses that in amino acids, making it the highest reported to date, and is accompanied by high in-plane piezoelectric coefficients, $|d_{21}|$ & $|d_{22}| > 100$ pm/V and highly strain-tunable shear piezoelectric coefficient d_{15} ranging from -90 pm/V to 210 pm/V. The monolayers exhibit rich band structures, including flat bands at the top-most valence band and a large spin splitting of ~100 meV, making them ideal for applications in LED and laser devices and opens up new exciting avenues for exploration in spintronics. The study presents an in-depth analysis of band flattening caused by tensile strain and demonstrates the strong integrability of ScP monolayer with Si substrate, which promises significant advancements in various practical applications.

Reference:

H. Seksaria, A. Kaur, and A. De Sarkar, *Origin of Strain Tunability in Flat Valence Band and Ultrahigh Shear Piezoelectricity in Superflexible Non-van Der Waals Graphitic ScX Monolayers (X= P, As, Sb)*, Phys. Rev. B **108**, 075426 (2023).

Short range structural correlations and property anomalies in non-MPB compositions of the Pb-free piezoelectric $Na_{0.5}Bi_{0.5}TiO_3$- $K_{0.5}Bi_{0.5}TiO_3$

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Abstract

Among Pb-free piezoelectrics, $(1-x)Na_{0.5}Bi_{0.5}TiO_3$ (NBT)-based systems uniquely exhibit a complex interplay between ferroelectric and non-ferroelectric (in-phase octahedral tilt) instabilities, impacting their dielectric and electromechanical properties. This complexity is pronounced in morphotropic phase boundary (MPB) systems like $(1-x)Na_{0.5}Bi_{0.5}TiO_3$-$xK_{0.5}Bi_{0.5}TiO_3$ (NBT-KBT), wherein composition driven rhombohedral-tetragonal ferroelectric-ferroelectric instability occurs around $x \sim 0.20$. Interestingly, beyond the MPB composition at $x \sim 0.40$, within the tetragonal regime, the system shows notable structural disorder and property anomalies. Using a combination of x-ray, neutron, and electron diffraction, along with microscopy techniques, we reveal that these anomalies stem from the emergence of short-range rhombohedral ferroelectric correlations. HAADF imaging further highlights local polar displacement fluctuations that explain the unusual behaviour. Based on these findings, we also propose a revised phase diagram for the NBT–KBT system.

Keywords: lead-free piezoceramics, structure-property correlation, Crystal structure, Transmission electron microscopy, Neutron diffraction, HAADF imaging, Phase diagram

Abstract-

Investigation of Electrical and Electromechanical Properties in High-Entropy BFO–BTO–STO Perovskites

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Abstract- High-entropy oxides (HEOs) have recently emerged as promising materials for multifunctional applications due to their unique configurational entropy-driven phase stability and tunable physical properties. In this work, we report the synthesis and characterization of a novel high-entropy perovskite oxide solid solution system based on $BaTiO_3$ (BTO), $BiFeO_3$ (BFO), and $SrTiO_3$ (STO) viz., 0.25BFO-0.30BTO-0.45STO. The multicomponent A-site cation distribution (Ba^{2+}, Bi^{3+}, Sr^{2+}) and B-site Ti^{4+} and Fe^{3+} occupancy result in significant lattice distortion, enabling the stabilization of a single-phase perovskite structure across a wide compositional range. Notably, in the bulk form, this system exhibits a stable single-phase cubic perovskite structure over a wide composition window.

Electrical and electromechanical measurements reveal that the system exhibits a high recoverable energy density of 56.41 J/cm³ and a large electromechanical strain of 0.75% at 3.02MV/cm, demonstrating its strong potential for advanced capacitor and actuator applications. These enhanced functional properties are attributed to the synergistic effects of entropy-driven lattice distortion, polarization dynamics, and local field fluctuations.

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Analysis of the comparative scaling behaviour between slanted and square-type polarisation loops in Nb^{5+}/Ho^{3+} co-substituted NBT systems for enhanced energy storage performance

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Generally, a slanted type of P-E loop is desired to achieve enhanced energy storage properties. Researchers are giving special focus on altering the square loop of various ferroelectrics to a slanted loop through chemical modification, which transforms macro-domains to polar nano-regions [1]. This distinct domain configuration of the slanted P-E loop led to a polarisation reversal mechanism different from that of the square P-E loop. To highlight the clear difference in polarization reversal mechanics of a slanted P-E loop from the square loop, the scaling behaviour of the polarization loop is studied by plotting the area of loop <A> with E_0. Given this, for comparative work, in this work, square loop and slanted loops have been taken from the same type system $N_{0.5}Bi_{0.495}Ho_{0.005}Ti_{(1-x)}$ Nb_xO_3 with a slight variation of Nb^{+5} at Ti^{+4} site (x=00 (NBHT, Nb00), 0.03 (Nb0.03) and 0.06 (Nb06) [2]. The Nb00 has been selected for a square type of P-E loop of the ferroelectric owing to the macro-domain. Nb^{+5} substituted $N_{0.5}Bi_{0.495}Ho_{0.005}TiO_3$ compositions (Nb03 and Nb06) possess the slanted type of loop due to the creation of polar nanodomain regions (PNRs) in their domain configuration.

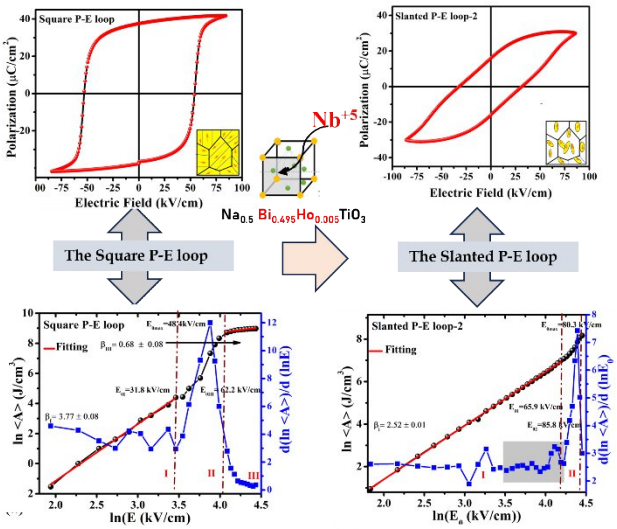

Fig Schematic illustration of the scaling behavior of square and slanted polarization loops, corresponding to the evolution of ferroelectric domains under varying electric fields

In the first and third stages, the scaling exponents (β), which represent the domain response, are calculated by linear fitting in these stages according to the power-law relationship $\langle A \rangle \propto E_0^{\beta}$. In the first stage, β (3.14 ± 0.01 and 2.52 ± 0.01) decreases for Slanted P-E loop-1 and 2, respectively, compared to the Square P-E loop (3.77 ± 0.08). In the third stage, a relatively high β (1.86±0.3) is obtained for Slanted P-E loop-1 compared to the Square P-E loop (β=0.68±0.08). Additionally, the critical electric fields E_{01} (59.6 kV/cm and 65.9 kV/cm) and E_{02} (80.7 kV/cm and 85.8 kV/cm) for Slanted P-E loop-1 and 2, respectively, increased compared to those of the Square P-E loop (31.8 kV/cm and 62.2 kV/cm). Thus, the distinct features of scaling behaviour of the slanted hysteresis P-E loop from the square loop, characterised by different domain response (β) and critical electric fields E_{01} and E_{02}, are explained by their distinct domain configurations (polar nanodomains and macroscopic domains). Similarly, the scaling behaviour of recoverable energy storage density (W_{rec}) is studied

for both square and slanted hysteresis P-E loops by plotting $\ln W_{rec}$ versus $\ln E_0$. Thus, understanding the polarization reversal of polar nano-domains of slanted P-E loops and macro-domains of square P-E loop, along with a qualitative analysis through scaling, can provide valuable insights into how doping and material modifications can be utilized to optimize energy storage properties.

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Epitaxial In-Plane Ferroelectric $BaTiO_3$ integration on Silicon through a single MgO buffer layer for On-Chip Electro-Optic Applications

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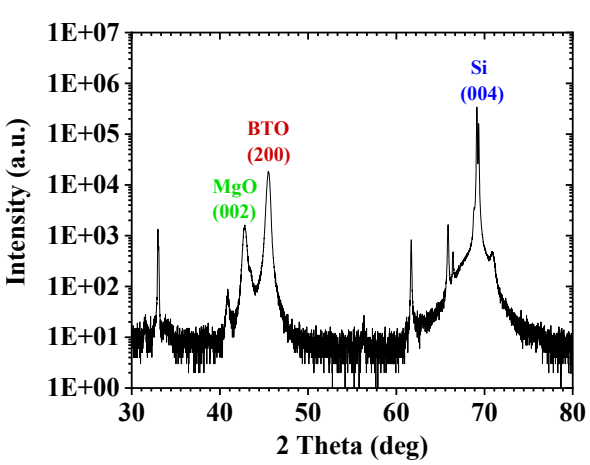
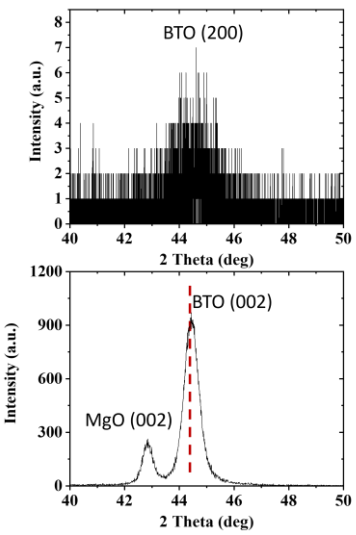
Barium titanate ($BaTiO_3$), a lead-free, CMOS compatible ferroelectric material with a large Pockels coefficient (r_{42} ~ 1300 pm/V), is highly desirable for on-chip electro-optic (EO) modulators. The device architecture necessitates $BaTiO_3$ polarization to be oriented in-plane with the substrate. Traditional integration on Silicon (Si) using a $SrTiO_3$ (STO) buffer via Molecular Beam Epitaxy (MBE) often leads to mixed c+a-axis orientations due to compressive epitaxial stress, thereby reducing the electro-optic response.

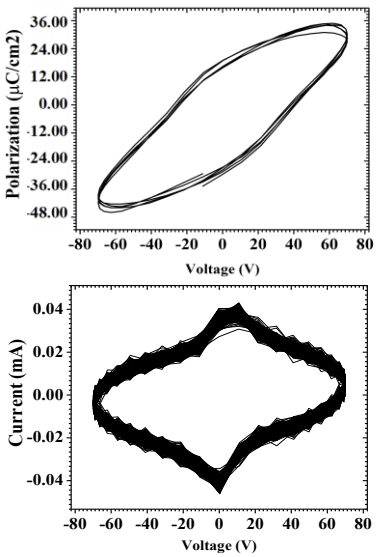
This work presents an alternative approach for integrating pure c-axis in-plane (c-IP) $BaTiO_3$ on (100) Si using a single magnesium oxide (MgO) buffer layer. The choice of MgO is due to its larger lattice parameter (4.214 Å) relative to $BaTiO_3$'s 'a' and 'c' parameters, combined with the tensile coefficient of thermal expansion (CTE) mismatch between $BaTiO_3$ (11.6×10^{-6}/K) and Si (2.6×10^{-6}/K), promotes the desired in-plane tensile strain, resulting in enhanced tetragonality and pure c-IP orientation. Furthermore, MgO's insulating properties enable in-plane electric field application for polarization control, and its refractive index (1.7) is ideal for optical waveguiding between $BaTiO_3$ (2.2-2.4) and Si (3.9).

The $BaTiO_3$/MgO stack was grown on (100) Si using Pulsed Laser Deposition (PLD). A 50nm MgO buffer layer was epitaxially deposited at 400°C under 1×10^{-5} mbar P_{O2}, confirmed by in-situ Reflection High Energy Electron Diffraction (RHEED). Subsequently, a 250nm $BaTiO_3$ film was grown at 800°C and 1×10^{-1} mbar P_{O2}. The resulting $BaTiO_3$ exhibited an in-plane lattice parameter of 4.0402 Å and an out-of-plane lattice parameter of 3.992 Å, indicating a strong c-IP orientation with 1.2% tetragonality. X-ray rocking curve (XRRC) FWHM values were remarkably low at 1.5° (200 plane, on-axis) and 1.9° (111 plane, off-axis), representing the best reported for PLD-integrated BTO on Si via MgO. The epitaxial relationship was determined as (200) BTO || (002) MgO || (001) Si and <001> BTO || <100> MgO || <110> Si.

In-plane ferroelectric response was validated with 500nm separated electrodes, yielding coercive fields of ~ 80 KV/cm and a remanent polarization of ~10 µC/cm². The film demonstrated good endurance, remaining stable for up to $\sim3\times10^6$ cycles. Finally, a Mach-Zehnder interferometer structure incorporating a pre-patterned Si waveguide below the $BaTiO_3$ was fabricated to extract the electro-optic response, losses, and effective Pockels coefficient, along with studying the direction dependency of the EO response, along the substrate plane. The inferences and insights from these findings shall be discussed.







Structural, relaxor behaviour, dielectric and energy storage properties of lead-free $(1-x)Ba_{0.95}La_{0.05}TiO_3–xBi(Zn_{2/3}Ta_{1/3})O_3$ ferroelectrics

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Abstract

The dielectric capacitors possess high power density, fast charge/discharge rate, high breakdown strength, efficient storage, compactness in size, fatigue resistance and excellent stabilities against temperature and frequency. Lead-free $(1-x)Ba_{0.95}La_{0.05}TiO_3–xBi(Zn_{2/3}Ta_{1/3})O_3$ (BLT–*x*BZT) ceramics have been designed based on a combined approach of partial La substitution for Ba of BT and the introduction of BZT into the BLT matrix. The design ideas of the present work are summarized in Fig. Le Bail refinement for X-ray diffraction patterns confirmed that the BLT–*x*BZT samples have the cubic ($Pm\bar{3}m$) structure at room temperature as a result of the relaxation of the tetragonal distortion of BT. Slim polarization-electric field loops characteristic of relaxor ferroelectrics with a suppressed remnant polarization were obtained. Burns temperature determined by the temperature dependence of dielectric constant increased with increasing BZT content, which suggests that BZT doping in BLT matrix promotes the formation of polar nanoregions. A recoverable energy density (U_{rec}) of 1.60 J/cm³ at 190 kV/cm was achieved in BLT–0.04BZT ceramics, along with an ultrahigh energy storage efficiency of 94 % due to low hysteresis loss. The BLT–0.02BZT ceramics also exhibited excellent frequency stability in energy storage properties across 1–100 Hz, demonstrating their potential for use in pulsed power systems.

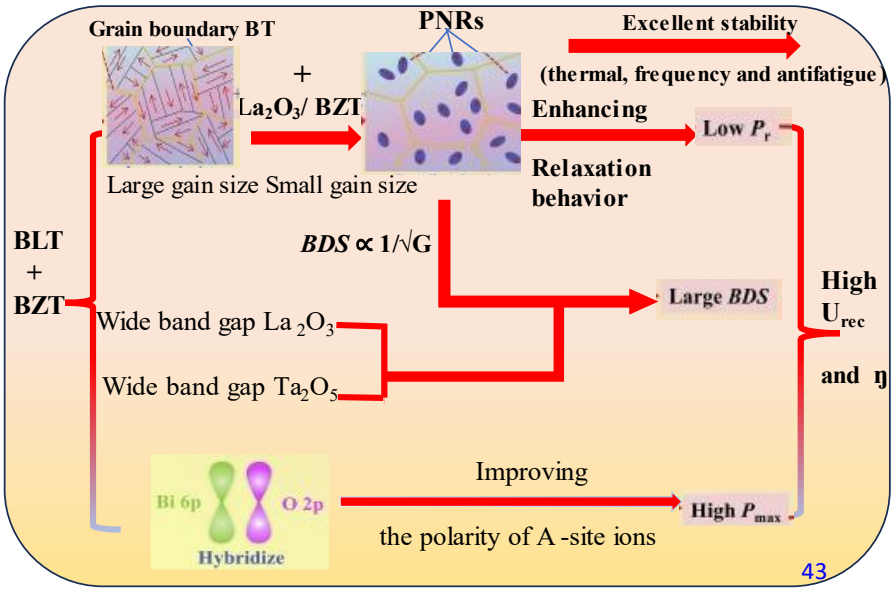

Fig. Schematic diagram of BLT-BZT ceramics showing parameters that improve energy storage properties.

Antiferroelectric to Ferroelectric Phase Transition and Electrocaloric Effect in Epitaxial $PbZrO_3$ Thin Films

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ABSTRACT

In this work, we investigate the antiferroelectric (AFE) to ferroelectric (FE) phase transition and associated electrocaloric effect (ECE) in epitaxial $PbZrO_3$ (PZO) thin films deposited on $SrRuO_3$-buffered layer on $SrTiO_3$ (100) substrates using pulsed laser deposition. Structural and phase transition behaviour were analysed through temperature-dependent X-ray diffraction, reciprocal space mapping, and polarization-electric field (P–E) measurements. The films exhibit a reversible AFE to FE transition under applied electric field, accompanied by a significant entropy change. A strong electrocaloric response was observed near the phase transition temperature, with a notable adiabatic temperature change (ΔT), demonstrating the potential of epitaxially strained AFE thin films for solid-state cooling applications. The influence of lattice strain and domain dynamics on the phase transition and ECE performance is discussed in detail. These findings suggest that engineered AFE materials such as PZO are promising candidates for integration into on-chip electrocaloric cooling technologies.

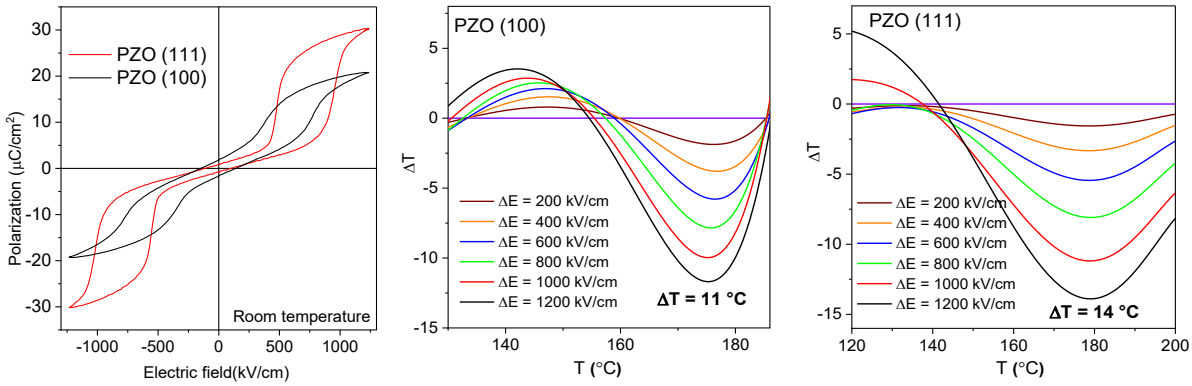

Figure 1. (P-E) hysteresis curves for PZO thin films grown along (001) and (111) orientations, respectively, measured at driving voltage of 10V. We are also measuring temperature dependent (P-E) and calculate Electrocaloric. A large EC response is recorded with the maximum ΔT = 11 K for PZO (100) and ΔT = 14 K for PZO (111) for ΔE = 1200 kV cm−1 for the PZO/SRO heterostructures.

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Re-entrant-like behavior in modified $BaTiO_3$ with pinched hysteresis loop

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In the present work, we have studied the re-entrant dielectric behavior in Fe-doped $BaTiO_3$. X-ray diffraction data show the formation of a single phase of the studied compound, which was further fitted with the Rietveld refinement by considering a tetragonal structure (space group *P4mm*). Temperature-dependent dielectric measurements have been carried out from 450-100 K and presented in Figure 1a. The cubic to tetragonal transition temperature comes out to be 370 K, whereas the tetragonal to orthorhombic transition is at 272 K. All these transitions are frequency independent and show a hysteresis loop when measured in heating and cooling cycles, thus reflecting its first-order phase transition [1]. However, when we further cool down the sample, *frequency dispersion* has been observed, with a peak at 218 K, which is unlike its pure phase ($BaTiO_3$). We have further analyzed this dispersion with the Vogel-Fulcher law, and the freezing temperature comes out to be 120 K. The transition from disordered to order and then disorder as we cool down the sample is essentially an anomalous behavior in such a class of ferroelectric materials and is called reentrant-like behavior [2]. Detailed analysis and some other measurements are underway for the studied compound. Additionally, ferroelectric analysis has also been carried out for the studied sample from room temperature to high temperature (450 K). The room temperature PE data shows the pinched type of hysteresis curves as shown in Figure 1 b. Such behavior of the curve can be understood in terms of the generation of the defect dipole as a consequence of the charge compensation of Fe^{3+} at the Ti^{4+} site [3].

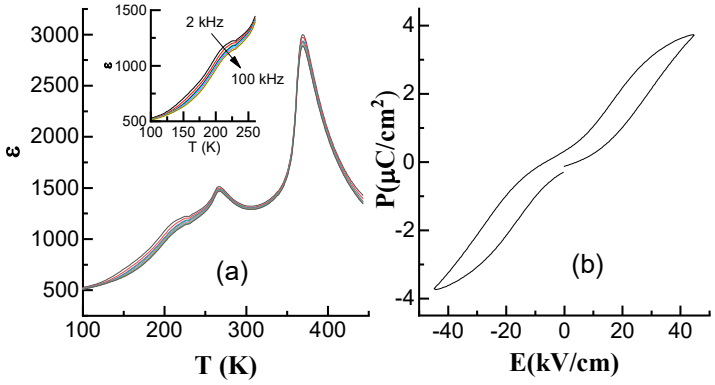

Figure 1: (a) Temperature-dependent dielectric data as a function of frequency and **(b)** ferroelectric hysteresis loop (*P-E*) at room temperature of $BaTi_{0.98}Fe_{0.02}O_3$. Inset of fig(a) shows the zoomed part across the temperature regime of dispersion.

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Enhancing Polarization and Reliability in HZO-Based FTJs Using WOx Electrodes and Interfacial Layers

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Abstract

HfO_2-based ferroelectric devices have gained significant attention due to their excellent scalability and compatibility with CMOS processes, making them promising for future memory and logic technologies. While Atomic Layer Deposition is currently the most widely used method for fabricating these devices, this study explores Radio-Frequency sputtering as an alternative, owing to its low carbon contamination, industrial relevance, and the advantage of room-temperature deposition [1].

TiN is commonly used as an electrode in HfO_2-based devices because it facilitates the stabilization of the orthorhombic phase, which is essential for ferroelectricity [2]. However, part of this stabilization arises from oxygen vacancies induced by TiN's oxygen scavenging behaviour [3]. While beneficial to some extent, excessive oxygen deficiency can introduce point defects and negatively impact device reliability—especially in ferroelectric tunnel junctions (FTJs), where direct tunnelling is the desired conduction mechanism.

To mitigate this issue, we investigate the use of a WO_x-based electrode or interfacial layer that acts as an oxygen reservoir [4], compensating for the oxygen vacancies caused by TiN. Various device structures were fabricated using a ferroelectric $Hf_{0.5}Zr_{0.5}O_2$(HZO) layer, incorporating different sequences of rapid thermal annealing, to study its impact on ferroelectric properties, structure, chemistry, and interfacial states of HZO devices. Initial electrical measurements showed promising ferroelectric characteristics, with a 2Pr value of 40 µC/cm² in films thinner than 6 nm, indicating suitability for tunnelling studies. Structural characterization using X-ray diffraction was performed to identify phase composition, while X-ray photoelectron spectroscopy was used to analyse chemical states and interfacial behaviour. Electrical characterizations were carried out to further evaluate polarization performance and overall device behaviour.

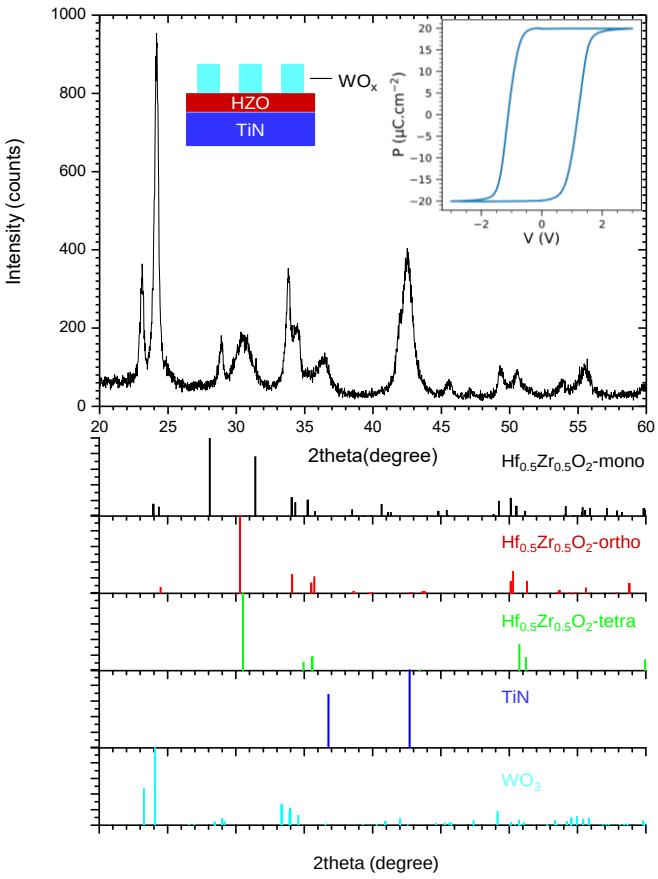

***Figure** 1: Schematic of the Ferroelectric Capacitor (FeCAP) structure: WO_X/HZO/TiN. Glancing Incidence X-Ray Diffraction scan of the FeCAP after annealing and associated reference patterns for the different phases of materials. Inset: Polarisation-Voltage loop from Positive-Up-Negative-Down measurements after annealing at 450°C*

These findings offer valuable insights into optimizing sputtered HZO devices for reliable FTJ applications and present a foundation for developing artificial synapses in neuromorphic computing systems.

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Tailoring Ferroelectric HfO_2 Thin Films: A Comprehensive Study of Deposition Parameters, Thermal Treatment, and Electrode Effects

Soumyajyoti Mondal, Asraful Haque, Shubham Kumar Parate, Pramod Yadav, Kaushal Tiwari, Pavan Nukala

Ferroelectric hafnia (HfO_2) is a highly promising material for next-generation FeRAM and FeFET devices due to its scalability and CMOS compatibility. Its non-centrosymmetric orthorhombic ($Pca2_1$) phase is essential for ferroelectric functionality. This work focuses on the controlled stabilization of this critical phase in HfO_2 thin films grown via pulsed laser deposition (PLD). We demonstrate that lower laser fluence directly promotes the formation of the ferroelectric orthorhombic phase during deposition. For films initially dominated by the non-ferroelectric monoclinic phase (grown at higher fluences), rapid thermal annealing (RTA) is effectively employed to induce a phase transformation to the desired ferroelectric orthorhombic phase. Furthermore, an investigation into electrode materials reveals that TiN electrodes significantly enhance device performance over W electrodes, exhibiting superior fatigue endurance and lower coercive fields. This study comprehensively elucidates the pivotal roles of PLD parameters, post-deposition thermal processing, and electrode selection in optimizing the ferroelectric properties of HfO_2 thin films for advanced memory and logic applications.

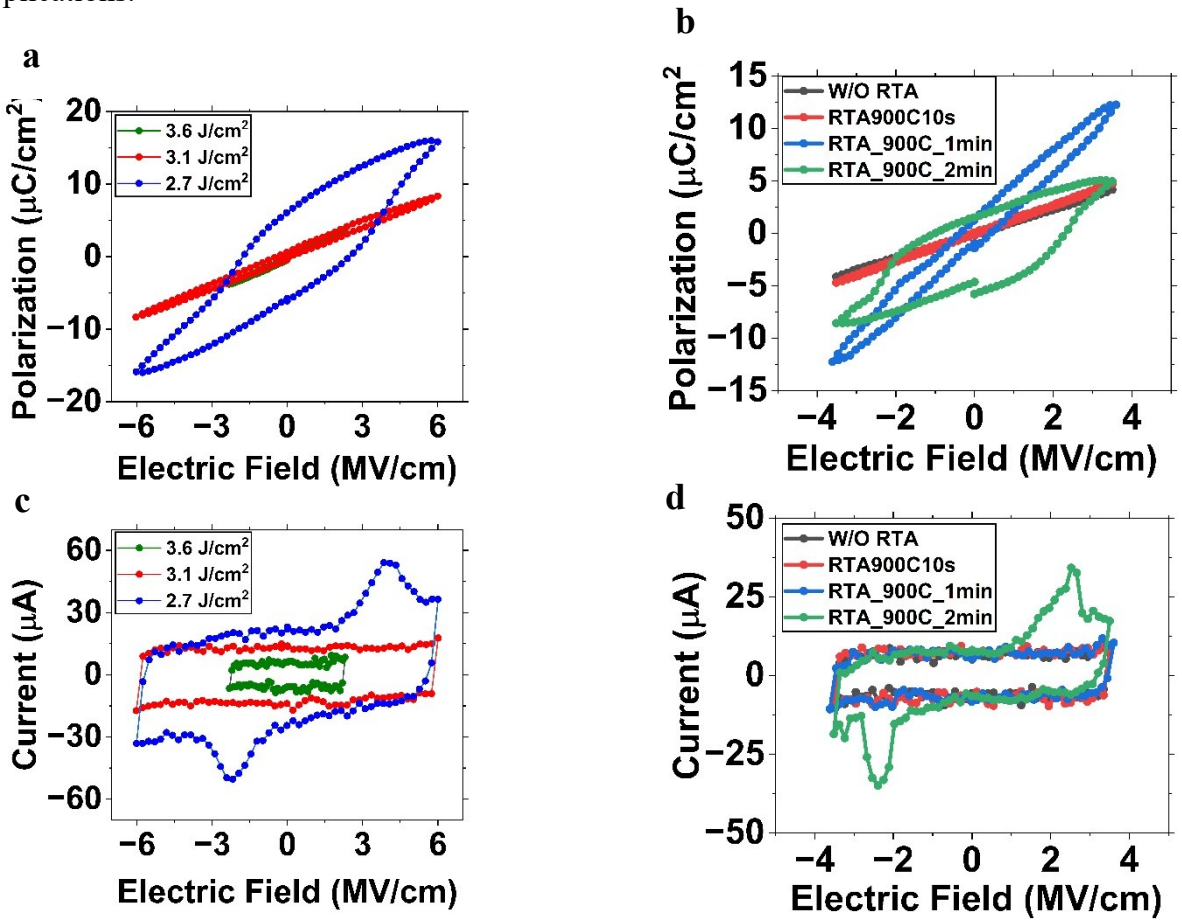

Figure: Electrical Characterization of Ferroelectric Y:HfO_2 Thin Films. Polarization-Electric Field (P-E) hysteresis loops (a, b) and Current-Electric Field (I-E) curves (c, d). Panels (a) and (c) illustrate the impact of laser fluence during deposition, while (b) and (d) show the effects of different post-deposition heat treatments.

Tuneable skyrmion liquid phase in polar skyrmions

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Abstract

Polar skyrmion are topologically protected swirling polarization textures showing exotic properties such as negative capacitance, chirality etc. Their stability and dynamic response under external stimuli (electric, and thermal fields) enable controlled manipulation, a crucial feature for device applications. While there have been few studies on the evolution of skyrmion under external stimuli the exact nature of polar skyrmion and their dynamics is still unknown. Here utilising piezoresponse force microscopy, scanning transmission electron microscopy, and phase field simulations we have drawn a detailed phase diagram of skyrmion with respect to electric field and temperature. The analysis of the translational and orientational correlation function reveals the polar skyrmions are in liquid phase. Also this liquid phase can be tune towards more ordered state with electric field and temperature. Through these studies, we have gathered significant insight into the manipulation of skyrmion with electric field and temperature, which provide a guiding principle for future nanoelectronics devices based on skyrmion.

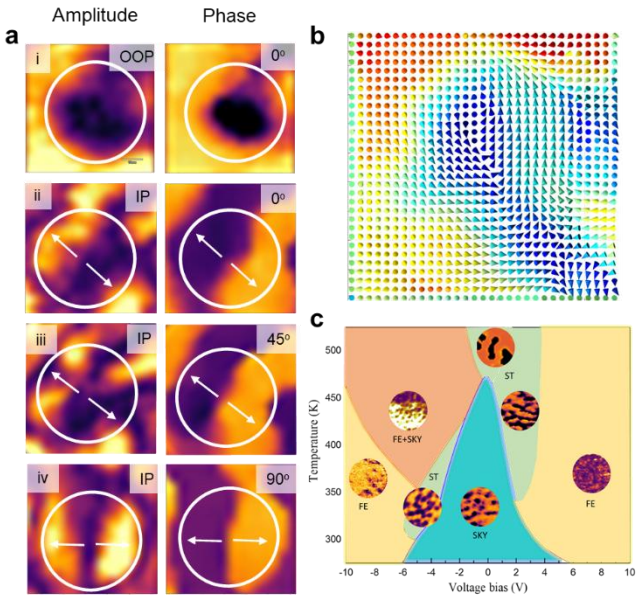

Fig1 Identification of polar skyrmions and phase diagram| a, Piezoresponse force microscopy (PFM) image. Vertical and lateral PFM images of single skyrmions at different orientations. **b,** 3-D vector PFM obtained from the combination of vertical and lateral PFM images. **c,** shows the detailed phase diagram of skyrmions using electric field and temperature dependent PFM.

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Ferroelectricity induced giant topological Hall effect in epitaxial multiferroic thin film heterostructures

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ABSTRACT

We report the emergence of a pronounced topological Hall effect (THE) in epitaxial thin-film heterostructures of ferromagnetic permalloy (Py, $Ni_{80}Fe_{20}$) and ferroelectric $BaTiO_3$ (BTO) interlayers grown on MgO (100) substrates. The observed topological Hall resistivity increases approximately 5 times in case of Py/BTO in comparison to single-layer Py films. Magnetic force microscopy reveals skyrmion-like spin structures, and previously it was demonstrated that Rashba-type spin–orbit coupling can be enhanced by broken inversion symmetry at the BTO interface which can give rise to pronounced topological Hall conductivity.[1, 2] These findings underscore how interfacial ferroelectric engineering with BTO can enable and control topological transport phenomena in spintronic heterostructures. Our comprehensive analysis involves epitaxial growth on MgO (100) substrates, pulsed-laser deposition, X-ray diffraction (to verify strain and film quality), and systematic Hall transport and magnetic measurements. The results conclusively demonstrate that the ferroelectric BTO layer is the pivotal ingredient triggering the topological response in Py achieving nearly five-fold enhancement over Py alone and turning THE in structures previously lacking such behavior. This work reveals a generalized route for inducing and controlling topological Hall signals via ferroelectric interlayers. By integrating BTO with conventional ferromagnets (Py), our approach opens up new avenues for skyrmion-based spintronic devices, where electric-field tunability is coupled to robust topological transport phenomena.

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Flexible and Wearable Polyvinyl Alcohol/Chitosan/$Ti_3C_2T_x$ MXene-Based Piezoelectric Hydrogels

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Abstract:

Conductive hydrogels have gained a lot of attention for their potential uses in flexible electronics, sensors, and electronic skins. However, highly low adaptation under cold or dry climatic conditions, along with poor reparability, substantially impedes the development of hydrogels in wearable electronics. Research on MXene reinforced hydrogels in flexible electrical sensing has made significant progress. However, there is a challenging systematic connection between production processes, network morphology, and hydrogel characteristics. Sensing performance is yet to be improved. Piezoelectric PVA/Chitosan/ $Ti_3C_2T_x$ MXene hydrogels represent a novel class of multifunctional materials that synergistically combine the exceptional electrical conductivity and mechanical robustness of MXenes with the intrinsic piezoelectric properties of chitosan (Cs). Characterization techniques revealed that the semi-IPN network crosslinking enhanced the mechanical resistance to deformation. Physico-chemical properties of hydrogel membranes were confirmed the uniform distribution of Cs and MXene within the hydrogel with improved conductivity as well as the material's piezoelectric response. The results have shown that the integration of MXene within a hydrogel matrix exhibited superior piezoelectric properties, maintaining the flexibility and stretchability inherent to hydrogels. For instance, these hydrogels can be employed in the development of flexible pressure sensors that convert mechanical stimuli into electrical signals, enabling real-time monitoring of physiological parameters. Additionally, their biocompatibility and responsiveness to mechanical deformation make them ideal candidates for flexible-wearable piezoelectric sensing applications.

Keywords: $Ti_3C_2T_x$ MXene, PVA hydrogel, Chitosan, piezoelectric hydrogels, energy harvesting, electrochemical studies

Curie - Weiss Crossover and Quantum Spin Liquid Behaviour in Multiferroic $TbInO_3$ Thin Film

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Abstract

Multiferroic materials that exhibit coupled electric and magnetic degrees of freedom are promising candidates for next-generation quantum and spintronic devices. Among these, $TbInO_3$ (TIO), a hexagonal perovskite crystallizing in the $P6_3cm$ space group, presents a unique coexistence of ferroelectricity and magnetic frustration, making it a compelling platform to explore emergent phenomena like quantum spin liquids (QSLs) in multiferroic materials.[1] The broken inversion symmetry and anisotropic exchange interactions mediated by strong spin–orbit coupling contribute to a highly frustrated QSL ground state, while the non-centrosymmetric structure supports ferroelectric polarization along the *c*-axis.[2] We successfully fabricated epitaxial TIO thin films on MgO (100) substrates via Pulsed Laser Deposition and compared the properties of the thin film with phase pure bulk sample. X-ray diffraction and Raman spectroscopy confirm the epitaxial growth and presence of hexagonal phase ($P6_3mc$) in thin film respectively. X-ray photoelectron spectroscopy reveals minimal disorder in the films, with a consistent chemical composition, oxidation states, and oxygen vacancies. Temperature-dependent DC susceptibility (χ-T) measurement for the thin film sample shows no magnetic ordering down to 0.4 K, supporting QSL behaviour which is reconfirmed with AC susceptibility measurements. Both the χ-T and reduced susceptibility (χT-T) plot reveal a C-W crossover, consistent with the presence of a QSL ground state. A large antiferromagnetic C-W temperature ($\theta_{CW} \approx -7.462$K) along with the absence of ordering down to 0.4 K indicates strong magnetic frustration and QSL behaviour, similar to bulk TIO.[1] Additionally, isothermal magnetization measurements fitted using the Brillouin function display notable deviations at low temperatures, indicative of persistent antiferromagnetic correlations—a key characteristic of QSL systems. These findings highlight the formation of multiferroic TIO thin film with QSL ground state. The dynamic spin fluctuations and absence of static magnetic order intrinsic to the QSL state can influence lattice degrees of freedom, offering a potential route to unconventional ferroelectric behaviour or enhanced tunability through magnetoelectric coupling which opens exciting possibilities for emergent functionalities in multiferroic quantum materials.[2]

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Way to achieve Highly Improved State-of-the-Art Ferroelectric Properties in $Hf_{0.5}Zr_{0.5}O_2$ at Low Processing Temperature

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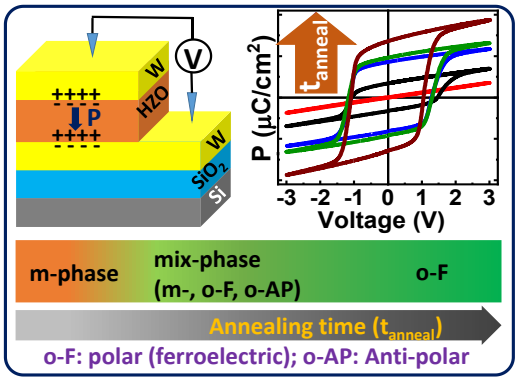
Abstract:-

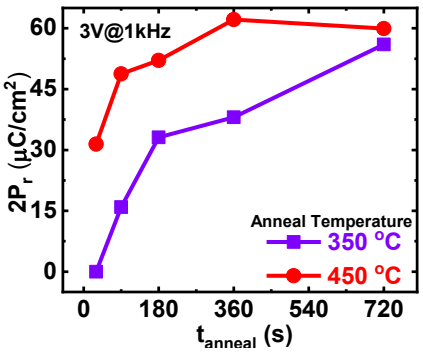
Ferroelectric HfO_2-based non-volatile memory devices such as Ferroelectric capacitor (FeCAP), tunnel junction (FTJ) and field effect transistor (FeFET) have been getting a lot of attention due to their low power-high performance operation and CMOS compatibility. Several dopants (Si, Al, Zr, La, Y, etc.) have been incorporated in HfO_2 to improve its ferroelectric properties. Among others, Zr has been reported to be the most effective dopant to enhance ferroelectric properties in HfO_2-ZrO_2 (HZO) system due to its structural similarities with HfO_2. However, the higher temperature annealing (≥ 500 °C) is required to obtain excellent ferroelectric properties in HfO_2-based ferroelectric devices, which is incompatible to the Back-End-of-Line (BEOL) process. The maximum process temperature of ≤ 450 or 400 °C is desired for BEOL processes. Hence, a novel approach to enhance ferroelectric properties in HZO processed at low temperature (≤ 400 °C) is necessary.



Generally, the low temperature annealing causes the low crystallinity of polar o-phase (O-III) in ferroelectric HfO_2 thin films, and therefore it is necessary to find new methods to increase crystallinity (more % of O-III phase formation) in ferroelectric HfO_2 thin films under BEOL process temperature.

Recently, different methods such as device stack engineering, interlayer engineering, and annealing and deposition temperature modulation at low temperature have been proposed to enhance the ferroelectric properties. The highest $2P_r$ of ~46 μC/cm^2 with strong fatigue limited endurance at 350 °C and and retention data was reported. The report with strong imprinted $2P_r$ of ~ 44.1 μC/cm^2 and endurance of 10^9 cycles (Imprint is the measure of horizontal shift of hysteresis loop during retention which implies data lost over time). However, the optimum process condition for higher remnant polarization, better endurance, and minimized imprint (which is a primary hindrance in marketing the ferroelectric based memories) with long retention and the impact of the process on these properties in HfO_2-based ferroelectric films has not been reported yet.

In this abstract, we propose a simple and novel process technique to improve ferroelectric properties in HZO processed under BEOL temperature limit. We discover the annealing time (t_{anneal}) as an isothermal crystallization method to enhance ferroelectric-orthorhombic-phase (O-III) even at low annealing temperature of 450 and 350 °C. As we increase the t_{anneal} from **30s, 90s, 180s, 360s, and to 720s**, we observe that $2P_r$ increases from **32 to 62 μC/cm^2 for 450 °C and from15 to 56 μC/cm^2 for 350 °C**, and the coercive voltage decreases to as low as $2V_c$ of 2.25V (360 s) and 2.54V (720 s) in 450 and 350 °C samples respectively. The principle O-III phase peak intensity at ~30.5° increases with increasing t_{anneal} as confirmed by GIXRD. However, the Raman spectroscopy reveals and segregates the different phases present in these samples. It shows that the dominant m-phase has disappeared beyond 90s of t_{anneal} and O-III modes' intensity increased with increasing t_{anneal} at the cost of m-phase in 350 °C annealed samples and the trend would be similar for 450 °C samples as well. The higher P_r value is associated with increasing polar o-phase (O-III) with increasing t_{anneal} and the low thermal expansion coefficient of tungsten (W) which applies tensile strain on the HZO film and it increases as t_{anneal} increases. HRTEM image helps determining the clear formation of O-III phase and EDS confirms no interfacial layer formation. The clean interface leads to the improved endurance of > 4x10^{10} cycles with almost full memory window open. Furthermore, the device demonstrates prolonged data retention of up to 10 years, making this FeCAP suitable for integration into the Back-End-of-Line (BEOL) of CMOS front-end transistor to implement Non-volatile DRAM (NVDRAM) devices.



Microstructure and piezoresponse force microscopy studies on neodymium titanate thin film - a high temperature ferroelectric

Sruti Muralikrishnan [a], *Manish Chandra Joshi* [a], *Sabarigresan Murugan* [a],

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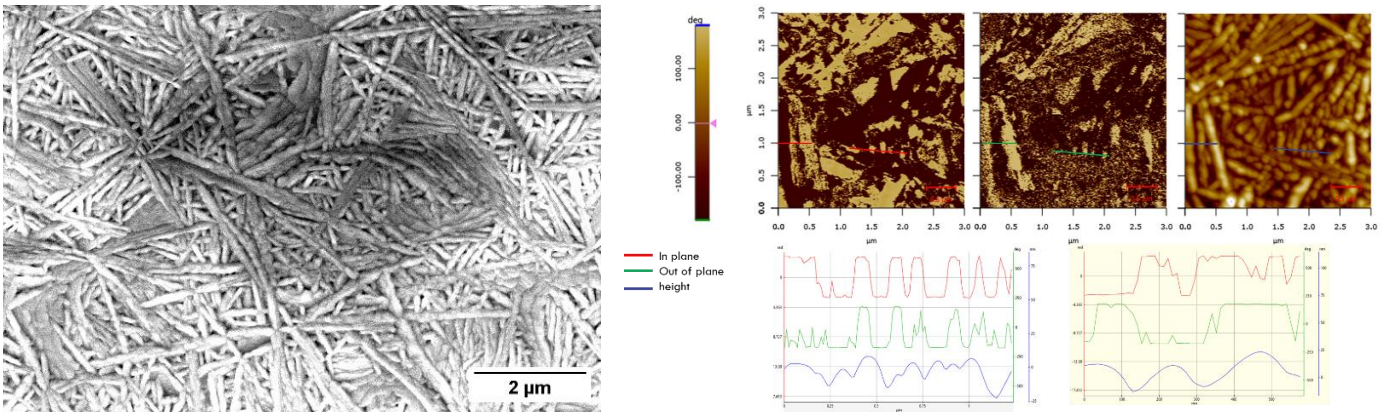
Neodymium titanate $Nd_2Ti_2O_7$ (NTO), a ceramic with layered perovskite structure, is a high temperature ferroelectric exhibiting thermal stability up to 1400 °C. It is extensively studied for its piezoelectric and pyroelectric applications in extreme environments.

In this study, $Nd_2Ti_2O_7$ thin film was deposited using the Pulsed Laser Deposition (PLD) technique at 800 °C maintaining oxygen partial pressure at 10 mTorr, on an alumina substrate, with $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) bottom electrode. Post deposition annealing at 1000 °C was performed to obtain a polycrystalline thin film. Thin film XRD analysis confirmed the formation of the monoclinic phase. Scanning electron microscopy (SEM) revealed that the grains coalesced into long, continuous dendritic arms forming nodal junctions, a morphology further confirmed through atomic force microscopy (AFM) imaging. While elongated needle-like morphology is expected for NTO, the dendrites forming nodal junctions could be attributed to varied deposition parameters.

The domains imaged using piezoresponse force microscopy (PFM) showed clear out-of-plane and in-plane domains, with evidence of 90° and 180° switching behaviour at room temperature and AFM morphology indicates the presence of twinned grains that may influence the local piezoresponse. The PFM phase analysis and its connection to polarization mapping will be presented.



Figures – SEM and PFM images showing in-plane and out-of-plane phase of NTO thin film

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A Highly Electrostrictive A_2BX_4-type Hybrid 2D Perovskite Ferroelectric and The Utility of its Composite Piezoelectric Nanogenerator in Wireless Mat-Sensor Technology

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Abstract: The quasi-spherical theory and ligand halogenation have emerged as effective strategies for promoting polar noncentrosymmetric structures with potential ferroelectric properties.[1] Here, we report a novel two-dimensional (2D) polar hybrid organic-inorganic perovskite, **[*p*-ClBnNH$_3$]$_2$CdBr$_4$** (***p*-ClBnNH$_3^+$** = 4-chlorobenzylammonium), which crystallizes in the orthorhombic noncentrosymmetric space group *Ccc*2. The structural polarity was confirmed via second harmonic generation (SHG) measurements, indicating a robust acentric arrangement, further supported by piezoresponse force microscopy (PFM) that revealed characteristic butterfly and hysteresis loops. Ferroelectric characterization through polarization–electric field (*P*–*E*) hysteresis measurements on thin films revealed a saturation polarization (P_s) of 1.28 μC cm^{-2} at room temperature. To assess its viability for energy harvesting, composite films were fabricated by embedding **[*p*-ClBnNH$_3$]$_2$CdBr$_4$** in a thermoplastic polyurethane (TPU) matrix. Devices incorporating 10 wt% of the perovskite yielded a piezoelectric nanogenerator (PENG) output voltage of 20.0 V and a power density of 67.6 μW cm^{-2}. Additionally, the material exhibited an exceptionally high electrostrictive coefficient (Q_{33}) of 3.6 m^4 C^{-2}, surpassing typical values observed in ceramic ferroelectrics and comparable to polyvinylidene difluoride (PVDF). A prototype "mat-sensor", which is a scalable smart force sensor, was developed using six parallel-connected device units integrated onto a flexible substrate, demonstrating rapid response and wireless functionality for real-time applications, including security systems. These findings position **[*p*-ClBnNH$_3$]$_2$CdBr$_4$** as a compelling multifunctional material for next-generation self-powered sensing and flexible electronic devices.

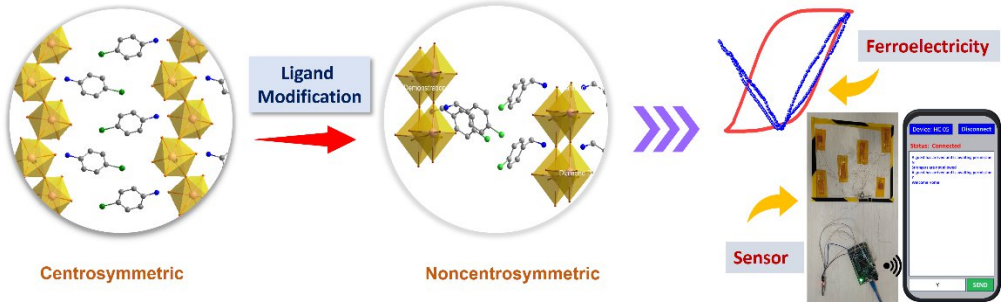

Figure 1. Designed 2D hybrid perovskite with tailored ligand demonstrating promising ferroelectricity and sensing capabilities.

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Two-Phase Energy Harvesting via Magneto-Pyroelectric Coupling

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The growing demand for sustainable energy solutions has led to interest in using overlooked waste energy sources, especially thermal fluctuations and stray magnetic fields produced by industrial machines and consumer electronics. Traditional energy harvesters often primarily focus on a single energy source, and thus, this results in their low efficiency. In contrast, hybrid energy harvesting systems can have the ability to capture multiple sources of energy forms at the same time through combined effects[1]. In this study, we present a flexible nanogenerator that combines electrospun polyvinylidene fluoride (PVDF) nanofibers with magnetostrictive ferrite nanoparticles to work together in harnessing energy via both pyroelectric and magnetoelectric effects. The PVDF matrix, which has a high electroactive β-phase content, effectively turns temperature differences into electrical energy. The dispersed ferrite nanoparticles convert weak ambient magnetic fields into mechanical strain. This strain can then be transformed into electricity through PVDF's piezoelectric response. This dual harvesting method shows a notable improvement in voltage output compared to single-mode devices, as shown by controlled thermal and magnetic field cycling experiments. The ability of nanocomposites to be processed in solution and their mechanical flexibility make them especially suitable for conformal integration in industrial IoT sensors and wearable electronics[2].

Keywords: PVDF nanofibers, Ferrite composites, Magnetoelectric, Pyroelectric, Hybrid nanogenerator

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Title: *Energizing Tomorrow: Biocompatible Ferroelectric Cu(II) Complexes for Sustainable Energy Harvesting*

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Department of Chemistry, IIT Bombay

Abstract: To tackle the growing global energy demand and the rapid exhaustion of non-renewable fossil fuels, it is crucial to develop sustainable alternatives. One promising strategy involves harvesting abundant but otherwise wasted environmental energies—such as mechanical vibrations, pressure, heat, sunlight, and tidal motion—and converting them into usable electricity through self-powered nanogenerators (SPNGs). A wide range of materials have been explored for this purpose, including inorganic oxides (e.g., perovskites and ceramics), polymers, organic molecules, peptides, and organic–inorganic hybrids. Among these, oxide systems exhibit strong piezoelectric and ferroelectric properties, making them highly effective for energy harvesting. However, they suffer from key limitations: high-cost, high-temperature synthesis, brittleness, limited tunability, and toxicity due to heavy metals. In contrast, polymers and peptides offer mechanical flexibility but often struggle to maintain stable polar states (e.g., the β-phase of PVDF) necessary for ferroelectric functionality. Hybrid organic–inorganic perovskites present a middle ground, combining low-temperature processability with excellent output performance, but are hampered by poor environmental stability and the presence of toxic components such as lead-based halides.

Through strategic molecular engineering and controlled design approaches, we have successfully addressed many of the limitations of traditional energy-harvesting materials by employing biocompatible, discrete molecular complexes. These materials are inherently lightweight, mechanically flexible, and readily polarizable under an external electric field—making them ideal candidates for integration into self-powered nanogenerators. Our synthesized Cu(II)-based molecular complexes exhibit impressive piezoelectric coefficients (d_{33} = 10–30 pm/V), comparable to benchmark materials such as $LiNbO_3$, ZnO, and widely used polymers like PVDF and PVDF-TrFE. They also display substantial spontaneous polarization, enabling efficient energy conversion in both single-crystal and composite configurations. In one of our flexible composite devices—fabricated by embedding a discrete ferroelectric complex into a non-polar polyvinyl alcohol (PVA) matrix—we achieved an impressive output peak-to-peak voltage of 4.94 V and an acoustoelectric conversion of 40 mV from 60 Hz soundwave. By leveraging the sensitive low-frequency detection limit of the AcNG combined with a Machine Learning (ML) approach, voices can be distinguished with a surprising accuracy of 95 %. Unlike conventional oxide single crystals, these molecular complexes are simpler to synthesize and exhibit desirable anisotropic properties. As such, they hold strong potential for a wide range of applications, including directional sensors, ultrasound transducers, and acoustic devices—where minimizing multidirectional mechanical and thermal noise is critical. This work underscores the versatility and promise of molecular materials for next-generation, soft, and sustainable energy technologies.

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ABSTRACTS

For

YOUNG RESEARCHERS' TALK

Heterostructure and interface design beyond epitaxy

Varun Harbola, Max Planck Institute for Solid State Research

The study of thin films, their interfaces and thin film heterostructures has been a cornerstone of experimental research at reduced dimensions. Advancements in epitaxial techniques have enabled the engineering of atomically precise and well-defined interfaces. However, the parameter space of interfaces enabled by epitaxy is determined by the lattice symmetry of the substrate and the plane on which epitaxy takes place. This for such interfaces is taken as a given. I will take this opportunity to focus on recent developments in oxide growth enabling the separation of the grown thin films from the growth substrate, resulting in freestanding oxide membranes. These membranes have allowed for unprecedented access to avenues in oxides, with novel symmetry disallowed interfaces, which go beyond the epitaxially possible atomically sharp interfaces . I will show striking phenomena we have observed with an exemplary SrTiO3 (001) on a sapphire (0001) interface, through which I hope to convey how these developments in oxides promise a fertile ground for remarkable discoveries in material science and physics.

From Delusion to Reality: The Isosymmetric Transition in $BiFeO_3$-$PbTiO_3$ and Its Complex Phase Diagram

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Morphotropic phase boundary (MPB) ferroelectric systems are of significant interest due to their enhanced electromechanical properties. In general, the MPB marks a critical point in the composition-temperature phase diagram of ferroelectric alloys, where a symmetry-breaking ferroelectric instability occurs, leading to a region of enhanced dielectric and piezoelectric responses. However, the $(1-x)BiFeO_3-(x)PbTiO_3$ alloy exhibits an intriguing deviation from this behavior, manifesting as a symmetry-preserving isostructural transition between two tetragonal phases (T_1 to T_2) upon heating. We resolve this anomaly by conducting a comprehensive study of the structural evolution under thermal cycling, the temporal changes in structure under isothermal conditions, and Landau-Devonshire phenomenological modeling. Our findings challenge traditional understanding by revealing that: (i) the apparent high-temperature tetragonal phase (T_2) is not in equilibrium, (ii) the true equilibrium phase at elevated temperatures is rhombohedral in symmetry, and (iii) the rhombohedral phase, though thermodynamically stable, is kinetically suppressed during heating due to internal strain effects, but becomes stabilized upon cooling. These findings provide crucial insights into the role of internal strain in controlling phase stability and suggest that strain-driven phase behaviors play a pivotal role in determining the structure-property relationships in multiferroic and piezoelectric materials. This study paves the way for the design of functional materials where phase stability can be manipulated via strain engineering, offering new possibilities for advanced device applications.

Ferroelectric Size Effects on Statics and Dynamics of Domain Wall

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Domain walls separating differently oriented polarization regions of ferroelectric materials are known to greatly impact nanoscale materials and device functionalities. Though the understanding of size effects in ferroelectric nanostructures has progressed, the effect of thickness downsizing on domain wall scaling behavior has remained unexplored. Using piezoresponse force microscopy, epitaxial $BaTiO_3$ film thickness size (2-90 nm) effects on the critical scaling universality of the domain wall dynamical creep and static roughness exponents including dimensionality is demonstrated. Independently estimated static roughness exponents ranging between 0.34 and 0.28 and dynamical creep exponents transition from 0.54 to 0.22 elucidate the domain wall dimensionality transition from two- to quasi-one-dimension in the thickness range of 10-25 nm, which is later validated by evaluating effective dimensionality within the paradigm of random-bond universality. The observed interdimensional transition is further credenced to the compressive strain and long-range strain-dipolar interactions, as revealed by the structural analyses and additional measurements with modified substrate-induced strain. These results provide new insights into the understanding of size effects in nanoscale ferroelectricity, paving the way toward future nanodevices.

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Large longitudinal electrostrain and electrobending deformation in polycrystalline piezoelectrics

Gobinda Das Adhikary* and Rajeev Ranjan

Piezoelectric ceramics are key to technologies such as SONAR, MEMS, and ultrasound imaging. While single crystals like $Pb(Zn_{1/3}Nb_{2/3})O_3$–$PbTiO_3$ (PZN-PT) and $Pb(Mg_{1/3}Nb_{2/3})O_3$–$PbTiO_3$ (PMN-PT) exhibit large electrostrains (~1.7%), they are expensive and difficult to produce. In contrast, non-textured polycrystalline ceramics are cost-effective but typically limited to ~0.3–0.4% electrostrain due to grain boundary constraints. We demonstrate a novel method to achieve significantly enhanced electrostrain (~1.2%) in polycrystalline $PbZr_xTi_xO_3$ (x = 0.52) by reducing sample thickness to 0.2 mm. This approach relaxes intergranular clamping and leverages the enhanced response of surface grains, which behave differently from the bulk. Additionally, we explore electrobending in $BaTiO_3$, $Na_{0.5}Bi_{0.5}TiO_3$-, $K_{0.5}Na_{0.5}NbO_3$-, and $BiFeO_3$-based systems, arising from asymmetric domain switching driven by oxygen vacancy gradients. These insights open new pathways for designing advanced piezoceramics with high strain and bending capabilities.

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Engineering Phase transitions in La doped HfO_2 films for cryogenic refrigeration and FEFETs

Ferroelectric Hafnia has garnered significant attention in the landscape of nanoelectronics with its excellent nanoscale ferroelectricity and seamless CMOS integration. Ferroelectric nanofilms are being well explored towards advanced memory and logic devices. However, there lacks a comprehensive study on the thicker hafnia for its pyro and piezoelectric counterparts. In this talk, I will present the recent advances in the development of high quality, 40nm thick La doped hafnia (LHO) films by a simple and cost-effective solution processing, quite a challenging deposition method for growing hafnia films, in ferroelectric orthorhombic phase.

The talk focuses on the fabrication of MIM devices with ferroelectric LHO layer sandwiched between bottom TiO_XN_y (magneli), and top TiN contact layers and their capability to use in potential applications including cryogenic cooling and ferroelectric field effect transistors (FE-FETs). The careful engineering of the MIM devices, by incorporating the magneli layer, a Mott Insulator, induces a polar to non-polar phase transition in LHO via proximity effect in the ferroelectric layer. The talk also highlights the strategy to tune the polar to non-polar phase transition temperature from 140 K to 260 K by introducing an Al_2O_3 capping layer and controlling its thickness.

Notably, the devices exhibit record pyroelectric and electrocaloric effects with a peak refrigerant matrix as high as of 106 K at 140 K under the applied electric field of 5 MV cm^{-1}. Furthermore, the talk presents a phase change ferroelectric field effect transistor integrated on a 2D MoS_2 channel. Near the induced phase transition temperature, the devices show steep sub-threshold slopes surpassing the Boltzmann limit indicating its potential for low power switching applications.

Gelatin Exfoliation Process: Enhance The Potential of Ferroelectric Component in Electronic Skin Applications

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[1] *Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan*

To enable next-generation electronic skin (e-skin) with sensing, actuation, and memory capabilities, integrating ferroelectric and piezoelectric oxide materials onto flexible platforms is essential. However, their high-temperature epitaxial growth is often incompatible with conventional flexible substrates. In this work, we employ mica substrates combined with a gelatin-assisted exfoliation method to fabricate freestanding epitaxial functional thin films, including Pt, ZnO, and high-entropy PMNTHZO.

With the aim of better understanding and controlling the exfoliation behavior induced by gelatin, we conducted a series of experiments, including varying the gelatin concentration, performing finite element simulations, and applying Stoney's equation to estimate the contraction stress of the gelatin layer. These results help optimize the stress range suitable for exfoliating functional thin films with varying mechanical properties. Under these optimized conditions, the exfoliated films preserve excellent crystallinity and functional properties, including conductivity, piezoelectric and ferroelectric responses. Moreover, the films demonstrate stable performance under repeated bending cycles, endure compressive bending radii and maintain retention over a period, validating their suitability for flexible device applications.

This technique offers an environmentally friendly, low-energy solution to integrate high-quality ferroelectric and piezoelectric materials into flexible devices, supporting broader applications in wearable electronics and smart robotics.

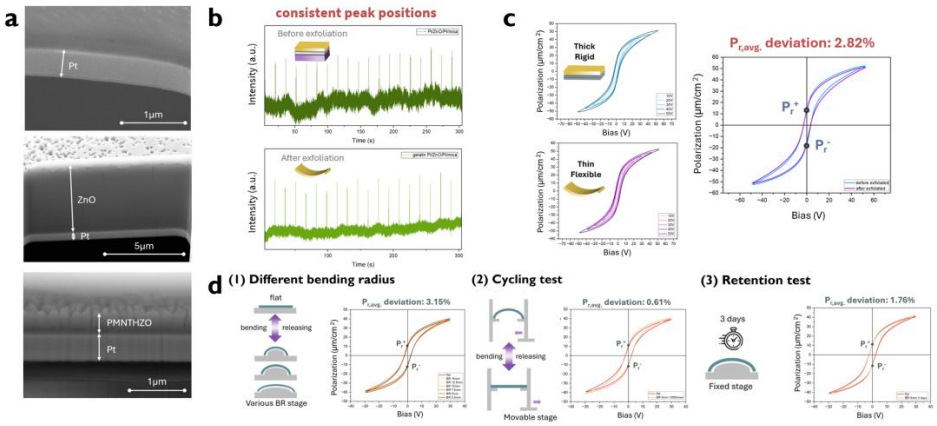

Figure 1. (a) Freestanding Pt, ZnO, and PMNTHZO films. (b) Piezoelectric response of ZnO and (c) Ferroelectric response of PMNTHZO before and after exfoliation. (d) Bending durability of PMNTHZO ferroelectric response.

Observation of Akhiezer and Landua-Rumer Regimes in the Temperature Dependence of Longitudinal Wave in BST on Sapphire BAW Resonator

Kongbrailatpam Sandeep Sharma[1], Akhil Raman T.S[2], James Raju K.C[2], and Gayathri Pillai[1]
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High quality factor acoustic resonators operating in the microwave frequency are of prime interest for applications of quantum sensing[1], transduction[2], and memory operations[3]. Achieving ultrahigh quality factor required for such quantum applications need a careful study of the various loss mechanisms (intrinsic and extrinsic) in the resonator. In this work, using a high overtone bulk acoustic resonator (HBAR), we study the absorption of longitudinal acoustic waves through a three-phonon process[4]. The wide spectra of HBAR excited using the ferroelectric BST film permits excitation of coherent phonons modes from few GHz to 10's of GHz. Through a temperature (T) sweep from 4 K to 200 K, we observe the evolution of temperature dependence of the Q^{-1} from $T^{1.48}$ to $T^{4.75}$ from 2 GHz through 9 GHz modes which confirms the Akhiezer and Landua-Rumer Regimes occurring in modes of the same resonator[4].

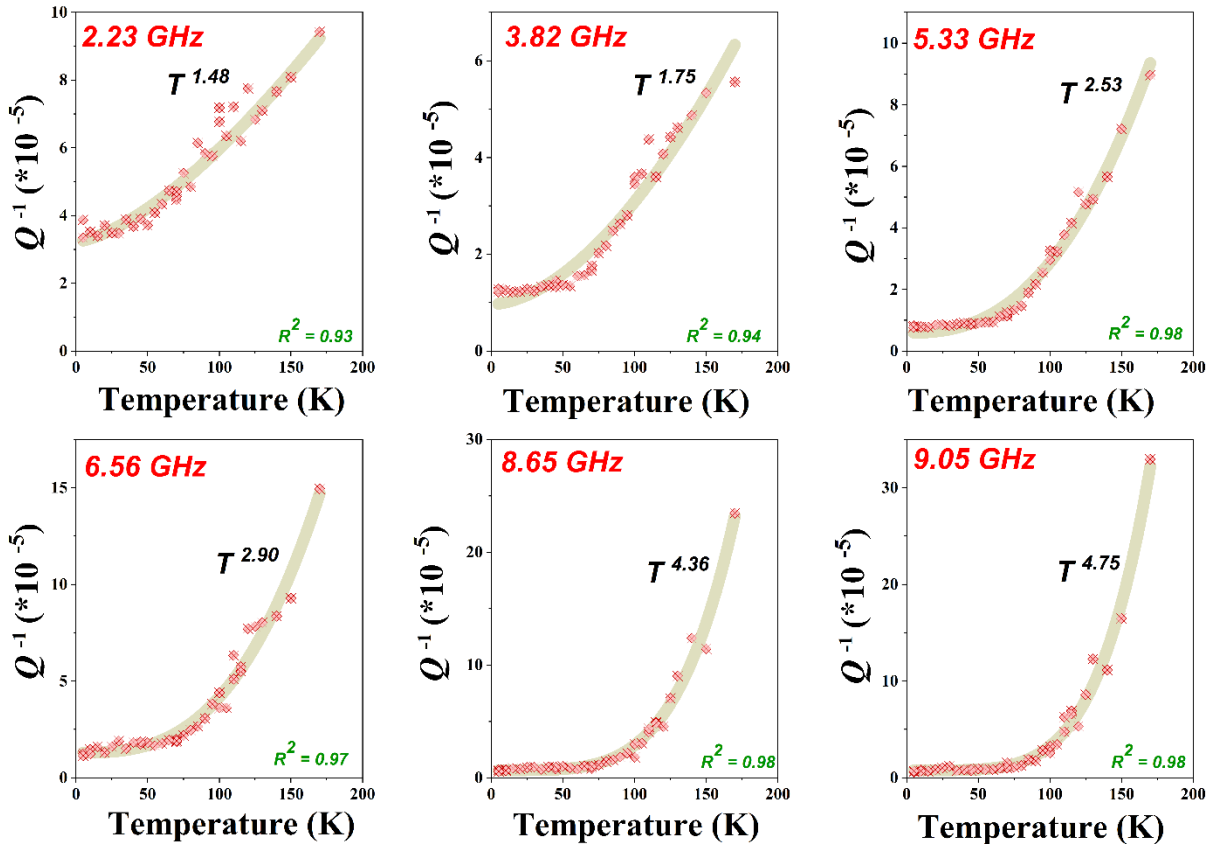

Figure 1. Q^{-1} vs temperature for different longitudinal acoustic modes of the HBAR.

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Generation of Phononic Frequency Combs via Nonlinear Mode Coupling in Curved Circular Piezoelectric MEMS Resonators

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In recent years, there has been growing research interest in phononic frequency combs (PFCs) generated in microelectromechanical systems (MEMS) resonators, inspired by the remarkable progress made in their optical counterparts. PFCs have typically been demonstrated using nonlinear modal interactions and parametric driving schemes [1–5]. As a result, MEMS resonators with tunable resonance frequencies and rich nonlinear characteristics are considered highly suitable platforms for comb generation. Furthermore, the use of single-tone actuation is desirable for practical implementation. Hence, the present work investigates phononic frequency comb generation in a curved circular piezoelectric MEMS resonator under single-tone excitation, demonstrating comb signatures at low input power levels.

The curved circular resonator was fabricated using a standard MEMS process, while retaining the oxide layer beneath the device layer. This approach enables controlled curvature in the resonator structure through stress imbalance between the thin-film layers, without resorting to complex fabrication steps. The curved profile plays a critical role in enhancing the nonlinear modal dynamics of the resonator. Figure 1(a) shows a schematic of the curved circular MEMS resonator. Experimental measurements were carried out using a UHFLI lock-in amplifier. The bidirectional electrical amplitude–frequency response of the fourth flexural mode under 300 mV AC excitation exhibited prominent nonlinear hysteresis behavior and revealed strong intermodal interactions between two modes, as shown in Fig. 1(b).

To detect phononic frequency comb signatures, the fourth mode was excited using a single-tone input swept across its nonlinear bandwidth. At each excitation frequency, the output signal was analyzed using the FFT spectrum module of the lock-in amplifier. Clear spectral signatures of phononic frequency combs were observed, particularly near 204.8 kHz, where equally spaced spectral lines emerged, confirming the formation of a comb, as shown in Fig. 1(b). These observations highlight the potential of curved MEMS resonators as promising platforms for efficient and tunable phononic comb generation with simplified single-tone excitation. The results pave the way for the further development of compact phononic devices for sensing, metrology, and signal processing applications.

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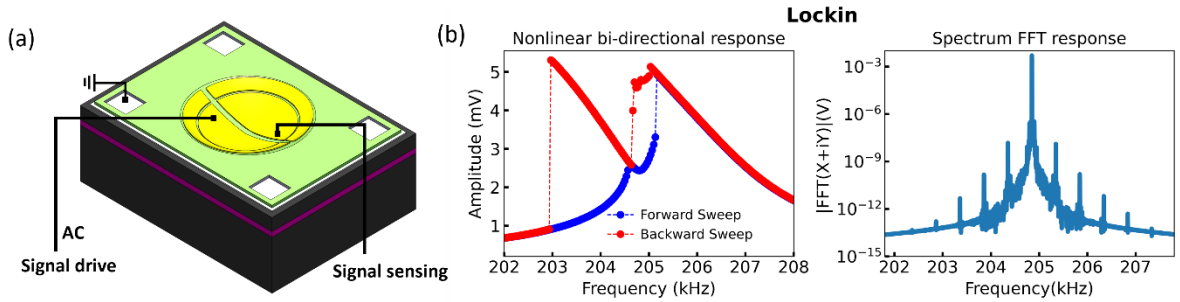

Figure 1: (a) Schematic of the curved circular piezoelectric MEMS resonator. (b) Bidirectional amplitude–frequency response of the fourth mode, and the corresponding spectral signature of phononic frequency combs at a 204.8 kHz input fréquence.

Different textured PZT films grown on Si/Pt substrate

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Abstract

Growing ferroelectric films with different textures under identical process conditions poses a significant materials challenge. The texture of ferroelectric films is largely influenced by the underlying substrate. Ti/Pt deposited on silicon is widely used as a bottom electrode and substrate for the growth of PZT thin films. In this study, we developed a novel two-step deposition process to engineer the surface of the Ti/Pt bottom electrode, enabling the growth of distinct (100) and (111) textured PZT thin films on different regions of the same silicon wafer. Using photolithography, we successfully sputter-deposited mono-layer and bi-layer Ti/Pt on separate regions of the wafer, allowing for controlled texture formation under identical processing conditions. We found that the bilayer Ti/Pt bottom electrode effectively suppressed Ti diffusion and oxide formation—critical factors for achieving (100) textured PZT growth. In contrast, the mono-layer Ti/Pt exhibited Ti diffusion and oxide formation, leading to the growth of (111) textured PZT. Ferroelectric measurement shows different polarization values and different dielectric constant. These findings highlight the potential of surface-engineered Ti/Pt electrodes in optimizing PZT thin films for piezoelectric MEMS applications.

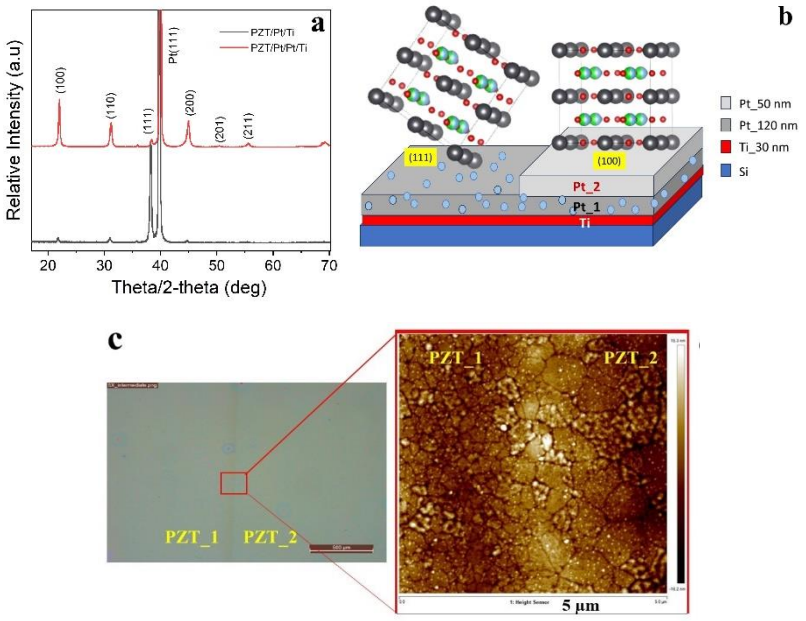

Fig. 1 (a) X- ray diffraction (b) Schematic diagram of PZT films on Si/Pt substrate and (c) Optical image and AFM topography at the interface region of different textured PZT films grown on same Si/Pt substrate

Photo-Induced Properties in Ferroelectric Oxides: From Fundamentals to Applications

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Interaction between light and ferroic order parameters in nanostructures leads to new physical functionality. In this respect, the quest for opto-electronic control of energy-efficient ferroelectric materials is gaining importance for fast memory applications. We explored the light-induced polarisation switching behaviour in epitaxial freestanding $BaTiO_3$ (18 nm) films. It is observed that after writing the domains with positive and negative voltage, the materials always return to their original downward polarisation state under illumination for both polycrystalline and epitaxial films. The material also exhibits significant enhancement in the amplitude response, which is confirmed by the imaging and spectroscopy analysis under dark and illumination conditions. Importantly, the freestanding $BaTiO_3$ film illustrates domain-switching immediately after illumination. The optically controlled domain switching response is compared between a clamped film and freestanding membrane. It is established that the fast domain switching response in the freestanding film compared to the clamped film is attributed to the removal of substrate-induced strain and the subsequent increase in domain wall velocity. Additionally, ferroelectric fatigue behaviour is not observed in our system even after 75 electrical and optical cycles, demonstrating the robustness of the observed phenomenon. Our work provides a step forward towards wireless sensing and dual optical and electronic control for computing. In addition, I will talk about a few other ferroelectric systems designed for photovoltaic (PV) applications and how strain influences the PV outcomes. Also, I will go through the strategy on how to design suitable PV materials for photovoltaic and optical control memory applications.

A new approach of ferroelectric ionic displacement detection using polarized Raman spectroscopy

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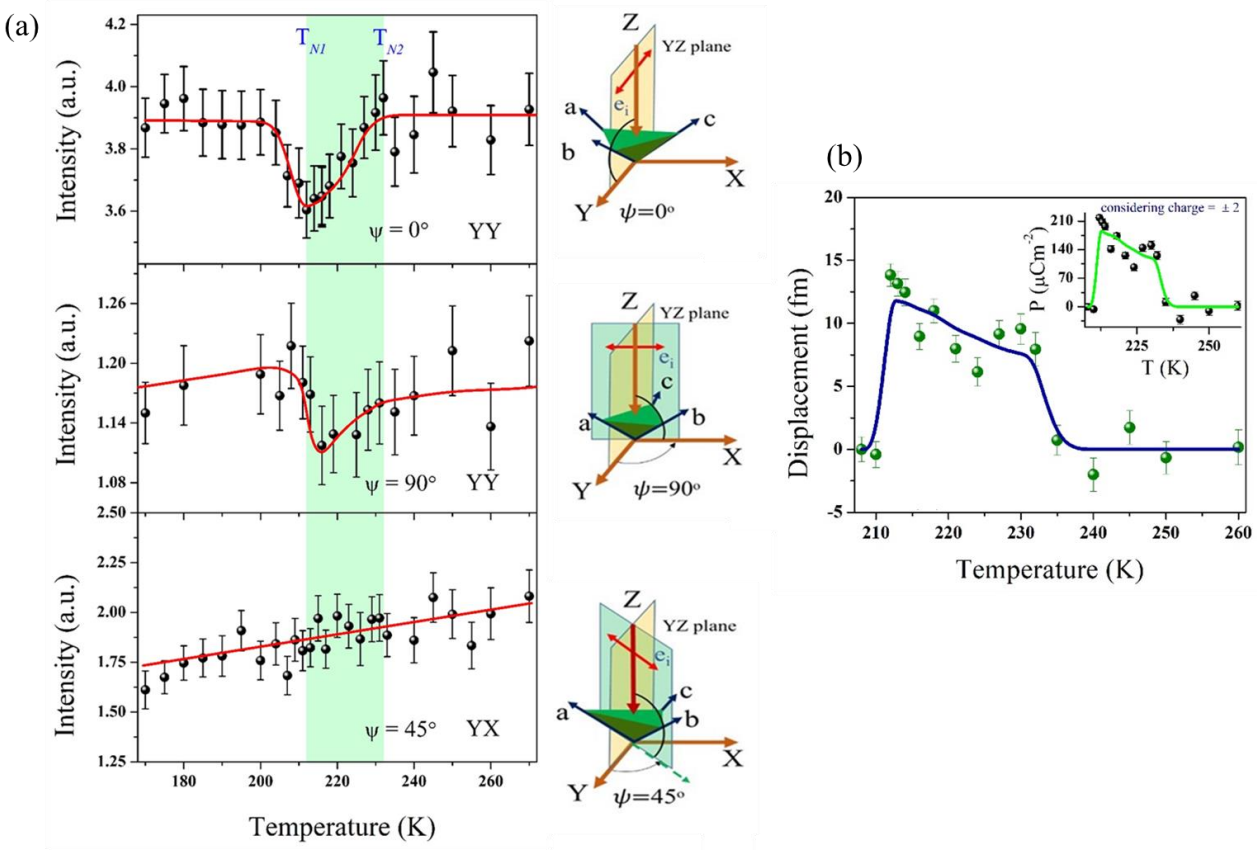

Fig 1: (a), (b) Temperature evolution of Raman intensity and shift of A_g modes in CuO, respectively.

Raman spectroscopy basically probes the changes in polarizability induced by lattice vibration, popularly known as Raman tensor, which are highly sensitive to the interatomic distances [1], can be used to detect very small (femto-meter) and precise directional atomic displacements and associated ferroelectricity which are very difficult using conventional methods like X-ray diffraction and Extended X-ray Absorption Fine Structure study. Fig 1 (a) shows the variation of Raman intensity of Ag mode of CuO as function of temperature, which depicts an ionic displacement along *b*-axis. The amount of displacements is detected using the change in Raman shift of this particular mode (b) and found that femto-meter ionic displacement is the microscopic origin of ferroelectricity in high temperature magnetic induced multiferroic CuO. Ti displacements associated to the ferroelectric polarization in $BaTiO_3$ [2] is also probed using this new method to validate the method.

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Insights into Multifunctional Properties of Ferroelectrics from Atomistic Simulation

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Ferroelectrics exhibit a rich spectrum of multifunctional properties. In tailored systems, their coupling with electric, magnetic, optical, mechanical, and thermal fields unlocks diverse opportunities across electronics, sensing, energy, and information technologies. In this talk, I will present the strategies we have pursued to uncover fundamental mechanisms underlying new multifunctional behaviors in ferroelectrics using modeling and atomistic simulations based on both first- and second-principles methods.

In particular, magnetoelectric-multiferroic materials with intrinsic cross-coupling between electrical and magnetic order parameters are promising candidates for next-generation memory devices, offering enhanced speed and reduced power consumption [1]. However, despite intensive research efforts, only a handful of bulk materials with electric-field-switchable magnetization have been predicted and observed in experiments, and aside from $BiFeO_3$, none of them orders magnetically at room temperature. Using group-theory-led first-principles calculations, we have predicted the possibility of room temperature electric field reversal of magnetization in the family of $A_4B_3O_9$ layered oxides, enabled by a rare Γ-point magnetoelectric coupling scheme [2].

While traditional approaches focus on discovering new properties in bulk ferroelectrics, recent research has shifted toward heterostructures, a premier example being ferroelectric/dielectric oxide superlattices. Lately, it has been shown that $PbTiO_3/SrTiO_3$ superlattices can host complex polar topological textures analogous to magnetic skyrmions [3]. These electric bubble (e-bubble) skyrmions can exhibit natural chirality arising from the in-plane Bloch-type polarization at the skyrmion wall around the out-of-plane polarization at the core. In our recent work, we investigate the soft-mode chiral phase transition of e-bubbles in $PbTiO_3/SrTiO_3$ superlattices driven by strain using second-principles simulations [4]. As chiral structures interact differently to left- and right-circularly polarized light, the chiral phonon modes, located in the sub-THz frequency range, may be optically active, suggesting potential applications in low-power communication technologies.

The results I will present are based on research conducted in collaboration with, and under the guidance of, Dr Emma E. McCabe and Dr Nicholas C. Bristowe from Durham University, as well as Dr Natalya S. Fedorova, Dr Hugo Aramberri and Prof Jorge Íñiguez-González from Luxembourg Institute of Science and Technology.

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Nanoconfinement Driven Mechanical and Thermal Properties of Ferroelectric Molecular Complex

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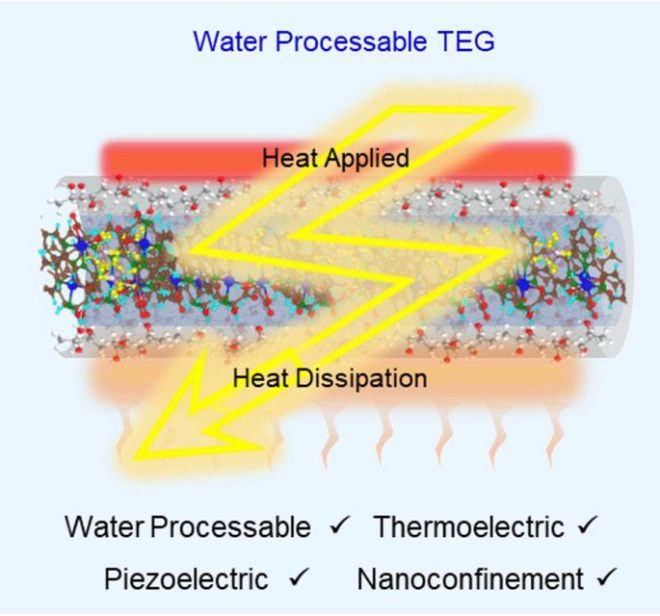
Keywords: Nanoconfinment, molecular complex, thermoelectric, nanofiber, piezoelectric

Abstract:

Water-processable hybrid piezo- and thermo-electric materials advances the range of applications of self-powered sensing and energy conversion devices. We acquaint, the nanoconfinement effect of ferroelectric discrete molecular complex [Cu(L-phe)(bpy)(H_2O)]PF_6·H_2O (**1**) in a non-polar polymer 1D-nanofiber to envision the high-performance flexible hybrid piezo- and thermo-electric nanogenerator (TEG). The 1D-nanoconfined crystallization of 1, enhances piezoelectric throughput with high degree of mechano-sensitivity, i.e., 710 mV/N up to 3 N of applied force with 10,000 cycles of unaffected mechanical endurance. Thermoelectric properties analysis shows a noticeable improvement in Seebeck coefficient (~4 fold) and power factor (~6 fold) as compared to its film counterpart, attributed to the enhance density of states (DOS) near the Fermi edges as evidenced by ultraviolet photoelectric spectroscopy and density functional based theoretical calculations. We report for an aqueous processable hybrid TEG that provides an impressive magnitude of Seebeck coefficient (~793 μV/K) and power factor (~ 35 mW/mK²)in comparison to the similar class of materials.[1]



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Latent electronic (anti-) ferroelectricity in $BiNiO_3$

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Metal to insulator transition (MIT) and an associated structural transition from *Pnma* to $P2_1/n$ in rare earth nickelate compounds $RNiO_3$ (except R = La), is mediated by NiO_6 breathing distortion and a consequent charge disproportionation at the nickel sites. Interestingly, at odd to that a very distinct type of MIT is observed for $BiNiO_3$, where charge disproportionation is instead appeared at the Bi sites, with an associated *Pnma* to *P-1* structural transition.

In this study, relying on first principles calculations, we first rationalize the phase transition from *Pnma* to *P-1*, revealing the existence of an overlooked intermediate $P2_1/m$ phase and a very unusual phase transition mechanism. Going further, we point out that the C-type charge ordering at Bi sites in the *P-1* phase is not unique. We highlight the existence of an alternative G-type charge ordering that breaks inversion symmetry and gives rise to a ferroelectric $Pmn2_1$ phase nearly degenerated in energy with the ground state. The $Pmn2_1$ phase shows a spontaneous polarization of 53 $\mu C/cm^2$, which mostly arises from charge ordering. The close energy of the $Pmn2_1$ and *P-1* phases, together with the low energy barrier between them, make $BiNiO_3$ a potential candidate to host electronic antiferroelectricity in which the field-induced transition from non-polar to polar would relate to inter-site electron transfer.

Acknowledgements: Work supported by F.R.S.-FNRS Belgium (PDR project PROMOSPAN).

Reference:

See "*Latent Electronic (Anti-)Ferroelectricity in $BiNiO_3$*, Subhadeep Bandyopadhyay and Philippe Ghosez, Physical Review Letters 133 (14), 146801 (2024)" for more details.

Towards room-temperature ferroelectric-spin-orbit (FESO) devices based on perovskite ferroelectrics

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The power consumption of logic and memory components is a key challenge for the microelectronics industry, a problem expected to intensify with the growing demands of artificial intelligence and machine learning. Alongside the impending end of Moore's law, this calls for new low-power computing paradigms beyond conventional CMOS. In-memory computing—where logic and memory operations are co-located—offers a promising solution to overcome the inefficiencies of traditional von Neumann architectures. For such systems, non-volatile memory elements are essential, and ferroelectric materials are particularly attractive due to their intrinsically low-power, electric-field-driven switching.

One proposed device architecture is Intel's magnetoelectric spin-orbit (MESO) device[1], in which information is encoded in the magnetisation of a ferromagnetic layer and switching is driven by a magnetoelectric material. However, the scarcity of robust room-temperature multiferroics limits practical implementation. An alternative concept is the ferroelectric spin-orbit (FESO) transistor[2], which bypasses magnetisation entirely and operates through ferroelectric control of spin-orbit coupling and spin-charge conversion. In this architecture, polarisation at the interface between a ferroelectric and a spin-orbit coupled layer modulates carrier density and enables current control via the inverse Edelstein effect.

Building on our earlier demonstration of non-volatile electric-field control of spin-charge conversion in a $SrTiO_3$-based Rashba two-dimensional electron gases (2DEGs), where ferroelectric polarisation was shown to reverse the sign of the inverse Edelstein effect via spin pumping measurements at low temperatures[2], we now extend this concept toward device integration. In our subsequent work[3], we demonstrated full electrical injection and detection of spin-charge conversion in nanoscale $LaAlO_3/SrTiO_3$ 2DEGs, establishing a robust, gate-tunable readout mechanism compatible with scalable architectures. These advances provide the foundation for the development of FESO devices, which integrate polarisation-driven spin-charge conversion with fixed ferromagnetic readout layers to achieve direct, non-volatile electrical translation of polarisation into output current—without requiring magnetisation switching.

In this presentation, we will detail our efforts to build room-temperature FESO devices based on Rashba-type 2DEGs formed in perovskite ferroelectrics. 2DEGs at oxide interfaces have emerged as versatile platforms for spin-orbitronics, combining strong Rashba spin-orbit coupling with gate-tunable transport. Here we describe the growth and characterisation of ultra-high-quality epitaxial $BaTiO_3$ thin films displaying Curie temperatures above 300 °C, switching voltages in the 100 mV range and endurance exceeding 10^{11} cycles. We show how 2DEGs can be generated at their surface using X-ray photoelectron spectroscopy and magnetotransport and demonstrate spin-charge conversion at room temperature in such 2DEGs interfaced with a ferromagnetic layer, with spin-charge conversion efficiencies comparable to the best $SrTiO_3$-based systems. We will demonstrate the integration of these materials into nanoscale FESO architectures fabricated via electron beam lithography. This technology offers a compelling pathway toward high-endurance, magnetic-field-insensitive in-memory computing with attojoule-level power consumption.

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ABSTRACTS

For

POSTER PRESENTATION

Crystallization of Ferroelectric Thin Films on Polymer Microwave Substrates for Tunable Microwave Device Applications

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Ferroelectric Barium strontium titanate, $Ba_{0.5}Sr_{0.5}TiO_3$ (BST5), thin films are suitable for microwave tunable applications because of their unique properties, such as high dielectric constant, low loss in the microwave range, high tunability, and electric-field induced piezoelectricity. However, the elevated crystallization temperature of the BST5 thin films makes it difficult for their integration into polymers and integrated circuits. The processing temperature of the ferroelectric oxide films can be brought down below 300°C through the laser-induced crystallization (LIC) method.

RT/Duroid is a high-frequency circuit material based on PTFE mixed with random glass or ceramic to form a composite that is laminated with copper on either side. It exhibits low loss and stable dielectric constant over a wide frequency range and is appropriate for the fabrication of planar microwave devices. However, at present, devices like varactors are added to them as lumped elements, as there is no technology to monolithically integrate them on such flexible polymer substrates to realize active integrated circuits over them. Rogers RT/Duroid 5880 is an excellent choice for the development of tunable microwave devices and provides the advantage that copper laminate can act as the bottom electrode and avoid the need for the deposition of the bottom metal electrode.

BST5 thin films are deposited over RT/Duroid 5880 substrate using the pulsed laser deposition technique, using a 248 nm KrF excimer laser of pulse width 20 ns with a repetition rate of 10 Hz at a temperature of 250 °C. The deposited BST5 thin films are in the amorphous state and are then irradiated with a defocused 248 nm KrF excimer laser beam for crystallization at the deposition temperature. The laser-annealed BST5 films are XRD crystalline(Figure 1). Using the laser-annealed BST film, a microwave varactor has been fabricated and is tested in the microwave frequency range using a Vector Network Analyzer (VNA). A dielectric tunability of 33% was achieved for the fabricated varactor (Figure 2). Achieving the crystallization of BST5 thin films on RT/Duroid substrates marks a significant advancement toward the direct integration of functional oxides for fabricating tunable microwave devices on flexible polymer substrates.

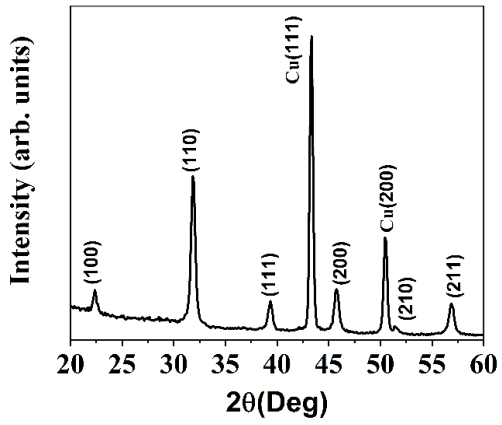

Figure 1. XRD pattern of laser annealed BST film on RT/Duroid 5880

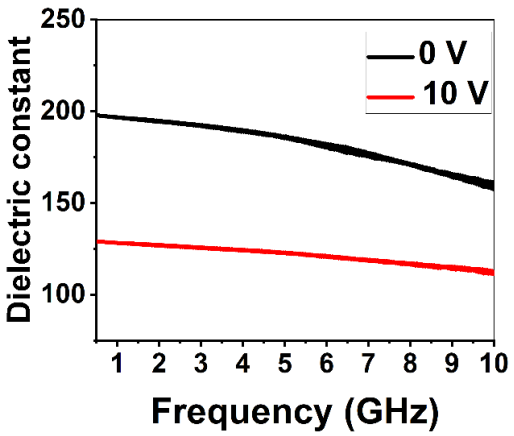

Figure 2. Dielectric constant vs frequency of fabricated varactor at 10 V dc bias

Dependence of Transient Negative Capacitance on Domain Switching Kinetics in La-doped $Pb(Zr_{0.4}Ti_{0.6})O_3$ Ferroelectric Capacitor

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The types of domains – 60°, 90°, and 180° – as well as lattice strain (epitaxial and chemical) influence the domain switching kinetics in multidomain ferroelectric capacitors. We noted in our study that these factors not only influence the domain wall speed and switching timescale versus bias voltage characteristics, but also the magnitude of transient negative capacitance in the (111) oriented La-doped $Pb(Zr_{0.4}Ti_{0.6})O_3$ ferroelectric capacitor. Ferroelectric capacitors undergo negative capacitive state during switching between two stable states of positive and negative saturation polarization both of which are associated with positive capacitance. The free energy – polarization energy landscape governs the switching process and depending on the landscape different switching pathways open up to reach the switched state. Bias voltage pulse profile – amplitude and frequency – determines the pathway followed and this, in turn, yields bias-voltage-pulse-profile-dependent transient negative capacitance. It, therefore, reflects the dependence of transient negative capacitance on domain switching kinetics. The switching process involves nucleation of reverse domains and their growth and the energy barrier associated with the switching process, therefore, varies depending on the switching pathway. The pathway of minimum energy barrier yields maximum domain wall density because of maximization of the nucleation sites resulting from minimization of energy barrier of nucleation. In a multidomain ferroelectric capacitor, maximization of domain wall density yields maximum transient negative capacitance (Fig. 1) since difference in polarization and polarizability between the domain and domain walls gives rise to negative capacitance. Phase-field simulation using time-dependent Ginzburg-Landau equation shows dependence of the domain wall density during switching on the bias voltage amplitude and its maximization at a specific bias voltage amplitude. The observation of maximum negative capacitance depending on domain switching pathway and kinetics has important implications in the context of different applications as, for example, it could be exploited to internally amplify the gate voltage in a negative-capacitance-field-effect-transistor (NC-FET) device for reducing the subthreshold swing (SS) 60 mV/decade or to develop electrostatic supercapacitors (comprising ferroelectric and dielectric capacitors) capable of producing enormous energy and power density.

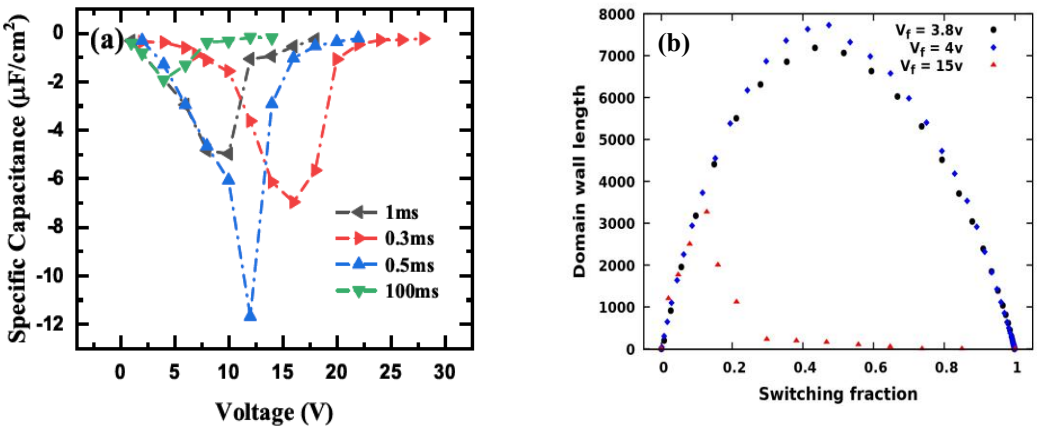

Fig. 1. (a) Variation of specific capacitance with applied voltage and time scale and (b) phase field study results of domain wall length as a function of switching fraction.

Coexistence of Negative Differential Resistance and Resistive Switching mediated by Phase change in a FeSFET Device

Indium Selenide (In2Se3) is recently discovered ferroelectric 2D semiconductor which holds immense potential in nanoelectronics and allied applications. The inherent polarization property along with semiconductor nature made it a desired candidate for FeS-FET(Ferroelectric semiconductor field effect transistor) , FTJ(ferroelectric tunnel junction), Different semiconductor heterostructures and non-volatile memory applications. All these works exploited the polarization property of In2Se3 which can be altered by applying external electric field. Along with tuneable polarization property it also exists in different polymorphs (Alpha, Beta, Gamma) which makes it a good candidate for Phase Change Memory devices. In this work for the first time, we observed the Coexistence of Negative Differential Resistance and Resistive Switching mediated by phase change in a In2Se3 based back-gated FeS-FET device. The observed NDR is also Gate tuneable and consistent with all temperature range. Since the discovery of the Esaki tunnelling diode, the negative differential resistance (NDR) effect has been widely applied in designing various devices such as logic switches, computer memory, and high-frequency oscillators. In addition to typical semiconductor-based tunnelling diodes vertically integrated two-dimensional (2D) layered van der Waals (VdW) heterostructures has also been used that involve the recently well-studied 2D transition metal dichalcogenides (TMDs) like MoS2-MoTe2, MoS2-WSe2, and MoS2-WSe2-graphene. However, to simplify the fabrication process and to have more practical applications in the future, it is better to possess the NDR effect at room temperature using a single type of material via a simple method. In this work we fabricated a planar transistor using Alpha phase Indium Selenide (2H- In2Se3) which is very much compatible with existing CMOS circuitry and process flow. Ferroelectric materials exhibit a spontaneous polarization in the absence of an external electric field. This polarization can be reoriented by ion displacement in the crystal, and polarization switching can be triggered by an external electrical field such that ferroelectric materials can have different conductance state. Our experiment shows that this NDR phenomenon occurs as an intermediate event during the switching process between two different conductance states. This Phase change assisted NDR phenomenon is quite different from other NDR devices in terms of mechanism. The subtle atomic configuration of the central Se atom in Se-In-Se-In-Se sequence leads to emergence of ferroelectricity in In2Se3 and a unique correlation between the Out-Of-plane and In-Plane dipoles. In our back-gated architecture we explored this interlocking between the OOP and IP polarization to achieve NDR and Resistive Switching through a vast range of Gate and Drain voltages. Further High-resolution TEM studies reveal the detailing of phase change process which includes Structural change of the material at different zones of the channel. To explore the possible changes in the microstructure TEM studies was done in Pristine sample as well as in samples after biasing with back-gate. A high density of stacking defects, along with Moire patterns were observed. Furthermore, Sliding between layers and dislocation of atoms were detected which could be associated with charged defects that couple to lateral electric field,. Such defects alters both carrier concentration and mobility leading to change of conductance along the channel. We also observed a unique zipping and unzipping mechanism between Van der wall layers in channel region. Diverse electrical measurements at different ambient conditions along with TEM studies in this work will be helpful to understand the actual mechanism of polarization modulation and future application of In2Se3 based nanoelectronics devices.

CMOS-Compatible $Hf_xZr_{1-x}O_2$ Ferroelectrics for Tunable Band-Pass Filters in Space Applications

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ABSTRACT

This project aims to develop ferroelectric-based thin films that function as band-pass filters within the microwave frequency range, with potential applications in satellite systems. The dielectric permittivity (ε) of ferroelectric materials is highly dependent on the applied electric field, enabling a tunable response. We have successfully grown Hafnium oxide with different doping of Zr ($Hf_xZr_{1-x}O_2$, HZO) and achieved ferroelectric orthorhombic phase. HZO is a CMOS-compatible ferroelectric with low-voltage tunability (~15% at < 10V), low dielectric loss, and stable behaviour at nanoscale (~10nm) thickness. HZO-based coplanar waveguide (CPW) filters have demonstrated reliable operation from kHz to GHz with low insertion loss, making them suitable for compact, low-power RF systems. (Fig.2)

To enhance overall tunability and voltage range, a complex perovskite ferroelectric $0.25BiFeO_3$–$0.30BaTiO_3$–$0.45SrTiO_3$ (BFBST)—was deposited on Nb:$SrTiO_3$ using pulsed laser deposition. CPW devices were fabricated and characterized using vector network analysis (S_{11}), showing dielectric tunability up to 72% at 200 V (2 GHz) with low loss tangent (<1). Combining HZO and BFBST enables a heterostructure filter design that offers both low-voltage operation and wide frequency tuning. This integration supports the development of reconfigurable, high-performance microwave filters for space communication and adaptive RF electronics.

Keywords: HZO, BFBST, tunable microwave filters, ferroelectric thin films, CMOS compatibility, satellite systems.

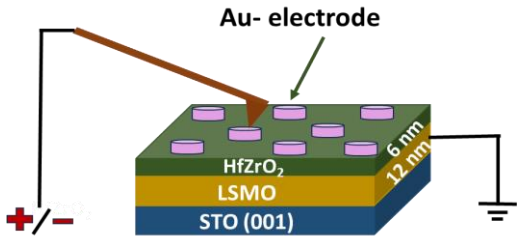

Fig.1

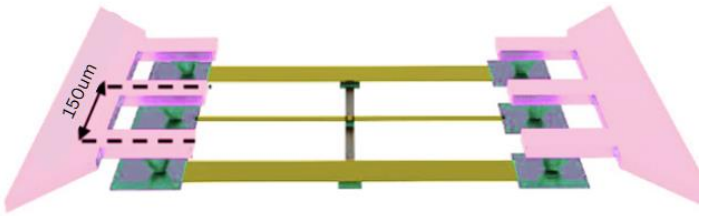

Fig.2

Fig.1 HZO/LSMO/STO ferroelectric thin film stack.

Fig.2 CPW band-pass filter with integrated ferroelectric varactors for voltage tunability.

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Enhanced Energy Storage Density in Lead-Free $Ba_{0.7}Sr_{0.3}TiO_3/Ba_{0.6}Sr_{0.4}TiO_3$ Multilayer Thin Films

(https://doi.org/10.1002/adem.202402610)

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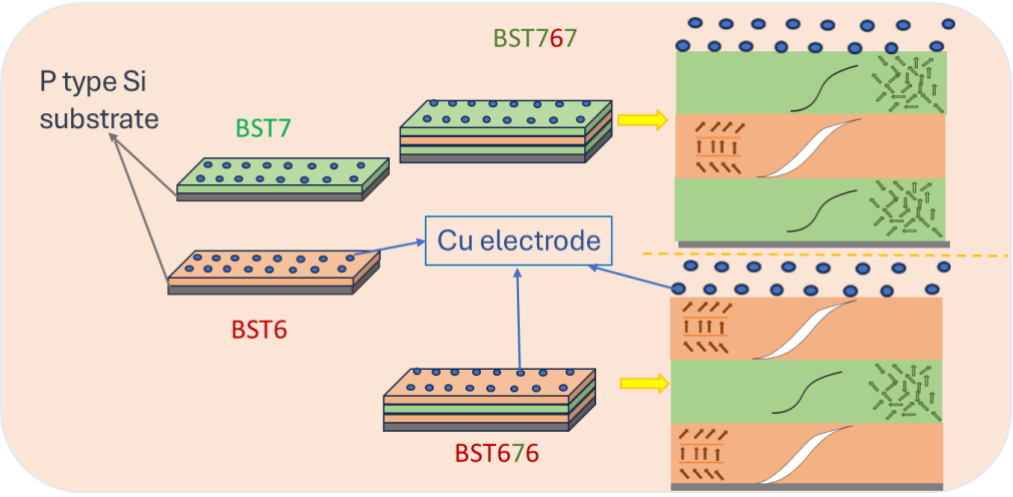
Ferroic thin films: structure-property correlations

Abstract

Lead-free dielectric thin-film capacitors are widely pursued for their promising applications in high-power electronic and electrical systems. However, achieving both high recoverable energy density (W_{rec}) and temperature stability remains a significant challenge. In this study, a trilayer structure comprising $Ba_{0.7}Sr_{0.3}TiO_3$ (BST7) and $Ba_{0.6}Sr_{0.4}TiO_3$ (BST6) is engineered using a solution-based process. The optimised BST767 configuration achieves an ultrahigh recoverable energy density of ≈56.9 J cm^{-3} and maintains ≈50 J cm^{-3} at 160 °C, with a high energy efficiency of ≈72%. The outstanding performance arises from electric-tree-assisted breakdown behaviour and pronounced interfacial effects, enhancing charge trapping and dielectric strength. The structure also demonstrates excellent stability under varying humidity and UV exposure. These results confirm the potential of BST-based multilayer systems for next-generation temperature-insensitive pulsed power and energy storage applications.



Schematic diagram of the fabricated monolayer and multilayer thin films

Energy Storage and Harvesting Potential of Eco-friendly Ca-substituted $Ba_{0.8}Sr_{0.2}TiO_3$/PVDF Ferro-Flexible Composite Films

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Abstract

Eco-friendly, lead-free $Ba_{0.8}Sr_{0.2}TiO_3$ based ferroelectric ceramics were synthesized via conventional solid-state sintering by substituting Ca^{2+} at the A-site, resulting in compositions of $Ba_{0.8}Sr_{0.2-x}Ca_xTiO3$ (x = 0, 0.06, 0.08). X-ray diffraction (XRD) analysis confirmed the formation of a tetragonal perovskite phase across all compositions. Notably, partial incorporation of Ca^{2+} at the Ti^{4+} site was observed in BSCT08, as evidenced by XRD and further supported by scanning electron microscopy (SEM). Among the compositions, BSCT06 exhibited optimal relaxor behavior, characterized by a slim P–E hysteresis loop with a remnant polarization (P_r) of 5.25 μC/cm². The same composition demonstrated a high recoverable energy storage density (W_{rec}) of 0.41 J/cm³ and an electrostrictive coefficient (Q_{33}) of 0.0223 m⁴/C². To explore energy harvesting applications, BSCT06 was incorporated into a PVDF matrix via solution casting to fabricate composite thin films. XRD patterns of the composites revealed characteristic γ-phase PVDF peaks along with reflections corresponding to the BSCT06 phase. The composite films showed enhanced mechanical flexibility under bending and twisting, and the relative permittivity increased with ceramic filler content. An improved dielectric breakdown strength (E_b) of 698 kV/cm was achieved in the 10 wt% BSCT/PVDF composite, compared to pure BSCT06 ceramic. The film also exhibited a W_{rec} of 0.31 J/cm³ with an energy efficiency of 48%, highlighting its potential for energy storage applications. Furthermore, a prototype piezoelectric energy harvester was fabricated using the ceramic-infused PVDF ferro-flexible films. The device incorporating 20 wt% BSCT/PVDF generated a peak-to-peak output voltage of ~9.3 V and a power density of ~2.86 μW/cm² under a known impact force, demonstrating its promise for use in self-powered sensors and energy harvesting systems.

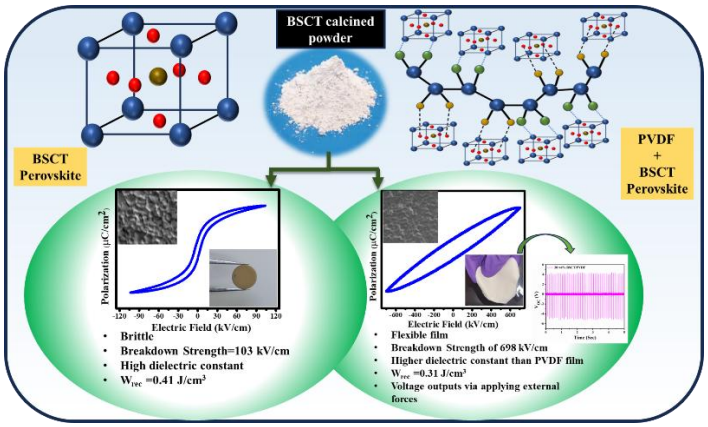

Figure 1. Graphical abstract of BSCT/PVDF composite film for energy storage and harvesting application

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Jena, L.K., Chahal, S., Sahoo, S., Boomishankar, R. and Asthana, S., 2025. Energy Storage and Harvesting Potential of Eco-Friendly Ca-Substituted Ba0. 8Sr0. 2TiO3/PVDF Ferro-Flexible Composite Films. *ACS Applied Electronic Materials*.

Emotion-Responsive Neuromorphic Behavior in $SrTiO_3$/Nb:$SrTiO_3$ Heterostructures

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Abstract

Neuromorphic systems emulate the functional principles of the human brain, offering promising routes toward adaptive, energy-efficient computing.[1–4] In this work, we demonstrate emotion-responsive neuromorphic behavior in epitaxially grown $SrTiO_3$ thin films deposited on Nb-doped $SrTiO_3$ substrates. The heterostructures exhibit memristive switching, synaptic plasticity, and dynamic conductance modulation under electrical stimuli—key features of neuromorphic hardware. Beyond conventional resistive switching, we integrate a framework for real-time emotion detection, where variations in input stimulus patterns representing different emotional states modulate the device's synaptic response. The observed behavior is primarily governed by electric field-driven oxygen vacancy dynamics and the interfacial charge transport across the $SrTiO_3$/Nb:$SrTiO_3$ interface. Our findings open new directions for the development of intelligent, emotion-adaptive systems leveraging complex oxide heterostructures.

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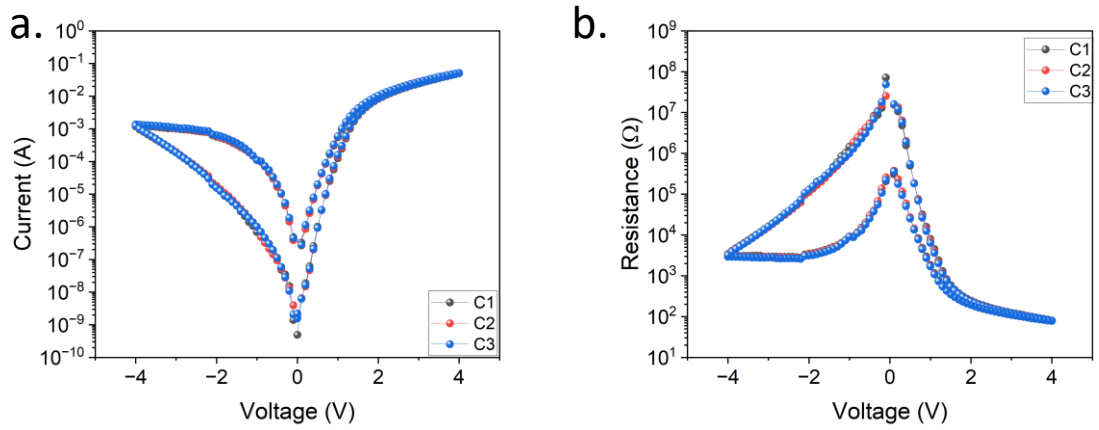

Figure 1 | **a.** Current–voltage (I–V) sweep measurements exhibiting clear resistive switching behavior. **b.** Corresponding resistance–voltage (R–V) sweep derived from the I–V data, further confirming the switching characteristics.

Strategies for Optimization of Negative Output Conductance and Gate-Induced Drain Lowering in Ferroelectric Negative Capacitance FET

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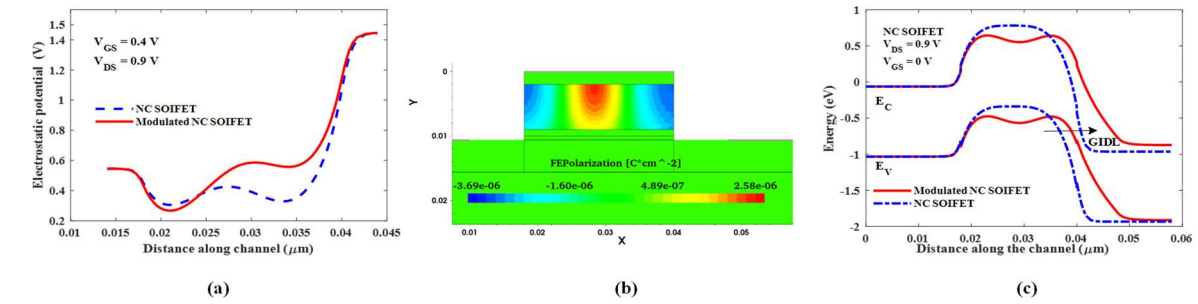
Abstract: The ferroelectric(FE) Negative capacitance (NC) Field effect transistor (FET) exhibits improved subthreshold swing, low power consumption, and enhanced drive capability. However, Negative Output Conductance (NOC) and Gate-Induced Drain Lowering (GIDL) in FE NC FET are undesirable in analog and low-power applications. This study proposes two strategies to mitigate/optimize NOC and GIDL in ferroelectric NCFET.



Ferroelectric NCFET (a) Surface potential modulation, (b) Enhanced ferroelectric polarization profile along the channel, (c) Drain doping modulation.

1. The gate metal work function of ferroelectric NCFET is tuned at the channel's drain end to modulate the channel's surface potential near the drain end. The modulated surface potential enhances ferroelectric polarization, which drops when the drain voltage increases at a particular gate voltage. The modulated electrostatic potential and enhanced ferroelectric polarization at the drain end optimize the NOC and improve GIDL compared to normal ferroelectric NCFET. Surface potential modulation improves the minimum and average subthreshold swing at a specific gate metal work function tuning, alongside optimizing the NOC and GIDL.

2. GIDL and NOC in ferroelectric NCFET are optimized using Drain doping modulation. Drain doping modulation improves ferroelectric polarization at the drain end of the channel, lowering the gate-to-drain coupling capacitance and improving NOC at higher drain voltages. The modulated drain doping reduces band-to-band tunneling (BTBT) and improves I_{GIDL}. The average subthreshold swing is improved compared to the conventional ferroelectric NCFET.

Keywords: Ferroelectric, Negative Output Conductance (NOC), Gate-Induced Drain Lowering (GIDL), Negative Capacitance FET (NCFET), Miller capacitance, surface potential, band-to-band tunneling (BTBT).

Abstract

Sub-Coercive Field Switching in Ferroelectric PZT Capacitors via Stochastic Resonance

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Stochastic resonance (SR) is a phenomenon in which the presence of noise enhances the response of a non-linear system to a weak sub-threshold signal as illustrated in Fig. 1(a). In bi-stable systems, SR can facilitate noise-assisted transitions between states, enabling signal detection or switching that would otherwise not possible. In this work, we leverage SR to achieve synchronous switching under sub-coercive electric fields in a ferroelectric lead zirconate titanate (PZT) thin-film capacitor. Fig.1(b) shows the PE loop of the ferroelectric PZT capacitor (V_c =2.1V and P_r = 17μC/cm^2) and Fig.1(c) shows the extracted double well using Landau model. Next, we apply sub-coercive voltage signal of amplitude 0.75V_c of different frequencies 75Hz with added white gaussian noise of varying standard deviation. The response of the PZT device under the application of noisy signal is shown in Fig.1(d)-(f). For low noise intensity: V_{rms} = 0.3V, the polarization (P) does not switch and modulates in a well that represents only the dielectric contribution to the P. On the other hand, at high noise i.e., V_{rms} = 2.56V the polarization switches randomly. However, at an optimum V_{rms} = 1.05V, the polarization switches synchronously (green) with the input weak sub-threshold noisy signal shown in red. We further confirm the point of SR by quantifying it through three metrics: Cross-covariance, output power and signal to noise ratio as shown in Fig1(g)-(i). This represents the point of stochastic resonance. This result shows how noise can be used positively to help detect or amplify weak signals in ferroelectric systems. Such a mechanism could be useful for designing low-power ferroelectric signal detectors in noisy environments, such as for weak signal recovery in communication systems.

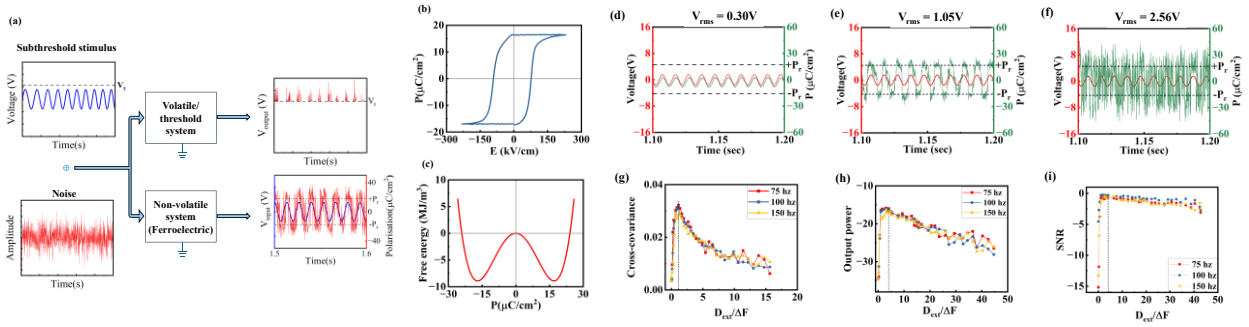

Figure 1. (a) Schematic of the stochastic resonance in a volatile/threshold and non-volatile bistable systems. (b) Polarization vs electric field hysteresis loop measured for our PZT device of area 4000 *mm*^{2}. (c) Free energy vs polarization plot representing the bistable potential well of the PZT device modeled using Landau theory. (d)-(e) Polarization switching at different noise intensity. (g)-(i) three different metric to quantify SR.

C-axis Oriented AlN Thin Films for High-Frequency Acoustic Resonator Applications

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Abstract

Aluminum Nitride (AlN), a group III-V compound semiconductor, has emerged as a promising material for next-generation microelectromechanical systems (MEMS), radio frequency (RF) components, and quantum technologies owing to its remarkable material properties. In this work, we report the deposition and characterization of highly c-axis-oriented wurtzite AlN thin films grown via reactive magnetron sputtering [1].Structural and surface analyses of the deposited films were conducted using X-ray diffraction (XRD), atomic force microscopy (AFM), and scanning electron microscopy (SEM). XRD confirmed the sharp and narrow (0002) peak, reflecting strong c-axis texture essential for high acoustic velocity and coupling efficiency. AFM and SEM further revealed smooth and densely packed grains with 60-80nm size, which are vital for minimizing acoustic scattering losses. To evaluate the dielectric and piezoelectric performance, electrical measurements such as current-voltage (*I-V*), capacitance-voltage (*C-V*), permittivity, and loss tangent (*tanδ*) were performed using a semiconductor device analyzer and vector network analyzer (VNA). The extracted dielectric constant was found to be in the range of 10–11, consistent with high-quality AlN thin films [2]. Figure 1(b) shows the resonance spectra of the high overtone bulk acoustic resonator (HBAR). We observe strong resonance responses spanning a broad microwave frequency band (from L band to X band). Such high-frequency devices with further device design optimization are suitable for Quantum Acoustodynamics applications such as quantum sensors, transducers, and memories.

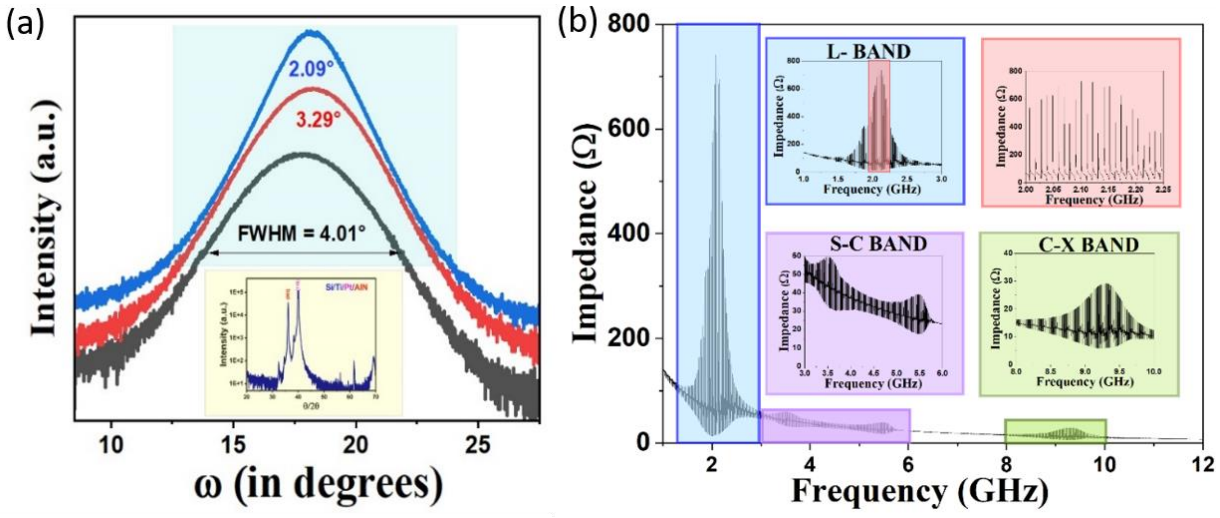

Fig.1. (a) Rocking curve (ω-scan) of AlN (002) peak deposited under different sputtering conditions showing improvement in c-axis orientation (intensity in log10 scale). (b) Resonance spectra of HBAR.

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A HYBRID MEMS - COMBINING PIEZOELECTRIC AND FERROELECTRIC THIN-FILM FUNCTIONALITIES

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Abstract: This paper introduces a new fabrication platform for the lateral integration of two distinct piezo/ferroelectric materials within a single circular PMUT. This leverages the high transduction efficiency of lead zirconate titanate (PZT) alongside the low permittivity of aluminum nitride (AlN) to optimize device performance. The concept is validated using the first resonant mode, showing higher output when AlN senses and unpoled PZT is driven with AC voltages compared to the reverse combination. Poled PZT is expected to further enhance performance.

Background: Piezoelectric materials differ in properties—high- piezoelectric coefficient (e) materials like PZT suit actuators, while low-permittivity (ϵ) materials like AlN are preferred for sensors. Hence, the figure of merit (FoM) for a resonator is given by the ratio e^2/ϵ. Achieving a good FoM in resonators requires balancing a large piezoelectric coefficient and low permittivity, and it is a challenge for single-material designs. Various approaches have been used to improve the FoM in resonators, including structural modifications and fabrication techniques. Integrating separate AlN and PZT devices enhances transceiver performance but increases the device footprint [1]. Recently, one study reported vertical stacking of PZT and ALN in a single resonator [2]. Here, we demonstrate a novel resonator design that improves transceiver performance by laterally stacking a ferroelectric material(PZT) with a high piezoelectric coefficient alongside a non-ferroelectric material(AlN) with lower permittivity, side by side within the same device.

Experimental Results: The electrical frequency response of the first mode was recorded using a lock-in amplifier, with simultaneous driving and sensing of unpoled PZT and AlN at varying AC voltages, as shown in Fig. 1(c). Interestingly, the results validate the proof of concept by demonstrating that the output electrical voltage is higher for PZT drive and AlN sense compared to the reverse combination.

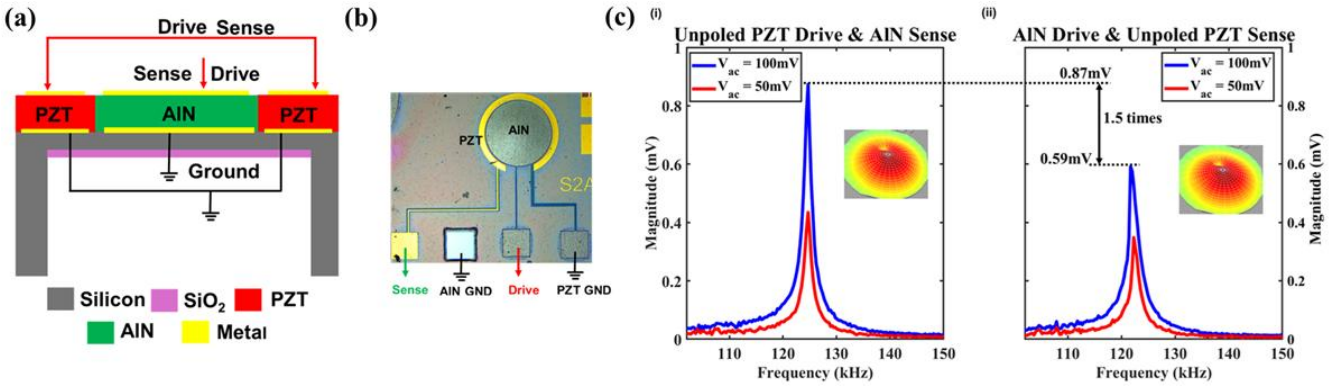

Fig. 1(a) *Schematic of cross-section of laterally stacked PMUT.* ***Fig. 1(b)*** *Optical Microscopic image of the fabricated device.* ***Fig. 1(c)*** *The electrical frequency response of the first mode of the laterally stacked PMUT using a Lock-in amplifier at different* AC *voltages without any DC bias, where PZT is not poled. (i) Driving the device using PZT and sensing by AlN (ii) Driving the device using AlN and sensing by PZT.*

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Unveiling ferrielectric and ferroelectric phases in $PbHfO_3$ thin films

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Abstract

While ferroelectricity is known to diminish in ultrathin ferroelectric films due to size effects, it is expected to emerge in ultra-thin anti-ferroelectric films, sparking researchers interest in using antiferroelectric materials as an alternative to ferroelectric materials for high-density data storage applications. $PbHfO_3$, the prototypical antiferroelectric, has been reported to exhibit ferroelectricity at the nanoscale; however, a fundamental understanding rooted in microstructural analysis remains elusive. Here, we investigate epitaxial $PbHfO_3$ films with thicknesses ranging from 50 nm to 200 nm. We discovered that film displayed a transition from antiferroelectric behaviour in the thicker films to ferroelectric behaviour in the thinner ones, intermediate thickness showing mixed phases. Moreover , we employed Piezoreponse force microscopy (PFM) to study the local electromechanical behaviour and distribution of ferroelectric and ferrielectric phase in $PbHfO_3$ thin films . These findings offer critical insight into the size-dependent polarization behaviour of antiferroelectric films and inform the design of nanoscale devices harnessing emergent polar phases

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Interfacial Compositional Analysis of Dielectric/Semiconductor Stacks Employing Electronic-Grade Metal Oxides

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Unavoidable interaction at the semiconductor/dielectric interface despite being both functional-inorganic materials such as metal oxides is mainly due to diffusion during thermal treatment. Although rapid thermal annealing step is performed to avoid the same, this also introduces undesirable metastable phases. In this investigation, we focus on the chemical compositional analysis of the interface formed by high-κ dielectrics and amorphous metal oxide semiconductors. This also becomes important in ferroelectric field effect transistors where ferroelectric/semiconductor interfaces are inevitable, the problem is severe for doped-hafnia ferroelectrics since the ferroelectricity is guided by the displacement of oxygen anions in the polar crystal. In this study, we investigate the role of the interface layer in Hafnium doped Aluminium oxide (HAO), Lanthanum doped Aluminium oxide (ALO)/Aluminium oxide (Al_2O_3), Zirconium Oxide (ZrO_2) deposited on to silicon wafer fabricated via the chemical solution deposition (CSD) method.. This work presents a systematic study aimed at correlating CSD processing parameters with the formation of different interfacial layers. The interfaces were characterized using X-ray Photoelectron Spectroscopy (XPS) to analyse compositional quality, while electrical behaviour was evaluated through capacitance–voltage (C–V) and impedance spectroscopy measurements.

Keywords: Dielectric, Interface layer, semiconductor , Heterostructure, Electro ceramics

Presenter: Mr. Dharnesh Alamanda

Electrical and Mechanical Switching of Ferroelectric Polarization in $BaTiO_3$ Ultrathin Films

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Electrically switchable spontaneous polarization in ferroelectrics has been in-depth explored in thin films for their potential application in non-volatile memory technology. The strong electromechanical coupling of ferroelectric polarization enables polarization switching through mechanical force, owing to the flexoelectric effect. In this study, we investigate electrical, mechanical, and coupled electromechanical switching of ferroelectric polarization in epitaxially grown ultrathin $BaTiO_3$ film using Piezoresponse Force Microscopy (PFM). An atomic force microscope (AFM) tip was employed to electrically and mechanically manipulate polarization with nanoscale precision. We systematically examined the influence of writing speed on both electrically and mechanically induced polarization switching and switching thresholds in terms of applied mechanical force and electric field under coupled electro-mechanical conditions. Additionally, using Scanning Kelvin probe force microscopy (SKPM), we investigated the role of surface charge accumulation and back-switching behavior influenced by related residual depolarization fields. These findings comprehensively contribute to the fundamental and pragmatic understanding of electro-mechanical polarization switching in ferroelectric thin films and offer prospects for their future integration into nanoelectronic and nanoelectromechanical systems.

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High Dielectric Tunability in Lead-Free $Ba_{1-x}Sr_xTiO_3$ Thin Films

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ABSTRACT

Lead-free $Ba_{1-x}Sr_xTiO_3$ (BST) thin films exhibit exceptional potential for advanced dielectric applications. This study demonstrates ultra-high dielectric tunability (~91%) with a high breakdown electric field (~800 kV/cm) and low loss (Fig.1A). Remarkable thermal stability (>473 K) and frequency stability (>1 MHz) were achieved through precise engineering of strain, composition, and thickness. The films exhibit relaxor ferroelectric behavior, with a diffused phase transition and low leakage current density, enabling clear ferroelectric hysteresis loops. Integration of BST films onto silicon substrates further highlights their scalability and industrial relevance.

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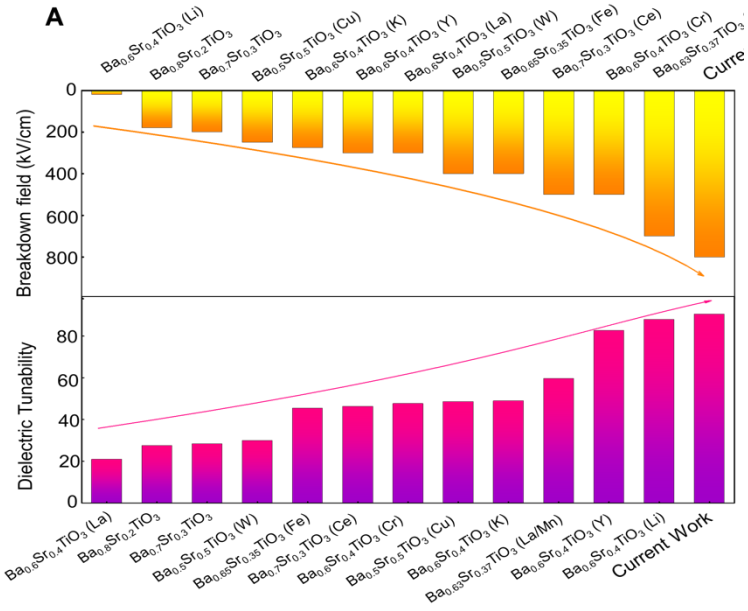

Fig.1: A, Comparison of dielectric tunability and breakdown electric field in the current work and other commonly used ferroelectric materials.

Facile Room-Temperature Synthesis of α-Quartz-like GeO_2 from Amorphous GeTe

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We successfully synthesized α-quartz-like GeO_2 microcrystals through a facile room-temperature sputter deposition of GeTe followed by exposure to an extremely high humidity (RH95%) environment. Spontaneous crystal growth was observed on the surface of the films, within few hours. Experiments were then conducted under varying substrates, duration and light exposure. Comprehensive characterization using X-ray Diffraction (XRD), Raman spectroscopy, and Scanning Electron Microscopy with Energy-Dispersive X-ray Spectroscopy (SEM-EDS) confirmed the formation of GeO_2 in the α-quartz phase. PFM was also done to check the peizoresponse of the microcrystals. This straightforward approach presents a novel low-temperature pathway for the synthesis of crystalline GeO_2 with potential applications in optics and electronics.

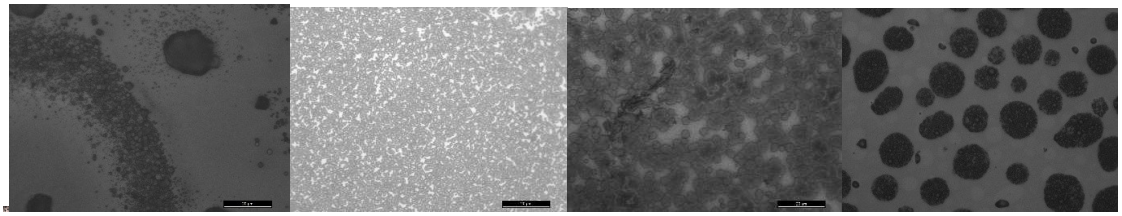

Fig. Optical Images of crystals

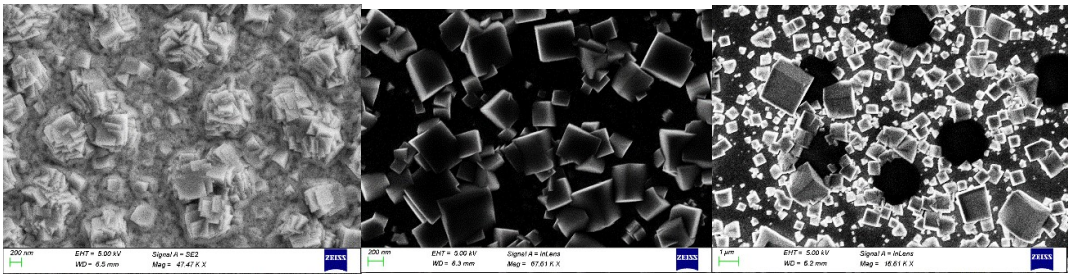

Fig. SEM Images of crystals

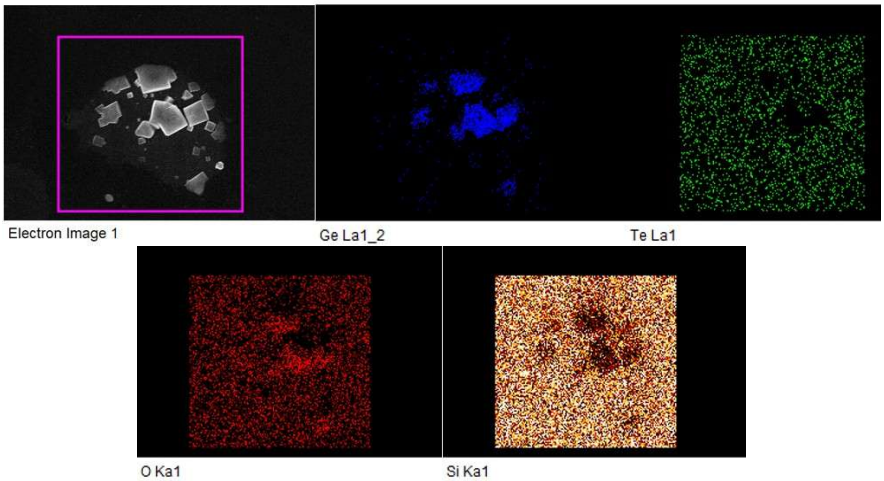

Fig. SEM EDS map of crystals

Sol–Gel Deposition and Rapid Thermal Annealing of Ferroelectric HfO_2 Thin Films on TiN-Coated Silicon Substrates

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Abstract

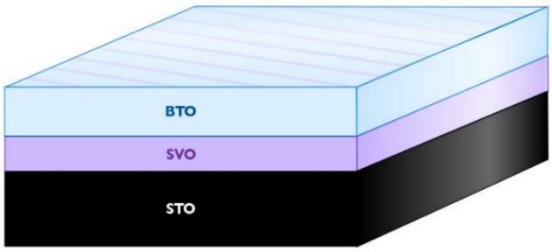
Ferroelectric Hafnium Oxide (HfO_2) has emerged as a next generation promising material for Non-Volatile memories, logic devices and neuromorphic computing due to its compatibility with CMOS processes, scalability down to nanometre thicknesses and robust ferroelectric properties even in ultrathin films. Unlike conventional perovskite-based ferroelectrics, HfO_2 offers enhanced thermal stability and process integration benefits. To enable efficient electrical characterization and device integration, titanium nitride (TiN) is commonly used as a bottom electrode owing to its high electrical conductivity, chemical stability, and ability to act as a barrier layer. In this work, a sol–gel method is employed for the deposition of ferroelectric HfO_2 thin films, providing a low-cost, scalable, and compositionally tuneable route to fabricate high-quality films. This approach enables uniform deposition over large areas and facilitates control over the film's microstructure, which is critical for optimizing ferroelectric performance.

In this study, titanium nitride (TiN) thin films were deposited on silicon substrates using RF sputtering, achieving uniform coverage with excellent electrical conductivity, as evidenced by a low sheet resistance in the range of 2–3 Ω/sq. A sol–gel precursor solution of HfO_2 was then synthesized and spin-coated onto the TiN surface, forming thin films with a thickness of approximately 40–50 nm. Post-deposition, the films underwent rapid thermal annealing (RTA) at various temperatures to induce the formation of the orthorhombic phase, which is essential for stabilizing ferroelectricity in HfO_2. The role of RTA was found to be critical in optimizing the crystalline phase and enhancing the ferroelectric response, making it a key step in achieving the desired functional properties.

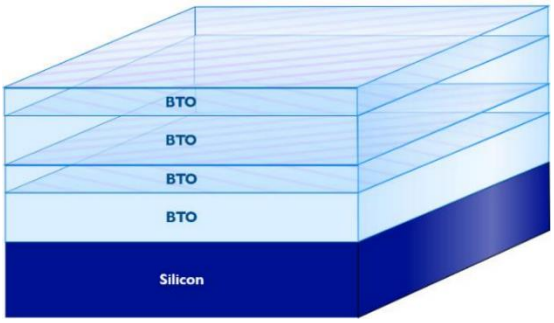
Heterogeneous Integration of Complex Epitaxial Oxides on to Silicon

Author: Jishnu NK, Asraful Haque, Pavan Nukala

Twisting angles in perovskite moiré structures provide a powerful way to engineer lateral strain modulations in nanoscale ferroelectric thin films, driving the emergence of high-density polarization vortices[1]. At certain “magic” twist angles, materials can exhibit properties like superconductivity, exotic magnetic states, and unusual electrical conductivity[2]. These phenomena arise because the atomic lattices align in a way that strongly influences electron interactions, leading to entirely new physical behaviors[2]. Heterogenous integration of complex epitaxial oxides is crucial for developing moiré patterns with functional oxides on conventional Si substrates. Such heterogenous integration of functional oxides by layer transfer technique and successful functional testing has been already demonstrated[3][4]. In this project this novel fabrication method is utilised to create moiré structures of Barium Titanate (BTO) on silicon substrates using a layer-by-layer transfer technique. Our approach utilizes Strontium Vanadate (SVO) as a water-soluble sacrificial buffer layer on top of Strontium Titanate (STO) substrate to epitaxially grow and transfer the BTO layer. Therefore, optimising the quality of SVO layer is crucial for the epitaxial growth as well as efficient transfer of BTO layer. So we have systematically explored the parameter space of Pulsed Laser Deposition (PLD) which includes fluence, target substrate distance, oxygen partial pressure and annealing time to optimize the SVO layer deposition. This presentation discusses the results obtained by optimization of various parameters for the deposition of SVO buffer layer.



BTO deposited on top of sacrificial buffer layer(SVO)



Heterogenous integration of epitaxial BTO layers on Si substrate

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Understanding strain relaxation behaviour in epitaxial neodymium nickelate thin films

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ABSTRACT

Perovskites $ReNiO_3$ (Re = Nd, Sm, Eu etc.) have attracted significant interest due to their fascinating magnetic, optical, and transport properties, including a metal-insulator transition (MIT) occurring within a broad temperature range of 100K to 500K. Among these, $NdNiO_3$ (NNO) shows temperature driven 1st order orthorhombic metallic to monoclinic insulator phase transition around 200K [1] and the MIT can be tuned by the application of chemical doping, epitaxial strain, etc [2]. Nickelates are typically unstable because of high ionization energy of Ni^{3+} ions, which makes it challenging to stabilize the NNO in perovskite structure. This often leads to the formation of secondary phases or oxygen-deficient structures. Strain engineering in epitaxial thin films offers an additional degree of freedom, allowing for stabilization of the desired phase and tuning of the MIT by modifying bond lengths and bond angles in the Ni–O–Ni network, which directly influences electronic bandwidth and correlations.

In this work, we have optimised NNO thin films with different thickness on $LaAlO_3$ (LAO) (001) and $(LaAlO_3)_{0.3}(Sr_2TaAlO_6)_{0.7}$ (LSAT) (001) single-crystal substrates using pulsed laser deposition. Thin films are characterized using X-ray diffraction and Raman studies and are found to be epitaxial in nature. Raman spectra show that lower-thickness film is in the perovskite phase; however, an additional phase appears for NNO/LAO with increasing thickness. The microscopic crystal structural the films are studied further using high-angle annular dark field (HAADF) imaging in an aberration-corrected scanning transmission electron microscope (STEM). It confirms the epitaxial growth of NNO/LAO thin film with a very sharp interface up to 10 nm. Resistivity (ρ) vs temperature (T) studies depict that all the films are metal at room temperature. However, strain-induced phase transitions are observed at lower temperatures: around 100 K for 6 nm NNO/LAO and 150 K for 6 nm NNO/LSAT. Electron energy loss spectroscopy (EELS) confirms the presence of $NdNiO_2$ as a secondary phase, in agreement with the Raman spectroscopy results. Recently, superconductive behavior has been found in $NdNiO_2$ thin film prepared by reducing the NNO [3].

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Understanding the Interface in Transparent Conducting Oxides with Dielectric and Semiconductor Capping Layers

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[*]*Corresponding Author*

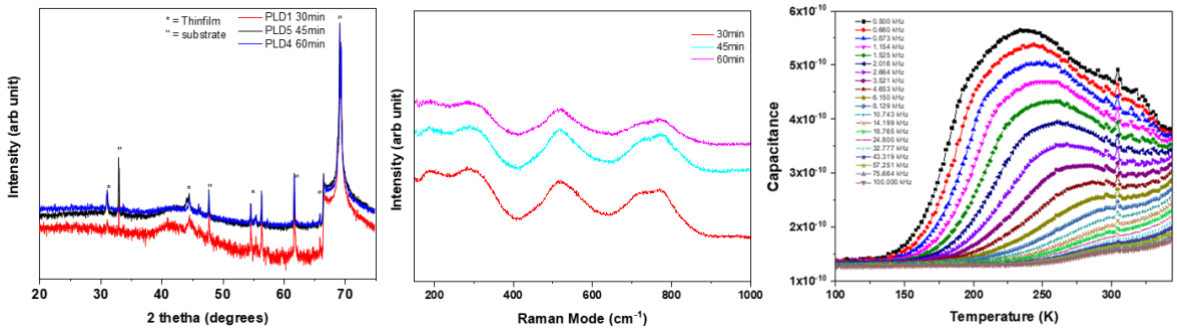
The study of transparent conducting oxide (TCO)/metal oxide(dielectric) interfaces is crucial due to the significant impact these interfaces have on the electrical and optical properties of TCOs. In this investigation, we focus on the interfacial characteristics of dielectric-capped TCOs. Highly conductive Aluminium-doped zinc oxide (AZO) thin films were developed via a low-cost, solution-based spin coating technique. These TCO layers were subsequently capped with dielectric materials such as Aluminium oxide (Al_2O_3) and Zinc oxide (ZnO). The interface quality and elemental composition were characterized using X-ray Photoelectron Spectroscopy (XPS), while the electrical performance of the multilayer structures was evaluated through four-point probe conductivity measurements. This study aims to provide insights into the role of dielectric capping in modulating the interfacial properties and electrical behaviour of TCOs.

Keywords: Dielectric, Interface layer, Semiconductor, Transparent Conducting Oxide, Thin films, Electro ceramics

Presenter: Mr. Mahiman Bansal

Temperature and Frequency-Dependent Field Effects on Polar States in $BaHf_{0.6}Ti_{0.4}O_3$ Thin Films

Relaxor ferroelectrics (FE) have attracted significant interest due to their distinct polarization characteristics and functional properties. Among them, lead-free relaxors, especially those based on barium titanate ($BaTiO_3$, BTO), are particularly promising due to their non-toxic nature, high dielectric permittivity, multiple phase transitions, and the ability to bring the transition temperature near room temperature. Notably, doped BTO materials exhibit relaxor behavior even without charge disorder. The distinctive frequency dispersion of dielectric constant values in relaxors has been attributed to the presence of polar nanoregions (PNRs). Recent findings in bulk polycrystalline $BaSn_{0.3}Ti_{0.7}O_3$, similar to BZT relaxors, reveal an intermediate temperature where structural modifications occur, aligning with numerical predictions. However, experimental studies investigating the effects of ac- and dc-fields on BTO-based relaxors are limited. This limitation is partly due to the difficulty of achieving the high electric fields required to identify polar states in bulk materials. Thin film studies may offer valuable insights into understanding the impact of these fields on barium titanate-based relaxors. To explore the effects of ac- and dc-fields as functions of both temperature and frequency to investigate the nature of the polar state in 40% Hf-doped BTO ($BaHf_{0.4}Ti_{0.6}O_3$) thin films were deposited on p-Si and Pt-si substrates. In the present work we report their basic characterization such as x-ray, Raman spectroscopy and dielectric measurement (shown in figure).



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Manipulations of multiferroic topology in self-assembled BiFeO3

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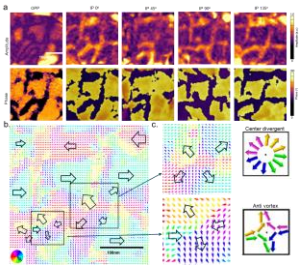
Abstract:

Self-assembled nanostructures in multiferroic materials are emerging as a frontier for advanced spintronic and nanoelectronics applications. However, effectively controlling and utilizing their complex topological features for practical device integration remains a significant challenge. In this study, we employed Reflection High-Energy Electron Diffraction (RHEED)-assisted pulsed laser deposition to grow $BiFeO_3$ (BFO) thin films on $LaAlO_3$ (LAO) substrates. The topography image confirms the formation of rectangular-shaped Nano islands. Electrostatic and boundary conditions give rise to stable topological features, such as center-convergent and center-divergent vortices and antivortices. Remarkably, we demonstrate that the application of a trailing electric field allows precise manipulation of these topological entities, including the merging and splitting of domain structures. Additionally, we show that pulsed electric fields can locally control these topological features with high precision. Moreover, DART SS-PFM reveals well-defined regions of distinct cohesive electric field and imprint field. Finally, we illustrate how the presence or absence of oxygen vacancies significantly influences the conductivity of nano-islands. Our results set the stage for the design of highly responsive, energy-efficient multiferroic devices with applications in memory and logic devices, paving the way for the next generation of smart materials.



Structural characterization of self-assembled BFO nanostructures. a, Vertical and lateral PFM images (at different angles 0º,45 º,90 º and 135º) confirm both out-of-plane and in-plane polarization components. **b,** Reconstructed Vector PFM using IP PFM Images, and **c,** reconstructed polarization vector map, indicating topologically nontrivial polarization textures like centre divergent Vortex and Antivortex.

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CMOS Compatible Ferroelectric Devices Featuring Amorphous Oxide Semiconductor Layer

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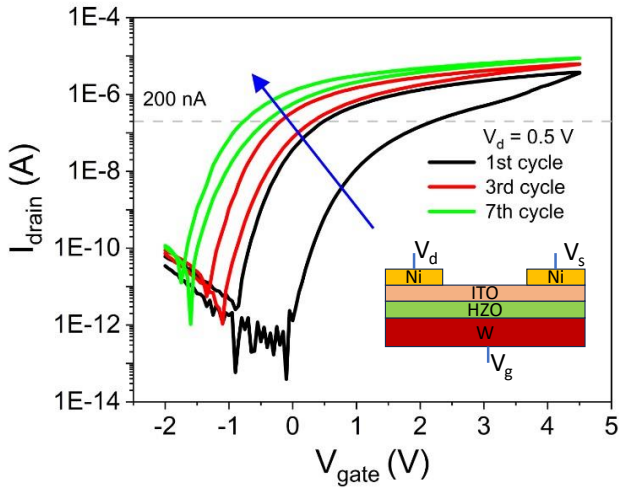
EE, IIT Bombay, Mumbai, India

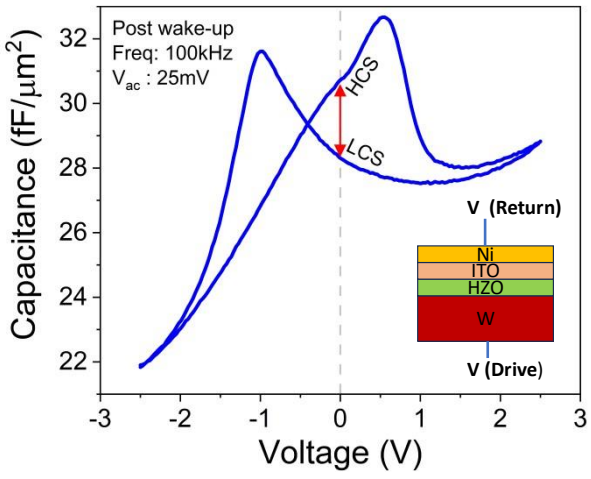
Abstract: -

Hafnium oxide based ferroelectric devices are emerging as low power embedded non-volatile memories. Owing to low crystallization temperature of $Hf_{0.5}Zr_{0.5}O_2$ (400-450°C), it is primary choice for ferroelectric devices that can be integrated on top of CMOS transistors in the back-end-of-line (BEOL). Among the various device architectures compatible with CMOS BEOL, ferroelectric capacitors and field-effect transistors (Fe-FETs) are gaining technological maturity. The BEOL integration requires, channel material with reasonable mobility (10-100 cm^2/V-s). Also, the capacitors need to allow non-destructive read out for technological applications. However, these two aspects have device level challenges. In this work, we demonstrate and analyse the electrical performance and cycling reliability of long-channel ferroelectric field-effect transistors (Fe-FETs) featuring a 10 nm $Hf_{0.5}Zr_{0.5}O_2$ (HZO) ferroelectric gate integrated with a thin 3 nm indium–tin–oxide (ITO) channel. While the Fe-FETs achieving a sizable memory window (MW) of approximately 1.7 V, repeated measurement cycles cause rapid degradation of this memory window, which is accompanied by a noticeable leftward shift in the threshold voltage. We will discuss the role of domain pinning particularly in context of oxide channel Fe-FETs that leads to such an observation and challenges to device operation.

We will also show metal–ferroelectric–semiconductor–metal (MFSM) capacitors fabricated alongside these Fe-FETs that demonstrate a robust capacitive window of approximately 3 fF/µm² between high capacitance state (HCS) and low capacitance state (LCS) post wake-up. This robust and stable capacitive contrast highlights significant potential for MFSM capacitors in capacitive-based non-volatile memory readout schemes, enabling low-power, scalable, and high-density memory array architecture.

These combined results provide critical insights into long-channel Fe-FET reliability and illustrate promising directions for capacitive sensing-based memory architectures.





Electric field-driven polarization extension phenomenon in multiferroic oxide

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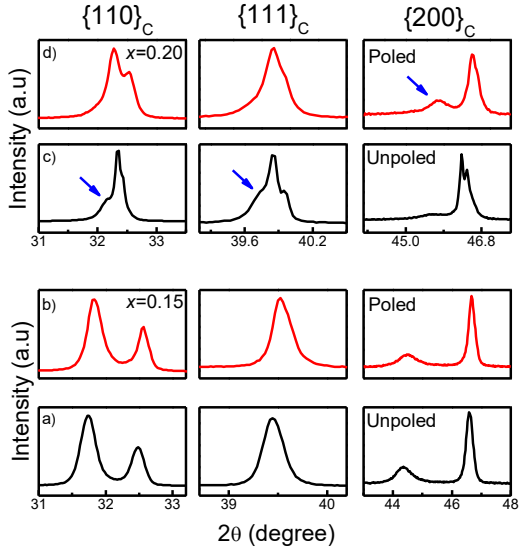
Abstract

A novel multiferroic solid solution of (1-*x*)$PbTiO_3$-(*x*)$TbFeO_3$, within the range of $0.0 \leq x \leq 0.25$, have been investigated. A composition-induced phase boundary from the tetragonal to the cubic phase is identified at $x = 0.20$. At this boundary composition, significant enhancements in ferroelectric properties ($P_r \sim 17$ μC/cm²), piezoelectric responses ($d_{33} \sim 130$ pC/N), and magnetic characteristics (~0.03 emu/g) are observed. Structural analysis reveals a coexistence of ferroelectric (Tetragonal: *P*4*mm*) and paraelectric (Cubic: *Pm*-3*m*) phases at the boundary composition. An electric field-dependent structural study indicates that these mixed phases transition to a single ferroelectric *P*4*mm* phase. An electric field-dependent structural study reveals that these mixed phases transform into a single ferroelectric *P*4*mm* phase. This transformation mechanism is associated with a one-dimensional change in polarization along the $[001]_C$ direction, following the polarization extension phenomenon.

Key words: Multiferroic materials, Piezoelectric coefficient, X-ray diffraction, Phase transformation.



X-ray powder diffraction Bragg's profiles of unpoled and poled samples of (1-*x*)$PbTiO_3$-*x*$TbFeO_3$ solid solution: a) Unpoled of x = 0.15, b) Poled of x = 0.15, c) Unpoled of x = 0.20, and d) Poled of x = 0.20.

Structural studies under an electric field demonstrate that these mixed phases fully convert into a single tetragonal phase. Specifically, after poling, 51% of the cubic phase transforms into the tetragonal phase, resulting in a predominantly tetragonal structure.

Epitaxial growth of AlN & AlScN on TiN(111) buffered Si (111) by Pulsed Laser Deposition

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Advisor: Prof. Pavan Nukala
Centre for Nano Science and Engineering, IISc

Abstract

AlN, a wurtzite crystal structure, is a piezoelectric material that can withstand high temperatures where other conventional piezoelectric materials reach their Curie temperature. The high-temperature stability and moderate d_{33} coefficient make them compatible with semiconductor processing. AlN's high acoustic velocity, moderate Electromechanical coupling coefficient (K_t^2 of 6-7 %)[2] and High-Quality factor find their applications in high-frequency filters, oscillators and resonators. But AlN polarity can't be switched under an electric field before its breakdown. Alloying with Sc can make AlN switch its polarity at fields below its breakdown field, making it a ferroelectric and increasing AlN functionality. Using Pulsed Laser Deposition, I have epitaxially grown AlN and AlScN thin films on TiN (111) buffered Si (111).

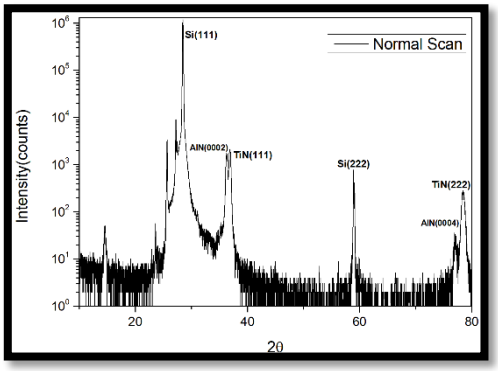
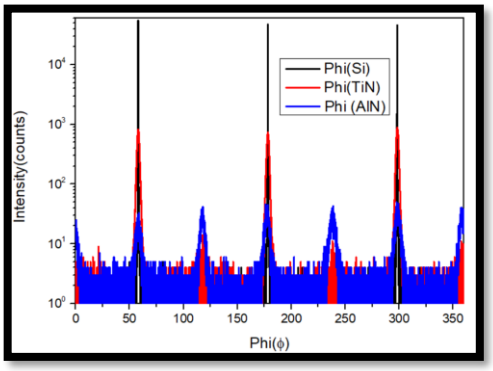


Fig. above. *Normal scan of AlN (0002)/TiN (111)/Si (111(which has the same orientation in out of the plane direction, please see...other peaks which are unindexed next to Si (111) are its K_β peaks).* ***Fig below*** *is a Phi scan of Si (004), TiN (002) and AlN (10-13), which have the same orientation relationship in the off axis.*

Growing AlN/AlScN on silicon is essential for integrating piezoelectric & ferroelectric functionalities into existing CMOS technology. A buffer layer is required to integrate functional nitrides (AlN) on Si, which can provide epitaxy and act as a bottom contact for vertical electric field measurements; one such material is TiN. I have optimised epitaxial Titanium Nitride (111) on Si (111) using pulsed laser deposition (KrF Laser, Fluence of 4.5 J/cm^2, repetition rate: 20Hz, pulse width: 25ns) in an in-house developed chamber that can go to low base pressures of 1e-6 mbar. We have used a strip heater setup to resistively heat the Si substrate(p++)to deposition temperatures (850°C, 950°C,1050°C).



On TiN/Si, using an Aluminium Nitride ceramic target, I deposited AlN thin films using pulsed laser deposition in the N_2 atmosphere (in the same chamber as TiN growth) using similar growth parameters as TiN growth. I have epitaxially grown AlN films on TiN buffered Si (111) [Epitaxial relation: AlN (0002)//TiN (111)//Si (111) (out of plane) & AlN [11-20]//TiN [1-10]//Si [1-10] (in-plane)]. Electromechanical and electrical measurements are performed to confirm that the AlN thin film grown is highly resistive and capacitive, and its d33 is nearly 2.5pm/V at 3 kHz. Later, using $Al_{0.3}ScN$ ceramic target, I have deposited AlScN thin film on TiN (111) buffered Si (111) substrate and confirmed its epitaxial growth using Normal scans & Phi scans. Electromechanical measurements on these films resulted in a d_{33} value of nearly -6.2 pm/V at 3 kHz (Nearly two and a half times increment in d_{33} at 30% Sc alloying content)

Abstract

Rahul Lakra

Freestanding Single-crystalline complex oxide membranes have emerged as a promising platform for exploring intrinsic material properties, owing to their elimination of substrate clamping effects. A critical step in fabricating such membranes involves the growth of the desired functional oxide atop a water-soluble buffer layer, typically strontium aluminate (SAO), which enables the release of the thin film from the substrate. In our study, we employ the Sol-Gel method to synthesize SAO buffer layers on strontium titanate (STO) substrates, focusing on the growth chemistry and material characterization of SAO.

Given SAO's high reactivity to moisture, even brief exposure to ambient air can lead to its decomposition. To address this challenge, we investigate various protective strategies to enhance the stability of SAO, ensuring sufficient preservation for subsequent structural characterization. Furthermore, we assess the epitaxial growth and crystalline quality of SAO films, aiming to optimize conditions for high-quality freestanding oxide membranes.

Precision-Transferred Flaky Hafnia Ferroelectric/High- κ Dielectric Heterostructures

Rahul Tiwari[1], *Dharnesh Almanda*[1], *Tribhuvan Kushwaha*[1], *Pavan Pujar*[*]

Emerging Electronic Materials and Devices Laboratory, Department of Ceramic engineering, IIT(BHU), Varanasi, 221005, Uttar Pradesh

The integration of ferroelectric materials with high-k dielectrics is central to the advancement of low-power and high-density nanoelectronics devices.[1] In this contribution, we present a mechanical transfer of flaky ferroelectric doped-hafnia and high-permittivity (κ) dielectric heterostructures for high performance electronics such as negative capacitance field effect transistors. Bulk-synthesized $Hf_{0.5}Zr_{0.5}O_2$ (HZO) flakes are mechanically exfoliated and deterministically transferred onto desired platforms such as silicon, glass, or flexible polymers. [2-3] This method enables clean, selective, and low-temperature integration, eliminating the need for high-vacuum processing or complex lithographic patterning. The transferred ferroelectric flakes retain their desired phase, exhibiting acceptable ferroelectric polarization, with marginal leakage current. Furthermore, when coupled with high-k dielectrics such as Al_2O_3 or ZrO_2, the resulting heterostructures show enhanced interface quality and dielectric performance, opening pathways for their use in FeFETs, MFM capacitors, and neuromorphic devices. The precision transfer of dielectric onto the pre-transferred HZO opens possibility of compound dielectrics/ferroelectrics approaches for futuristic electronics. This study demonstrates the effectiveness of the 2D transfer platform for engineering complex ferroelectric/dielectric architectures, offering a reliable and CMOS-compatible route.

Keywords: Ferroelectric, dielectric, Precision 2D transfer System, Heterostructure, Electroceramics

Presenter: Mr. Rahul Tiwari

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Influence of Nitrogen flow on CMOS compatible Sputtered Aluminium Nitride Thin Films for Piezoelectric Applications

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Abstract: Aluminum nitride (AlN) thin films are reactively sputtered on Si (111) substrate at low temperature (300 °C) for piezoelectric-based device applications. AlN thin films grown on Molybdenum coated Si (111) substrate with AlN-interlayer confirm the highly *c*-axis orientation for all the Nitrogen flow rates concentrations of 12.5% to 100%. The observed *c*-axis orientation in all the samples may be due to the higher sputtering power of 175 W. However, varied nitrogen concentration induces residual stress in the thin film. The lattice constant *c* was found to be lowest for the thin film grown with 37.5% of nitrogen concentration, and the estimated in−plane stress was in tensile state along with 50% nitrogen concentration. Compressive in−plane stress was observed in all other thin films grown. The FE-SEM surface view shows AlN thin films grown at 37.5% and 50% nitrogen have small circular grains with higher density, and cross-sectional view confirms the compact and columnar grain growth with smooth grain boundaries. The films grown at 12.5% and 25% have shown pebble like and triangular shape morphology respectively and columnar growth observed with broader grain boundaries. However, nitrogen concentration of 62.5% and above resulted in circular small grains with disordered columnar growth. The surface roughness (0.39 nm) and low leakage current were also found in thin film grown at 37.5% of nitrogen concentration i.e., 1.17×10^{-5} A/cm^2 measured at 100 kV/cm. This confirms the reduced defect densities. Therefore, AlN grown at low temperature 300 °C with 37.5% N_2 is suited for the complementary metal oxide semiconductor (CMOS) process based piezoelectric devices.[1][2]

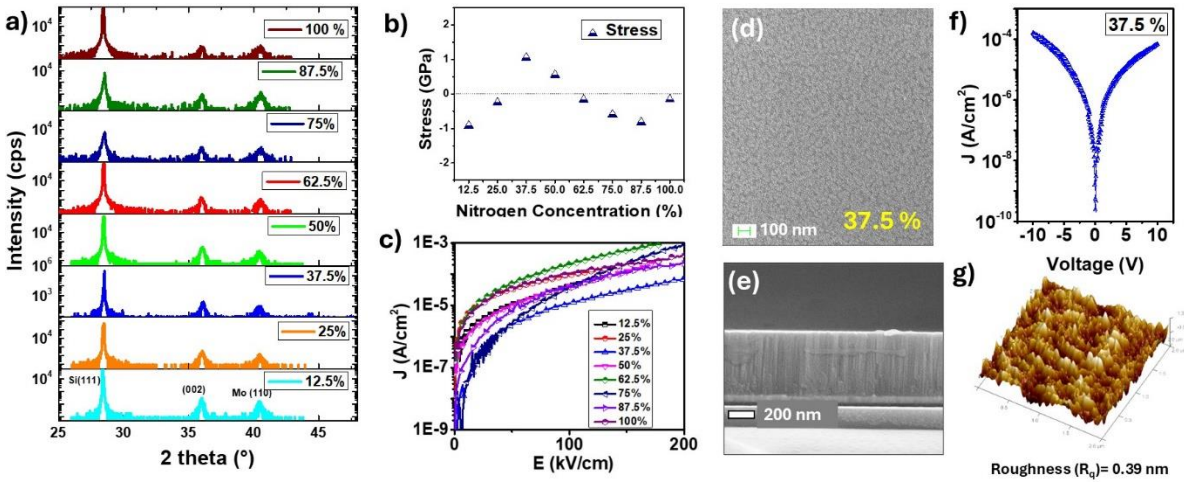

Figure 1. a) XRD Plot, b) Stress c) current vs electric field of MIM devices of AlN thin films sputtered deposited at different nitrogen flow rate, d) FE-SEM image top view and e) cross section view, f) JV curve g) AFM topography of 37.5% AlN

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Strain-Engineered Suppression of Meta-Magnetic Transition and Its Effects on Magnetocaloric Effect in Multiferroic Dy_2NiMnO_6 Thin Films

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Abstract

Double perovskites with the general formula $A_2BB'O_6$ have garnered considerable attention due to their rich interplay of spin, charge, and lattice degrees of freedom. Among existing double perovskites, Dy_2NiMnO_6 (DNMO) is known to exhibit type-II multiferroicity along with high magnetic entropy.[1,2] The co-existence of these two properties provides a unique platform for on-chip solid-state cooling technology. DNMO thin films are particularly appealing as they enable miniaturization, paving the way for potential device applications. Along with this, they also provide control over strain, which can be used to tune ferroelectric polarization, magnetoelectric coupling, magnetic, and magnetocaloric properties. The primary focus of our study is to enhance magnetocaloric efficiency in double perovskite thin films. Many double perovskites undergo first-order transitions due to field-induced metamagnetic transitions, which result in energy loss due to thermal hysteresis. One effective strategy to address this issue is to modify the magnetic interactions in double perovskite materials. In this work, we report the suppression of the meta-magnetic transition in DNMO epitaxial thin films grown on $SrTiO_3$ and $LaAlO_3$ using a pulsed laser deposition technique. Both thin films DNMO/$SrTiO_3$ and DNMO/$LaAlO_3$ show second-order transitions with $-\Delta S_M$ values 12.76 J/ kg-K and 10.386 J/ kg-K, respectively. In contrast, DNMO bulk shows a first-order transition with $-\Delta S_M \approx 14.17$ J/ kg-K. The change in the order of transition from the first order to the second order in thin films allows the thin films to work over multiple cycles with minimal thermal hysteresis loss. DFT calculations were performed to confirm the effect of strain on the magnetic ground state. The suppression of meta-magnetic transition in thin films is owing to the fact of weakening of Dy-Ni/Mn interactions, due to the change in Ni-Mn magnetic interactions from strain. Furthermore, our finding of suppressing the meta-magnetic transition in DNMO thin films opens a new avenue for enhancing the magnetocaloric properties of rare-earth-based double perovskites in multiferroic thin films.

Abstract

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Understanding the Interface in Transparent Conducting Oxides with Dielectric and Semiconductor Capping Layers

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The study of transparent conducting oxide (TCO)/metal oxide(dielectric) interfaces is crucial due to the significant impact these interfaces have on the electrical and optical properties of TCOs. In this investigation, we focus on the interfacial characteristics of dielectric-capped TCOs. Highly conductive Aluminium-doped zinc oxide (AZO) thin films were developed via a low-cost, solution-based spin coating technique. These TCO layers were subsequently capped with dielectric materials such as Aluminium oxide (Al_2O_3) and Zinc oxide (ZnO). The interface quality and elemental composition were characterized using X-ray Photoelectron Spectroscopy (XPS), while the electrical performance of the multilayer structures was evaluated through four-point probe conductivity measurements. This study aims to provide insights into the role of dielectric capping in modulating the interfacial properties and electrical behaviour of TCOs.

Keywords: Dielectric, Interface layer, Semiconductor, Transparent Conducting Oxide, Thin films, Electro ceramics

Presenter: Mr. Mahiman Bansal

Structural and Property Correlation in BCT-BZT Piezoelectric Thin Films at the Morphotropic Phase Boundary

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Abstract: BCT-BZT piezoelectric thin films have garnered significant attention for their potential in high-performance electromechanical devices due to their enhanced piezoelectric properties near the morphotropic phase boundary (MPB). Our study aims to investigate the interplay between structural characteristics and electromechanical properties of BCZT thin films, focusing on the MPB region. By employing advanced deposition techniques, such as pulsed laser deposition, we synthesized BCZT thin films with precise compositional control across the MPB. Structural analysis using X-ray diffraction and transmission electron microscopy revealed phase coexistence and lattice strain variations, which significantly influence the piezoelectric response. Our electrical and piezoelectric measurements, including polarization hysteresis and piezoresponse force microscopy, demonstrate enhanced piezoelectric coefficients and electromechanical coupling at the MPB, attributed to the structural instability and phase transitions. Notably, in the bulk form, this system exhibits tetragonal and orthorhombic phases for 50BCT-50BZT composition. The correlation between crystallographic orientation, domain structure, and functional properties will provide critical insights into optimizing BCZT thin films for applications in sensors, actuators, and energy harvesters. These findings underscore the importance of tailoring composition and processing conditions to exploit the MPB for next-generation piezoelectric technologies.

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Strain-Driven Ferroelectric Domain Evolution in Epitaxial BCZT Thin Films near MPB

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Abstract

BCZT a lead-free ferroelectric near its morphotropic phase boundary (MPB), exhibits enhanced electromechanical properties due to the coexistence of multiple phases (tetragonal, orthorhombic, and rhombohedral) at room temperature. The strong coupling between polarization and strain in such systems makes epitaxial misfit strain as an effective tool for tailoring ferroelectric domain structures in thin films.

In this study, epitaxial BCZT thin films were grown on $SrTiO_3$ (001) substrates with thicknesses of 20 nm and 70 nm. From reciprocal space mapping , the 20 nm film remains fully strained, while the 70 nm film is partially relaxed. Despite partial relaxation, both films exhibit a dominantly tetragonal phase due to substrate-induced biaxial compressive strain. Surface morphology of the film and ferroelectric domain structures were investigated using atomic force microscopy (AFM) and piezoresponse force microscopy (PFM). The thinner film exhibits coherently grown surface with out of plane polarisation variants. In contrast, the 70 nm film shows additional in-plane domain features with the emergence of 90°-oriented island ferroelastic domains, indicating partial strain relaxation.

To support experimental observations, a thermodynamic phase-field model was employed to simulate domain evolution under varying epitaxial strain conditions. The simulations reveal that under high compressive strain, only tetragonal 180° variants are stable. However, as the misfit strain reduces from -1% to 0%, orthorhombic ferroelastic domains emerge alongside the tetragonal variants, consistent with experimental results. Our findings demonstrate the critical role of epitaxial misfit strain in modulating the phase stability and domain architecture in BCZT thin films, offering insights for optimizing strain-engineered ferroelectric devices.

Electromechanical response and its dependance on stoichiometry of $BaTiO_3$

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Recently giant electromechanical (EM) responses have been observed in several defective systems due to the formation of site deficiency which is obtained either by creating geometrical or compositional modification [1]. One such report has been published [2] where the authors have integrated $BaTiO_3$ epitaxially on Si using single TiN buffer layer. They observe giant electromechanical response in $BaTiO_3$ (on TiN/Si stack) with electrostrictive response of $M_{31}=10^{-14}$ at 1kHz $(m/V)^2$ by the virtue of formation of defect dipoles, domain wall motion and polar nano-domains. However, there are a few studies on how the giant electromechanical response varies with stoichiometry of $BaTiO_3$. In this work we try to answer this question by studying other chemistries of $BaTiO_3$. We study three compositions: Ba/Ti=1, <1 and >1 and start with confirming the chemistry of these compositions by XPS and EDS followed by structural measurements by TEM. We then measured the electromechanical response, PE loops, IV characteristics and how ferroelectricity evolves with chemistry. Typically, stoichiometric $BaTiO_3$ is known to be ferroelectric [3] however surprisingly we find the off stoichiometric compositions too giving ferroelectricity on the stack. Effect of annealing has also been compared as there are significant changes in the resistive and electromechanical property of these films due to annealing. Overall, we explore various aspects of varying stoichiometry on the electromechanical properties of $BaTiO_3$.

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Design the Next-Gen, Flexible, Fiber-based Magnetoelectric composite of Zn-Doped BCZT-NZFO@PVDF for wireless power transmission application for implantable devices.

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Abstract: In the modern age, the growing demand of the wireless sensor and implantable devices has brought attention to develop the sustainable, flexible, ecofriendly, and affordable power source to run the WSNs and IoTs. Magneto-mechano-electric (MME) energy generator has recently gained attention due to its high-power density and potential for self- powered sensor networks. In this study we optimized Zn doped $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$ (BCZT) ceramics, and their impact on structural, dielectric, and electrical properties. Furthermore, to create magnetoelectric fiber composite via electrospinning method by adding different wt.% of $Ni_{0.5}Zn_{0.5}Fe_2O_4$ (NZFO), followed by material characterization. Subsequently, the MME generators were created in truncated cantilever shape using the fibers composites and underwent for energy harvesting characterization for device optimization. The optimized MME generators with 20 wt% of NZFO has demonstrated under the magnetic field of 6 Oe at 50 Hz which gives the output voltage, current and power density of 14.4 V, 1.1 μA, and 1.98 $\mu W/cm^2$, respectively. This power density is more than enough to run the low powered WSNs and implantable devices.

Work Function Engineered, Electrically Poled SnS–PVDF Nanofiber based nanogenerators for Enhanced Piezoelectric-triboelectric Energy Harvesting and Sensing

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Abstract:

In response to the increasing demand for sustainable power in wearable electronics, where traditional batteries are hindered by finite lifespans and upkeep requirements, we introduce a piezo-triboelectric hybrid nanogenerator (PT-HNG) designed for efficient biomechanical energy harvesting. A key innovation in this work lies in the enhancement of piezoelectric performance through the incorporation of tin(II) sulfide (SnS) into electrically poled PVDF nanofibers. The SnS inclusion plays a pivotal role in elevating the piezoelectric response of the PVDF matrix by inducing a high fraction of the polar β-phase and leveraging its intrinsic piezoelectric coefficient ($d_{33} \approx 16.7$ pm V^{-1}). This enhancement is further corroborated by ultraviolet photoelectron spectroscopy (UPS), which reveals an increase in work function from 8.34 eV (pristine PVDF) to 8.94 eV (SnS-PVDF), indicating a stronger dipolar alignment and improved charge generation efficiency. These modifications collectively result in a significantly improved piezoelectric output, positioning the PT-HNG as a promising solution for next-generation self-powered wearable systems. The PT-HNG efficiently converts low-frequency biomechanical motions such as tapping, writing, and finger bending into electrical energy, delivering an open-circuit voltage of ~55 V, a short-circuit current of ~20 μA, and an average output power of 0.576 mW—sufficient to light up four commercial LEDs. In addition to energy harvesting, the device functions as a self-powered pressure and strain sensor, exhibiting reliable performance in real-time human motion monitoring.

Effect of higher aspect ratio 2-D platelet filler on the electroactive phase fraction and ferroelectric characteristics of BiT/PVDF nanocomposite

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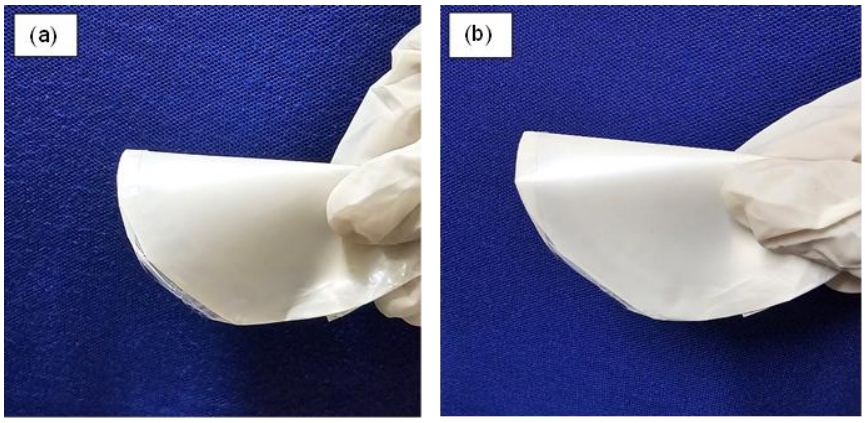
Abstract

Ceramic-polymer 0–3 composites, which combine ceramic particles known for superior electrical characteristics within a polymer matrix with high dielectric breakdown strength, have garnered significant interest for their applications in energy storage and harvesting. Among various influencing factors, the geometry and dimensions of the ceramic fillers play a crucial role in defining the overall performance of these composites. Particularly, two-dimensional platelet-shaped fillers are of interest due to their high aspect ratio, inherent anisotropy, and ability to align or texture within the matrix enabling enhanced electrical properties at relatively lower filler concentrations compared to spherical particles. In this work, Bismuth Titanate (BiT), a ferroelectric ceramic with an Aurivillius-type layered structure, that can be spontaneously grown into an anisometric shape was synthesized using the molten salt technique. The eutectic mixture of NaCl and KCl served as the reaction medium to facilitate anisotropic growth. By varying the salt-to-oxide weight ratio from 1:1 (denoted as BiT-1) to 5:1 (BiT-5), we tailored the aspect ratio of the BiT crystals, achieving ultra-thin, nanosheet-like platelets at higher salt concentrations. These synthesized platelets were then incorporated into a polyvinylidene fluoride (PVDF) matrix using a solution casting approach. The resulting nanocomposites—BiT-1/PVDF and BiT-5/PVDF—were examined to understand how filler morphology influences the microstructure, β-phase fraction and ferroelectric behaviour of the composite films.

Keywords

0-3 composites; 2-D platelet; aspect ratio; anisotropy; Aurivillius structure; molten salt synthesis; β-phase fraction



Photographs of (a) BiT-1/PVDF and (b) BiT-5/PVDF composite films prepared via solution casting

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Fiber-based flexible magneto-mechano-electric generators enhanced by UV and IR treatments for sustainable IoT sensors

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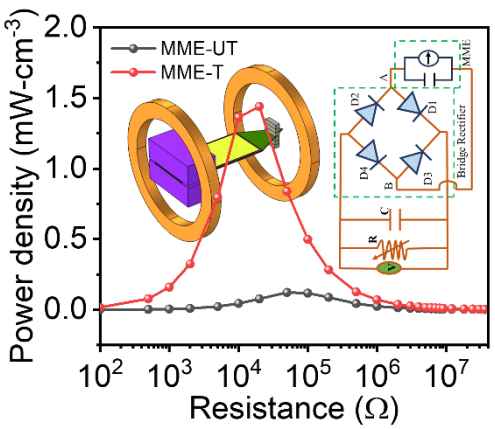
Abstract:

The rising reliance on the Internet of Things (IoT) highlights the need for reliable and sustainable energy sources to power sensors and communication modules. This study introduces a magneto-mechano-electric (MME) energy harvester with magnetoelectric (ME) coupling, capable of harvesting energy from low-intensity ambient magnetic fields. The device features a truncated cantilever design made of a flexible composite fiber composed of a piezoelectric AlN–PVDF polymer matrix combined with magnetostrictive Metglas. This configuration enhances magneto-mechanical vibrations and boosts energy conversion efficiency. To improve performance, the piezoelectric fibers undergo UV treatment to strengthen their electrical response, while the Metglas element receives infrared (IR) treatment to enhance its magnetic properties. These material improvements are confirmed through polarization–electric field (P–E) loops, dielectric analysis, and magnetic hysteresis (M–H) curves, supported by magnetic force microscopy (MFM). The developed MME harvester yields an open-circuit voltage of 32.8 V and a root-mean-square DC power density of 1.4 mW/cm³ under a low 6 Oe alternating magnetic field at 50 Hz. Finite element modeling with COMSOL Multiphysics 6.2 closely aligns with the experimental results. Compared to the untreated version, the optimized harvester shows about an 1100% increase in power output (0.1 mW/cm³ to 1.4 mW/cm³). Detailed structural and material insights are provided through XRD, FTIR, XPS, and HRTEM analyses. The generated energy is enough to power flame-detection microsensors, demonstrating the device's potential for integration into smart infrastructure and IoT systems.

Graphical abstract:



Piezoelectric Material for Energy Harvesting Application: Enabling Self-Powered Systems.

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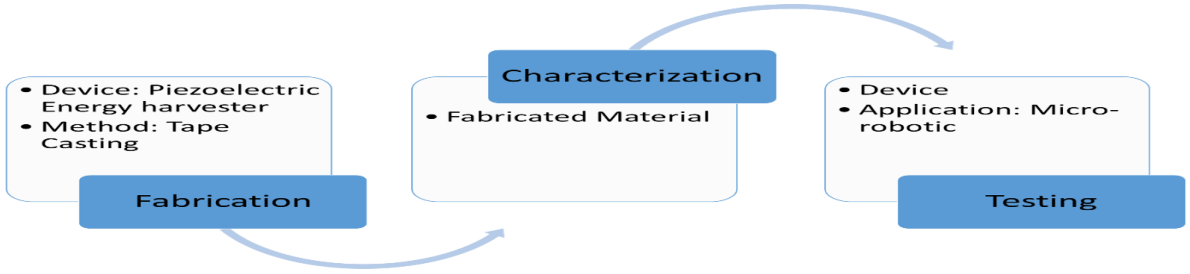
Piezoelectric materials have emerged as a highly promising candidate for electromechanical sensing, actuation, and energy harvesting, offering the ability to convert mechanical energy to electrical energy vice versa. Among these materials, traditional ceramics like Lead zirconate titanate (PZT) has been widely used for its high piezoelectric coefficients [1]. For the growing demand for sustainable and compact power sources for low-energy electronic devices and microsystems, Researchers have found significant research in developing thick film for piezoelectric energy harvesting devices. Thick film devices typically range from a few µm to a few mm and offer an attractive application in wireless sensor networks, wearable electronics, and micro robotics applications.

The main component in thick film Piezoelectric technology is a slurry, which is a composite of fine piezoelectric ceramic bound with polymer matrix and cured at ambient temperature[2]. One of the advantages of this is that it can be easily fabricated by sol-gel, tape-casting, and screen printing.

We have attempted to fabricated using tape-casting method, and then it was dried. The main concern for thick film fabrication is to produce a film of uniform thickness and to make them crack-free with high piezoelectric performance.

Methodology:



The outcome is expected to be validated in a miniature robotic application, a self-powered sensor.

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3D-Printed Microstuctred Triboelectricity induced Piezoelectric Handwriting Pad Based on MoS_2/PDMS Nanocomposites for AI-Driven Digital Text Conversion

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Abstract: We introduce a cutting-edge triboelectricity- induced piezoelectric writing pad (TPWP) equipped with advanced letter detection technology, converting handwritten input into digital text [1,2]. This device not only preserves the tactile and intuitive nature of traditional writing but also harnesses the efficiency of digital text, offering users the advantage of instant and accurate transcription for enhanced productivity and streamlined information management. A micro/nanostructured TPWP, featuring a 3D-printed surface texture, is engineered to function as an intelligent self-powered handwriting pad. The efficacy for handwriting conversion is systematically demonstrated through the acquisition of handwriting signals from three individuals encompassing English letters **A, B, C** and **D**, employing the micropatterned TPWP. TPWP fabricated using MoS_2/PDMS nanocomposite and Teflon tape is a triboelectricity induced layer placed on the micropatterned PDMS surface. Though, these signals exhibit detectable unique features for the same letters of different people, generated patterns also have basic similarity for a particular letter. To enhance the accuracy of letter recognition, handwritten data was filtered and trained up to 250 epochs. The time varying signal was transformed into a spectrogram for deep learning algorithm [3]. Convolutional Neural Network (CNN) integration allows the deep learning algorithm to successfully detect each individual letter. High classification accuracy is reached, with English letters "**A**" and "**B**" scoring 100% and "**C**" and "**D**" scoring 99%. Overall, the suggested model's precision is 99%. This study, strongly suggests that the use of 3D printed textured TPWP has great potential for handwriting to text conversion applications.

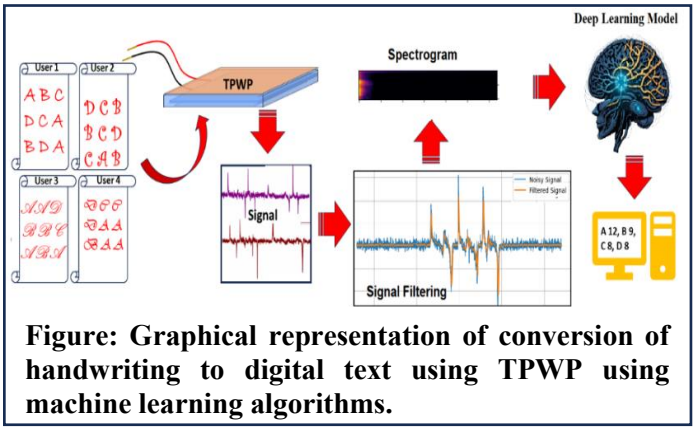

Figure: Graphical representation of conversion of handwriting to digital text using TPWP using machine learning algorithms.

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1D Monochalcogenide in Nanocomposite Fibers: A Hybrid Approach Toward Flexible Energy-Harvesting and Sensing Applications

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Abstract:

Low-power electronic devices are increasingly crucial for next-generation flexible electronics, with applications ranging from artificial intelligence systems to biosensors and energy harvesting. Among emerging energy conversion technologies, piezoelectric and pyroelectric nanogenerators have shown great promise for efficiently converting mechanical and thermal energy into usable electrical signals [1]. In this regard one-dimensional (1D) and two-dimensional (2D) nanomaterials are distinguished by their exceptional characteristics, including high charge carrier mobility and outstanding thermoelectric properties. In particular, 1D semiconducting monochalcogenides such as tellurium (Te) have attracted significant attention as promising materials for piezoelectric, ferroelectric, and optoelectronic applications [2]. In this study, we report a facile synthesis of one-dimensional (1D) tellurium nanorods (Te-NRs) with non-centrosymmetric crystal structure. These 1D Te were nano-confined within poly(vinylidene fluoride) (PVDF) nanofibers, leading to improved alignment of nanorods for optimized piezoelectric and pyroelectric responses to create a high-performance hybrid nanogenerator (HNG). The resulting HNG demonstrates a peak-to-peak voltage (V_{OC}) of approximately 8.5 V and a short-circuit current (I_{SC}) of 1.2 μA. Also, by employing organic PEDOT:PSS/Xyl electrodes, we achieve superior photothermal heat localization compared to traditional metal electrodes, which further amplifies the pyroelectric response and enables detection of small thermal variations. As a proof of concept, the HNG was successfully utilized for physiological signal monitoring, highlighting its potential as a self-powered biomedical sensor. The integration of monoelemental Te-NRs with ferroelectric PVDF nanofibers not only enhances device stability but also broadens the operational scope, making the system suitable for mechanical and thermal energy harvesting, infrared sensing, and respiratory monitoring.

Keywords: 1D-Tellurium, Nanofiber, Mechanical and Thermal energy harvesting, Healthcare monitoring.

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Self-Assembled Ferroelectric Nanodots in Imidazolium Tetrafluoroborate with Multiaxial Polarization

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Abstract

Molecular ferroelectrics offer a unique platform for designing low-dimensional, flexible, and environmentally benign functional materials. Here, we demonstrate room-temperature ferroelectricity in imidazolium tetrafluoroborate ($ImBF_4$), synthesized via a simple slow-evaporation method. Structural integrity and chemical composition were confirmed by FTIR spectroscopy, revealing characteristic N–H and C–H stretching modes alongside BF_4^- vibrational signatures. Thin films prepared by dispersing crystalline $ImBF_4$ in a sodium alginate matrix and spin-coated on Pt/Si substrates exhibit striking self-assembled nanodot arrays in Piezoresponse Force Microscopy (PFM) study. PFM study reveals robust switching of both out-of-plane (OP) and in-plane (IP) polarization components, evidenced by clear bipolar contrasts in amplitude and phase images. The presence of 180° domain walls and multidirectional polarization (head to head and tail to tail IP components) point to a multiaxial ferroelectric character, rarely observed in molecular systems. Furthermore, variation in spin-coating conditions modulates nanodot size without compromising ferroelectric order, highlighting morphological tunability. With a transition temperature (Tc) of 370.9 K, $ImBF_4$ stands out as a thermally stable, solution-processable molecular ferroelectric with potential applications in nanoelectronics, memory devices, and neuromorphic systems.

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Homochirality-Induced Piezoelectricity in a Single-Component Molecular System

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Abstract:
Organic piezoelectric materials have recently garnered significant attention as potential alternatives to ceramics.[1] However, there are only a handful of reports on single-component molecular crystals exhibiting piezoelectric properties. Introducing homochirality is one of the simplest approaches to achieving piezoelectricity in molecular crystals. Herein, we present an enantiomeric pair of compounds (*R*)-2-(((1-(*p*-tolyl)ethyl)imino)-methyl)phenol (^{R}PTIMP) and (*S*)-2-(((1-(*p*-tolyl)ethyl)imino)-methyl)phenol (^{S}PTIMP) crystallizing in the noncentrosymmetric $P2_12_12_1$ space group making them suitable for piezoelectric studies. In contrast, the racemic mixture of these compounds, *Rac*-2-(((1-(*p*-tolyl)ethyl)imino)methyl)phenol (^{Rac}PTIMP), crystallizes in the centrosymmetric $P2_1/n$ space group. The noncentrosymmetry of both ^{R}PTIMP and ^{S}PTIMP was confirmed through second harmonic generation (SHG) measurements, showing the SHG efficiencies of 0.11 and 0.12, respectively, relative to standard potassium dihydrogen phosphate (KDP). Piezoelectric coefficient ($d33$) measurements on a powder-pressed pellet of ^{S}PTIMP resulted in a $d33$ value of 4.7 pC N^{-1}. The piezoelectric energy harvesting experiments performed on the poled thermoplastic polyurethane (TPU) composite films of ^{S}PTIMP resulted in a maximum voltage output of 7.04 V for the 15 wt % ^{S}PTIMP-TPU composite device. The energy storage efficacy was also tested by successfully charging a 10 μF capacitor within 100 s using the best-performing 15 wt % ^{S}PTIMP-TPU device.

Figure 1. A pair of enantiomeric Schiff base compounds $^{R/S}$PTIMP were synthesized and shown to exhibit piezoelectric properties. The polymer composites of ^{S}PTIMP in thermoplastic polyurethane showed piezoelectric energy harvesting properties with good open-circuit output voltages, which were further utilized for capacitor charging experiments.

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Co(ii)complex promoted PVDF β-phase crystallization: innovations in pressure sensing and energy harvesting

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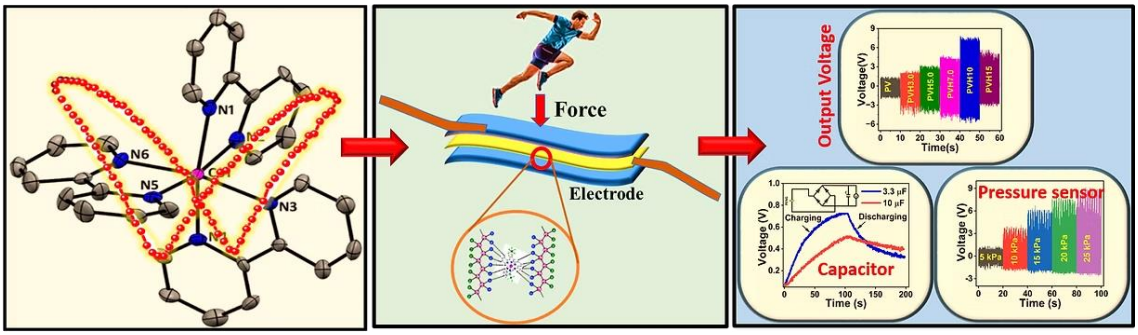
Conventional bulk oxides in PENGs face issues like toxicity, rigidity, and require harsh processing to induce the electroactive β-phase in PVDF. In contrast, the discrete Co(II) complex $[Co(bpy)_3]$ $(PF_6)_2$offers a flexible, low-toxicity alternative that crystallizes in a polar *P3₁* space group. Uniquely, Co-bpy promotes self-polarization of the β-phase in PVDF under mild conditions—more efficiently than bulk oxides. Among various composites, the 10% Co-bpy-loaded film (PVH10) showed the highest output (13.5 V), five times that of pristine PVDF, along with 1.16 μW cm^{-2} power density and 1.3 μA current. The device also enabled rapid energy storage and high-pressure sensitivity, highlighting the superior functional integration of Co complexes over traditional oxide fillers.



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Fabrication of high output performance piezoelectric nanogenerator based on PVDF/BFBT for energy harvesting

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Flexible piezoelectric nanogenerators (PENGs) are gaining attention as sustainable power sources for self-charging wearable devices due to their ability to harvest mechanical energy from the environment. We report a lead-free $BiFeO_3$–$BaTiO_3$ (BFBT) nanoparticle-embedded PVDF-based flexible piezoelectric nanogenerator (PENG). The β-phase of PVDF was stabilized by optimizing the doping of BFBT nanoparticles, eliminating the need for external electrical poling. Hydrogen bonding between the hydrogen atoms of PVDF and the oxygen atoms of BFBT induces rotation of $–CH_2$ bonds, promoting the formation of the β-phase. A low-cost solution casting method was employed to fabricate flexible BFBT/PVDF nanocomposites, which were then sandwiched between copper electrodes and encapsulated with a thin PDMS layer to form the final PENG device. X-ray diffraction (XRD) and Fourier transform infra-red spectroscopy (FT-IR) characterizations were employed for the identification and quantification of the piezoelectric polar phases. The β-phase content was found to increase from 46.9% in pure PVDF film to 90.6% in the PVDF/5wt.%BFBT composite film. The dielectric constant of the sample also increases from 7 to 31 as the BFBT content increases. To confirm the enhanced ferroelectric phase formation in PVDF-BFBT nanocomposite polymer films, the P-E measurements have been carried out. PVDF/5wt.%BFBT nanocomposite exhibits the greatest spontaneous polarization (P_s~5.42 μ C/cm^2) at 1MV/cm among all the nanocomposites, which could be due to the presence of highest concentration of the polar β-phase. The PENG based on PVDF/5wt.%BFBT achieved an output voltage of 5.3 V under a force of 50 N at a frequency of 15 Hz, demonstrating a sensitivity of 80 mV/N and a response time of 14 ms.

Keywords- Piezoelectric nanogenerators, PVDF, solution casting, piezoelectric sensor, BFBT

Towards Advanced Multiferroic Materials: Interplay Between Magnetism and Ferroelectricity

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Potential application of molecular magnetic materials in future electronic devices mainly depends on the "molecular bistability" that arises while switching between two easily accessible electronic spin states of the system *i.e.,* high spin (HS) and low spin (LS), typical examples include Spin Crossover (SCO) or Metal-to-Metal Electron Transfer (MMET)[1] systems. Specific attention is now being given on the systems that can exhibit multi-functional behaviour *e.g* SCO/ET with chirality, luminescence, photo-activity as well as polarizability.[2] Preparation of complexes that couple magnetic properties with inherent polarization from the ligand backbone or from counter cation or anion opens up possibilities for developing advanced multiferroic materials for magnetoelectric devices.[3] These systems show stimuli-responsive (heat, light or pressure) spin-state switching which also allows us to draw a correlation between polarization and magnetic properties to be applied in modern magnetoelectric devices. As an active research group working in molecular magnetism, we have lately started exploring this exciting aspect to correlate SCO and ferroelectricity in 3d transition metal-based molecular complexes. Herein, I present two distinct molecular systems: (i) an Fe(III)-based cyanometallate featuring a polarizable counter cation, and (ii) a mononuclear Co(II) complex incorporating a polarizable ligand substituent. Both the systems show indication of phase transition with polarization switching and their magnetic correlation is underway.

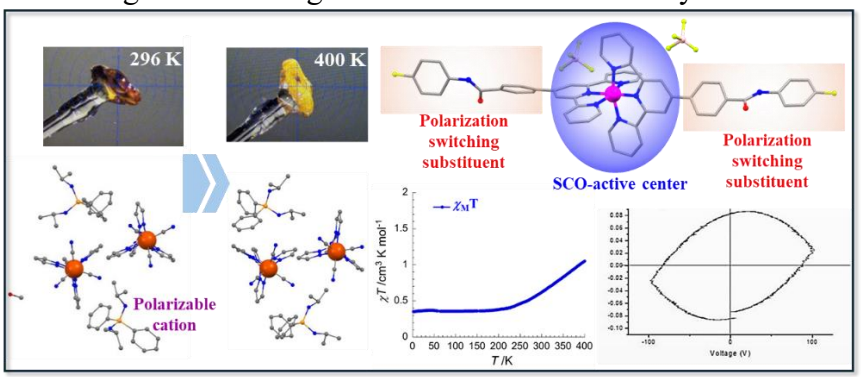

Figure 1 Single Crystal XRD structure and properties of the mononuclear complexes based on Fe(III) and Co(II) centers

Acknowledgement: We thank Solid State and Structural Chemistry Unit, Indian Institute of Science, Centre Franco-Indien pour la Promotion de la Recherche Avancé, CEFIPRA, CSRP Project 70T07-2, Prime Minister's Research Fellowship, INSPIRE Fellowship, Department of Science and Technology, Government of India for the research support.

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Harnessing Chirality: Piezoelectric $[Mn\text{-}Camp\text{-}4BPY]_n$ Metal–Organic Framework for Nanogenerator Applications

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Escalating global imperatives for sustainable and decentralized energy solutions has propelled research into piezoelectric nanogenerators (PENGs) that convert ambient mechanical input into electricity. Traditional ceramic piezoelectrics are limited by brittleness, high processing temperatures, and poor environmental compatibility. Metal–organic frameworks (MOFs) offer a compelling alternative due to their structural anisotropy, tunability, and mechanical compliance. We present a chiral 3D MOF, $[Mn\text{-}Camp\text{-}4BPY]_n$, synthesized using enantiopure D-camphoric acid and 4,4′-bipyridine. This homochiral assembly enables polar packing essential for piezoelectric response, supported by intramolecular hydrogen bonding. PFM confirms a longitudinal piezoelectric coefficient (d_{33}) of 6 pm/V. A fabricated PENG device delivers measurable electrical output under mechanical actuation. These findings position MOFs as promising candidates for next-generation soft energy harvesting technologies.

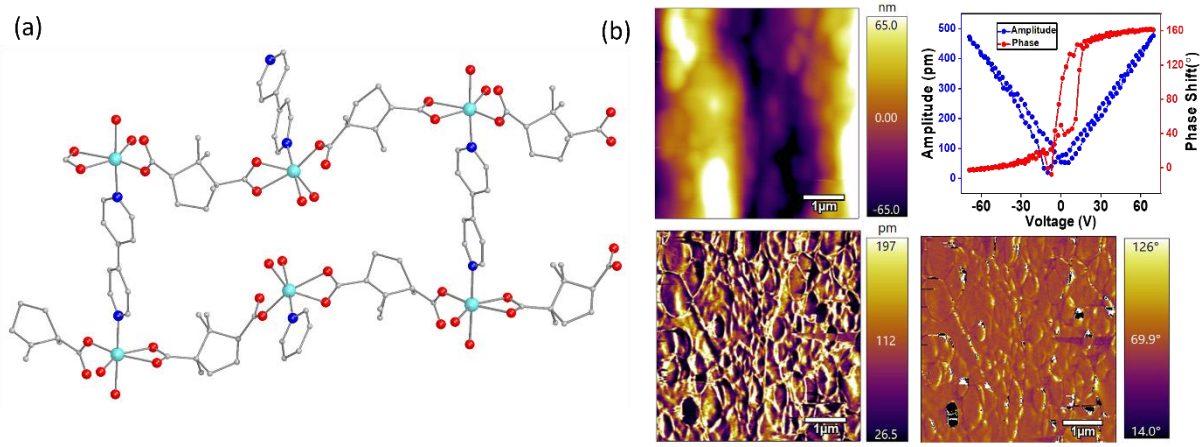

Figure 1: (a) Ball and stick representation of crystal structure of complex (b) Amplitude-Voltage butterfly loop, Phase shift-Voltage hysteresis loop with Lateral PFM amplitude and phase showing the different domains.

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Ferroelectric Polymer Nanocomposite Based Triboelectric Nanogenerators for Efficient Energy Harvesting Applications

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Triboelectric nanogenerators (TENGs) provide a low-cost and efficient approach for harvesting ambient mechanical energy. Polyvinylidene fluoride (PVDF), a widely used polymer in TENGs, offers excellent chemical stability and exhibits strong dipolar polarization in its electroactive β-phase. The incorporation of ferroelectric materials with high remnant polarization and large piezoelectric coefficients into PVDF facilitates β-phase formation and enhances its dielectric and ferroelectric properties. Moreover, the inherent piezoelectricity of the composite contributes to the overall voltage output, enabling a synergistic energy harvesting mechanism. This dual functionality results in a hybrid nanogenerator that combines triboelectric and piezoelectric effects (TENG–PENG), leading to enhanced performance. In this study, $0.94(Na_{0.5}Bi_{0.5}TiO_3)$-$0.06(BaTiO_3)$ (NBT-BT), a classical ferroelectric with high dielectric and polarization characteristics, is incorporated into the PVDF matrix. Structural characterization confirms increased β-phase content, and electrical measurements reveal significantly improved ferroelectric and piezoelectric responses compared to pristine PVDF. The PVDF/NBT-BT nanocomposite demonstrates strong potential to overcome the low output limitations of conventional TENGs and is a promising candidate for self-powered sensing applications.

Keywords: Triboelectric nanogenerators, ferroelectric, piezoelectric, PVDF, NBT-BT

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Engineering 3d metal Based Molecular Magnetoelectric Materials and its Applications

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Multiferroic (MF) materials exhibit coexisting ferroic orders such as ferroelectricity, ferro-/antiferromagnetism, and ferroelasticity, enabling magnetoelectric (ME) coupling.[1] In conventional inorganic systems like perovskites, strong ME coupling is limited due to symmetry constraints and incompatible electronic structures. Known single-phase ME oxides typically show low magnetic transition temperatures and weak ME effects.[2,3] In contrast, molecular complexes offer advantages such as structural tunability, soft synthesis, and environmental friendliness.[4] Here, we present a single-phase 2D layered molecular ME material, **[Cu(R,R-dacy)(N_3)$_2$]$_n$** (R,R-dacy = (1R,2R)-diaminocyclohexane), exhibiting a high ME coupling coefficient (α = 112 mV Oe^{-1} cm^{-1}). A magnetoelectric nanogenerator (MENG) fabricated from this material produces 200 mV under a 20 Oe AC magnetic field and can harvest stray magnetic fields to light up 3 LEDs, demonstrating its potential for low-field magnetic energy harvesting applications.

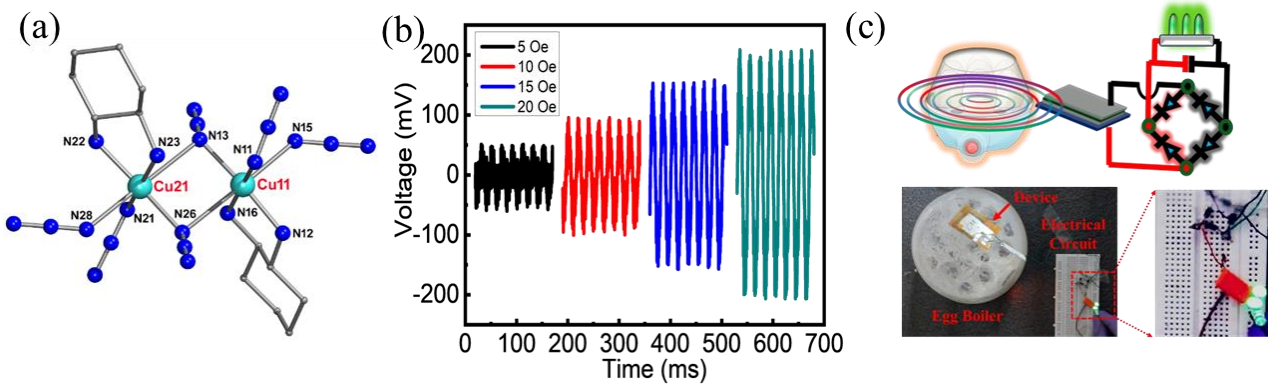

Figure.1. a) Ball and stick representation of crystal structure of complex. b) Open circuit voltage under different AC magnetic fields. c) Schematic showing stray magnetic field harvesting around a working egg boiler machine.

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Title of the paper: Mechanical Manipulation of Ferroelectric Domains in Molecular Ferroelectric

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Abstract

Ferroelectricity in inorganic materials has been widely explored for applications in energy harvesting, microelectronics, non-volatile data storage, and neuromorphic computing. However, their rigid structure, high coercive field, complex synthesis, and environmental toxicity limit their applications in flexible electronics. To address these issues, molecular ferroelectrics have emerged as a promising alternative due to their cost-effective processing, tunable flexibility, biocompatibility, and low coercive field. Herein, we synthesized imidazole perchlorate ($ImClO_4$) crystals and high quality thin film on silicon substrate where hydrogen-bond interactions predominantly govern spontaneous polarization. To overcome the problem of charge injection and dielectric field breakdown in thick films from high switching electric field, we demonstrate mechanical control of ferroelectric domains at the nanoscale. The switching mechanism is attributed to the flexoelectric effect, where strain gradient generates a trailing electric field under sufficient mechanical force. Additionally, we show that the flexoelectric field can be modulated by adjusting the atomic force microscopy (AFM) tip's scanning direction. Controlled mechanical manipulation reveals the anisotropic switching behavior of ferroelectric domains with complete switching of smaller domains and partial switching of larger ones at specific angles. These findings provide insights into the angular dependence of flexoelectric fields and their role in domain switching, proposing the possible contribution of anisotropic H-bonding network. This study offers a pathway to optimize molecular ferroelectrics for future flexible and biocompatible electronic devices.

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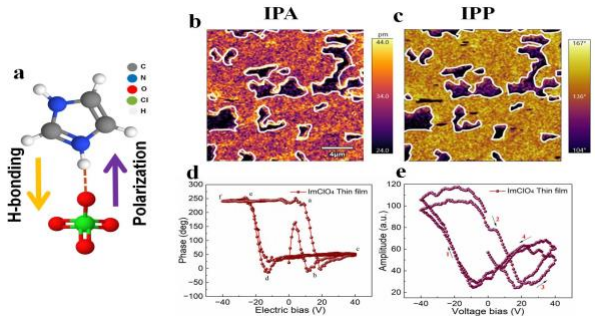

Figure 1| Spontanious polarization in $ImClO_4$, Domain mapping, and piezoelectric properties of ImClO4 thin film.

Spin Polarization in Lead-Free Ferroelectric Hybrid Halide Perovskite

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Hybrid inorganic-organic halide perovskites (HIOP) of the form ABX_3 (A = metal or molecule, B = metal or molecule, X = halogen) have been known for optoelectronic devices[1-2]. The ferroelectric property has added multifunctional features to these materials. Recently, a lead-free $MPSnI_3$ (MP = methylphosphonium ion = CH_3PH_3) have been experimentally synthesized and showed that it exhibits a narrow bandgap of 1.4 meV, and a spontaneous polarization of 3.94 μC cm^{-2}[3]. Using the first principle-based density functional theory (DFT) simulations as implemented in VASP (Vienna Ab-initio Simulation Package)[4], we have investigated the electronic structure of this material. The structural relaxation of the experimental structure led to a monoclinic phase with the Pc space group. The structural relaxation with various molecular orientations leads to several degenerate structures within the energy threshold, inferring the dynamical nature. The electronic band structure with relativistic effects within the PBE formalism shows the bandgap of 0.4 eV. Near the band extremum, the band structure shows spin splitting of 95 meV in the valence band and 45 meV in the conduction band. The spin texture analysis in the k_x-k_y plane has provided the partial persistent spin texture. The narrow bandgap and significant valence band spin-splitting may find application in spintronics devices.

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South Asia Ferroelectric Symposium
L-phenylalanine (LPA) -poly-ethylene-oxide (PEO) based piezoelectric electrospun nanofibers for energy harvesting applications.

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ABSTRACT

Several organic amino acid-based piezoelectric materials capable of generating electrical energy in response to mechanical deformation and vice versa has been extensively studied for power device, pressure sensors, transducers, etc [1]. In general, Piezoelectric materials are usually made of inorganic materials such as lead zirconate titanate (PZT), Barium Titanate (BTO), Lithium Niobate (LN), etc. However, these piezoelectric materials are not biocompatible and can harm living organisms. The application of this kind of material is limited due to the toxic nature of metals in their composition and the high-temperature synthesis procedure. Therefore, biocompatible piezoelectric materials are our focus of interest. Such kind of material includes biodegradable polymer, protein-based polymer, and amino acids. Although the piezoelectric response of organic materials is often smaller than that of inorganic materials, various methods have been proposed to increase their response [2]. Electrospun fibers have gained a lot of attention for energy harvesting applications because of their advantages, like flexibility, cost-effectiveness, adaptability to diverse shapes, and ability to be customized for multiple functions.

Electrospinning is one of the fiber preparation methods, which enhances crystallinity and dipole alignment in piezoelectric materials, leading to increased piezoelectric activity [2]. Using this technique, nanofibers composed of L-Phenylalanine (LPA) inside the polymer matrix of polyethylene oxide (PEO) have been synthesised. The x-ray diffraction pattern of LPA-PEO nanofibers confirms its non-centrosymmetric monoclinic crystal structure with $P2_1$ space group [3]. SEM image shows that fibers are continuous, uniform in nature, and the average diameter of the fiber is found to be ~246 nm. It is observed that LPA incorporated PEO nanofiber matrix enhances the mechanical strength of the sample when compared with bare polymeric PEO fiberous film of comparable thickness. Using the polymeric LPA-PEO fiber mat, a piezoelectric nanogenerator (PENG) has been fabricated to study its energy harvesting behaviour. The sample generates a peak voltage as high as 5 V during a finger pressing and releasing process. This study shows that the nanocomposite fiber-based flexible PENGs are promising mechanical energy harvesters and effective power sources for portable electronic and wearable devices.

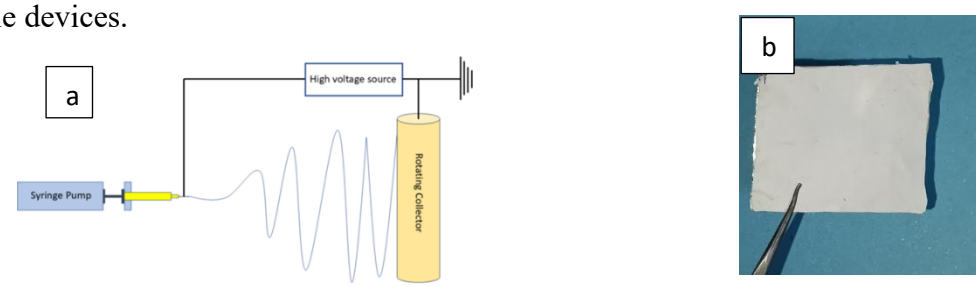

Fig 1.a) Schematic diagram of the Electrospinning setup and b) Electrospun LPA-PEO nanofiber mat.

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Ferroelectricity and Piezoelectric Energy Harvesting of an $A_3M_2X_9$ type 0D Bromobismuthate Hybrid with Bulky Organic Quaternary Amine

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Abstract

Organic-inorganic hybrid ferroelectric compounds of the halobismuthates family have emerged as a focal point of research owing to their reduced toxicity and distinctive optical characteristics. This study presents a novel ammonium hybrid perovskite, [BPMBDMA]·$[Bi_2Br_9]_1$, which exhibits both ferro- and piezoelectric properties and crystallizes in the polar noncentrosymmetric $Pca2_1$ space group. The nonlinear optical (NLO) activity of [BPMBDMA]·$[Bi_2Br_9]$ was corroborated through second harmonic generation measurements evidencing its noncentrosymmetric structure, which was further substantiated by piezoresponse force microscopy analyses. Ferroelectric P-E hysteresis loop investigations conducted on a thin film sample of [BPMBDMA]·$[Bi_2Br_9]$ revealed a saturation polarization (Ps) as much as 11.30 μC cm^{-2} at ambient temperature. To explore the piezoelectric energy harvesting capabilities of [BPMBDMA]·$[Bi_2Br_9]$, composite materials were fabricated using polylactic acid (PLA) as a matrix. Notably, a device comprising 10 wt% [BPMBDMA]·$[Bi_2Br_9]$ in PLA demonstrated a remarkable output voltage of 24.6 V and a peak power density of 13.65 μW cm^{-2}. The practical applicability of this device's output performance was further evaluated through a capacitor charging experiment, wherein a 10 μF capacitor was charged within 160 seconds.

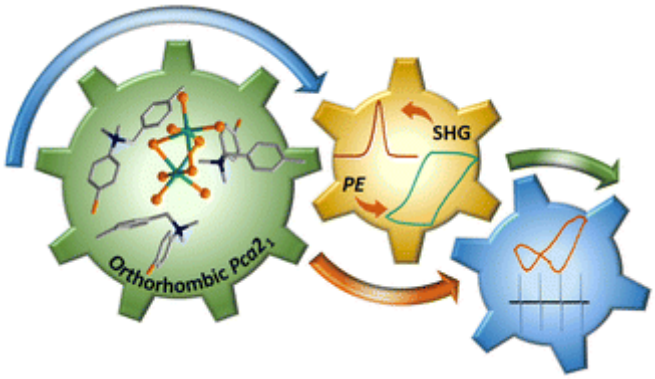

Figure1: A novel room-temperature ferroelectric Halobismuthate(III) compound, [BPMBDMA]·$[Bi_2Br_9]$, was synthesized and found to possess excellent ferroelectric and piezoelectric properties. Its polylactic acid (PLA) composites demonstrated strong potential for piezoelectric energy harvesting with high open-circuit voltage and power density, making it ideal for self-powered devices.

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Synergistic Effect of Ti_3AlC_2 MAX Phase and PEDOT-b-PEG on the Dielectric and Electrochemical Behavior of Flexible PVDF Nanocomposites

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Abstract

This study reports the successful fabrication of flexible, multifunctional polyvinylidene fluoride (PVDF)/poly(3,4-ethylenedioxythiophene)-block-poly(ethylene glycol) (PEDOT-b-PEG)/Ti_3AlC_2 MAX phase nanocomposite films via a facile solution casting approach. By tailoring the composition of the Ti_3AlC_2 within the PVDF/PEDOT-b-PEG matrix at varying loadings led to uniform dispersion and strong interfacial compatibility, enabling significant enhancement in structural, thermal, and functional properties. Comprehensive characterization through various physiochemical techniques confirmed structural integrity and improved filler–matrix interactions, while attaining the superior thermal stability and delayed degradation. Dielectric analysis over broad frequency (1 Hz–1 MHz) and temperature (30 °C–150 °C) ranges exhibited a substantial rise in dielectric constant and AC conductivity at low frequencies and elevated temperatures. Furthermore, cyclic voltammetry demonstrated enhanced electrochemical performance, including increased current density and specific capacitance, highlighting the electroactive nature of the nanocomposite. These comprehensive findings underscore the potential of PVDF/PEDOT-b-PEG/Ti_3AlC_2 nanocomposites as high-performance materials for energy storage and flexible electronic applications.

Keywords: Ti_3AlC_2 MAX, PEDOT-b-PEG, Polymer Nanocomposites, Energy storage, Dielectrics, Cyclic voltammetry

Lead-Free Piezoelectric Ceramics for Energy Conversion and Packaging Applications

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Abstract: This study presents the development of a self-powered sensor based on a polymer–piezoceramic composite, aimed at packaging applications. Lead-free barium titanate ($BaTiO_3$) nanoparticles were incorporated into a polyvinylidene fluoride (PVDF) matrix to enhance its piezoelectric, ferroelectric, and dielectric properties by promoting the formation of the electroactive β-phase. Composite films with varying weight percentages of $BaTiO_3$ were fabricated using the solution casting method to systematically investigate the effect of nanoparticle concentration on material performance. The morphology of the (1-x)PVDF–(x)$BaTiO_3$ composite films was examined using field emission scanning electron microscopy (FE-SEM), while phase composition and crystallinity were characterized via Fourier transform infrared (FTIR) spectroscopy and X-ray diffraction (XRD). In addition, key electrical and electromechanical properties were evaluated. The results revealed that the incorporation of functionalized $BaTiO_3$ nanoparticles significantly enhanced the dielectric, ferroelectric, and piezoelectric responses, with the 80PVDF-20$BaTiO_3$ composition exhibiting optimal performance. Specifically, this composition demonstrated a substantially higher dielectric constant compared to pristine PVDF, indicating notable improvements in energy harvesting and storage potential. Based on this composition, an impact sensor was fabricated and tested. The sensor exhibited a strong electrical response under applied mechanical impact, validating its potential use as a self-powered sensing element in smart packaging systems.

Keywords: Impact sensor, Piezoelectric, Dielectric, Ferroelectric, Energy harvesting, Smart packaging.

High Entropy Perovskite Ceramics for Capacitive Energy Storage

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Abstract: High Entropy perovskites ceramics represent a sub-class of ABO_3 perovskite ceramics, where atleast one sub-lattice consists of five or more than five multi-principal elements with nearly equal atomic proportions. Owing to specific characterises including high configurational entropy, high lattice distortion, slower diffusion, and existence of cocktail effect allowing them to preferred over traditional perovskite ceramics in numerous applications such as tribological, thermal and catalytic applications. With this motivation, this paper focus on synthesis of novel lead-free high entropy perovskite compositions and investigate their potential in energy storage for capacitor applications. This paper attempts to optimize the composition and/or processing conditions to maximize the capacitive energy storage performance of high entropy perovskites ceramics in order to cater large demand of energy storage and miniaturization of lead-free capacitors for future generations. Results of this study indicates that the increment of entropy resulted in broad dielectric characteristics during the dielectric study, which evidenced the relaxor behaviour in the sample. Moreover, the high entropy ceramics samples exbhited the higher energy storage along with lower storage loss during P-E loop study. This study could be a great guide to fabricate high performance and miniatured capacitors.

Keywords: High Entropy, ABO_3, Perovskite, Lead-Free Capacitors, Energy Storage.

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Tuning the switching dynamics through cation engineering in $PbZrO_3$-based materials for enhanced energy storage and electrostrain characteristics

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Antiferroelectric materials have recently gained more attention for their energy storage and actuator applications. Chemical substitutions are often used to enhance their dielectric and piezoelectric properties. While less exploration has been conducted on their scaling behavior and domain dynamics compared to ferroelectric materials, our study addresses this gap. We examined the switching dynamics of chemically modified $PbZrO_3$-based antiferroelectric materials, selecting dopants to significantly increase the antiferroelectric (AFE) - ferroelectric (FE) switching field. Our findings revealed a more gradual AFE-FE transition and a notable 61% increase in field-induced strain in the doped system, highlighting its potential for actuator applications also. These results underscore the promise of chemical substitution as a novel method for advancing AFE materials, making them suitable for actuator and energy storage uses.

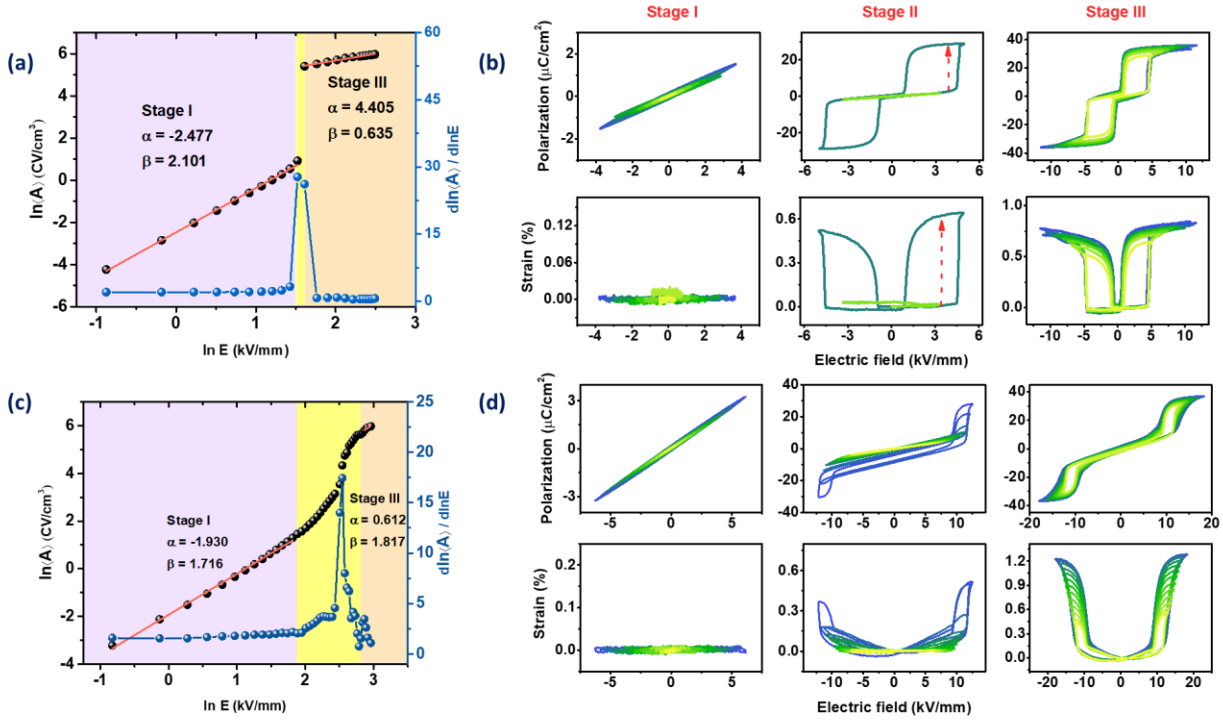

Figure 1: $\ln\langle A\rangle$ vs $\ln\langle E\rangle$ of undoped (a) and doped (c) $PbZrO_3$-based AFE material. The P-E loops and S-E curves of undoped (b) and doped (d) ceramics in three different stages.

Composition optimization for recoverable energy storage density performance, breakdown strength, relaxor nature, and thermal stability in eco-friendly Eu^{3+} substituted $Na_{0.2}K_{0.3}Bi_{0.5}TiO_3$

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Abstract

Environment-friendly ceramic capacitors with outstanding energy storage with thermal stability properties are greatly required for advanced high-temperature pulsed power systems. However, it is still a great challenge to develop lead-free dielectric materials with simultaneous excellent recoverable energy storage density (W_{rec}) and energy storage efficiency (η). A solid-state reaction technique is used to create lead-free Eu Substituted $Na_{0.2}K_{0.3}Bi_{0.5}TiO_3$ with x = 0 (Eu 0),0.02 (Eu 2),0.04 (Eu 4),0.06 (Eu 6). As dopant concentration rises, the polarization-electric field (P-E) loop, the strain-electric field (S-E) curve, and the dielectric curve all showed that the substitution improved the relaxor properties via transition from normal ferroelectrics. This transition is attributed to the rise in chemical inhomogeneity and site disorder, which led to a decrease in the correlation lengths of the built-in dipole moments. By introducing Eu^{3+}-based $Na_{0.2}K_{0.3}Bi_{0.5}TiO_3$ ceramic, we designed local compositional disorder and built quenched random fields to maximize the discrepancy between the maximum polarization, remanent polarization, and breakdown strength. The Eu^{3+} substitution widened the observed diffuse phase transition type relaxor property in the dielectric curve. With 20% and 40% variation, the plateau-type dielectric curve of Eu 4 substituted NKBT produces excellent dielectric constant stability over the temperature ranges of 120°C to 500°C and 90°C to 500°C respectively. The Eu 2 sample has a recoverable energy density of 1.02 J/cm^3 with a large electrical breakdown of 121 kV/cm, which makes it a promising candidate for energy storage. $Na_{0.2}K_{0.3}Bi_{0.5}TiO_3$ - based systems can be used for actuator applications with further development, according to the positive strain value. So, the Eu substituted systems are effective for both actuator and energy storage applications on improvising and tuning as necessary, according to research with the right dopants. The SRBRF model is exploited to understand the transformation from a normal ferroelectric to a relaxor in NKBT-Eu. These findings show that creating weakly coupled polar phases can increase the energy density and efficiency of bulk ceramics based on Bi-based, which may be a significant step towards utilizing Bi-based materials for energy-storage applications.

Key Words: Relaxor ferroelectrics, Energy storage, Thermal stability, NBT-KBT, PNRs

Synergistic Enhancement of Energy Storage Properties in 2D-3D Composites of Graphene and Barium Titanate

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ABSTRACT

Two-dimensional (2D) material-based composites have gained a lot of attention due to their ability to increase polarization properties, which are crucial for advanced flexible electronic applications. In this study, we explore the synergistic effect of graphene (G) on the polarization properties of Barium titanate ($BaTiO_3$ (BT)). The G-BT nanocomposites were synthesized utilizing the microwave-assisted solid-state method. XRD analysis reveals distinctive peaks of graphene and BT in G-BT composites. The addition of graphene enhances mechanical stability and reduces the flow of unwanted charge carriers, therefore increasing the overall ferroelectric behavior of G-BT composites. As a result, we observed an increased recoverable energy storage density, Wrec, of approximately 135.97 mJ/cm³ and 167.06 mJ/cm³ for 5 wt% and 10 wt% of graphene in BT, respectively. Additionally, the breakdown voltage (Eb) increases significantly from 38.2 to 52.71 kV/cm. Overall, combining graphene with BT yields composites with better polarization properties, making them attractive for advanced electronic and flexible ferroelectric applications.

Investigations of energy storage and thermal stability properties in eco-friendly B-site substituted $Na_{0.5}Bi_{0.5}TiO_3$

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In this work, $(Mg_{1/3}Nb_{2/3})^{4+}$ cationic substitution in lead-free polycrystalline $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) has been adopted to synthesize by the conventional solid-state reaction method. The cationic substitution was introduced into NBT through compositional modification, which significantly restricted grain growth and promoted a ferroelectric to relaxor ferroelectric phase transition. The substitution of $(Mg_{1/3}Nb_{2/3})^{4+}$ influenced the crystal structure, ferroelectric, dielectric properties, and micromorphology, which had been investigated systematically. The enhancement of relaxor nature is found with this substitution and further verified by dielectric curve, polarization (P) - electric field (E) hysteresis loop, and current (I)- electric field (E) curve. The recoverable energy density was determined to be 1.09 J/cm^3 and 1.24 J/cm^3 at 101 kV/cm and 114 kV/cm in the 10 mol% and 20 mol% of $(Mg_{1/3}Nb_{2/3})^{4+}$ substituted systems, respectively. Furthermore, over the 35 ˚C to 490 ˚C temperature range, the 30 mol% $(Mg_{1/3}Nb_{2/3})^{4+}$ substituted composition showed superior thermal stability in the permittivity. Therefore, this study concluded that these cationic substituted NBT compositions are appropriate materials for applications involving higher-temperature and energy storage in electronic devices.

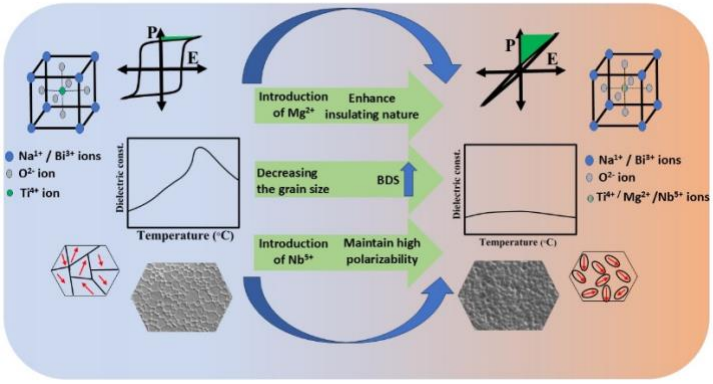

Figure 1. Graphical abstract of $(Mg_{1/3}Nb_{2/3})^{4+}$ cationic substituted in the $Na_{0.5}Bi_{0.5}TiO_3$.

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Improved Relaxor Characteristics in A and B-site Substituted Perovskite $BaTiO_3$ for Energy Storage Applications

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Abstract:

With the growing demand for efficient energy storage systems, ferroelectric ceramics like $BaTiO_3$ (BT) have attracted significant attention for dielectric capacitor applications [1]. The relatively low energy density of these materials, however, substantially restricts their potential domains of application. The introduction of lattice defects or the enhancement of polarization performance, which is achieved by converting nonlinear dielectrics into relaxed dielectrics (RFEs), emerges as a pivotal methodology for achieving superior energy storage capabilities. Various research studies indicate that the relaxor properties of BT can be improved through single or co-doping [2].

This study investigates the effects of Nd and Mg substitution on the structure and electrical properties of $BaTiO_3$. Pure and substituted $BaTiO_3$ were synthesized via solid-state reaction. The synthesis method utilized a stoichiometric combination of high-purity carbonate and oxide precursors, followed by calcination and sintering under carefully optimized conditions. The phase purity and crystalline structure were analysed using X-ray diffraction (XRD), which confirmed the development of a single-phase perovskite structure. The substituted samples exhibited minor peak shifts and broadening in their XRD patterns, suggesting the successful incorporation of substituents into the $BaTiO_3$ lattice. Raman spectroscopy demonstrated significant alterations in the vibrational properties of $BaTiO_3$ due to substituents. The substituted samples showed broader spectral features and displaced peak positions in comparison to pure $BaTiO_3$, suggesting considerable local structural disorder and the formation of polar nanoregions. These spectral alterations are linked to the relaxor-like behavior observed in electrical measurements, where the disruption of long-range ferroelectric order allows for easier dipole reorientation during charging cycles. Pure $BaTiO_3$ displayed typical square-shaped hysteresis loops characterized by a high remnant polarization ($P_r \approx 8\ \mu C/cm^2$), while the substituted samples showed progressively narrower loops with lower P_r values ($P_r \approx 1\ \mu C/cm^2$). This trend towards tighter hysteresis loops, along with decreased coercive fields (from 15.7 kV/cm to 2.77 kV/cm), suggests that the energy storage efficiency is improved in the substituted samples. These findings highlight the potential of carefully designed co-doped strategies to optimize $BaTiO_3$ -based materials for energy storage applications.

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The prominence of sintering temperature optimization in amelioration of densification and energy storage behavior in KNN based ceramics

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$K_{0.5}Na_{0.5}NbO_3$(KNN)-based ceramics are considered to be promising lead-free dielectrics for pulsed power systems, thanks to their notable breakdown strength linked to submicron grain structures. Yet, their full potential is often limited by the volatilization of alkali ions (K^+, Na^+) during sintering and difficulties in achieving optimal densification - factors that significantly hamper their energy storage performance. Careful optimization of sintering temperature offers a viable route to mitigate these issues and improve the functional properties of KNN based ceramics. This study investigates the influence of sintering temperature on the dielectric, microstructural, ferroelectric & energy storage properties of a novel lead-free ceramic composition, 0.875KNN–0.125BZO ($0.875K_{0.5}Na_{0.5}NbO_3$-$0.125BiZrO_3$) fabricated by solid state synthesis. Samples were sintered at three different temperatures (1140 °C, 1160 °C, and 1180 °C). All samples exhibited a perovskite structure as confirmed by X-ray diffraction (XRD) analysis. Dielectric analysis revealed a diffusive phase transition for all samples, indicative of relaxor-like behavior, which was further supported by the presence of slender P–E hysteresis loops. The composition sintered at 1160 °C exhibited the most favorable properties. The sample achieved bulk density ~ 4.69 g/cm^3 with highest relative density ~ 95.2%. FE-SEM studies revealed a uniform microstructure with fine grains (~0.43 μm), contributing to an enhanced breakdown strength (BDS) of ~145 kV/cm. Ferroelectric measurements for this sample showed the slimmest P–E loop with the lowest remnant polarization ($P_r \approx 2.67$ μC/cm²) and the highest maximum polarization difference ($\Delta P \approx 20.89$ μC/cm²), resulting in an energy density of ~1.68 J/cm³, recoverable energy density (W_{rec}) of ~1.25 J/cm³, and a high energy efficiency of ~74%. These findings demonstrate the strong potential of 0.875KNN–0.125BZO ceramics for high-energy storage applications and broaden the understanding of sintering temperature optimization as a key strategy for unlocking the optimal energy storage performance in KNN-based ceramics.

Keywords: Lead free; $K_{0.5}Na_{0.5}NbO_3$; Energy storage; Sintering Temperature; Relaxor ferroelectric.

Phase Transition and Ferroelectric Properties of KNN- $BiScO_3$ Ferroelectric System

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Piezoelectric materials are a class of dielectric material which have the ability to convert mechanical stress into electric signals and vice-versa. The harmful nature of traditional lead-based ceramics has intensified efforts to discover viable lead-free alternatives. Out of numerous lead-free materials, Potassium Sodium Niobate ($K_{0.5}Na_{0.5}NbO_3$(KNN)) stands most promising because of its high Curie temperature (420°C) and significant ferroelectric and dielectric properties showing implicit applications in piezoelectric sensors, actuators, high-temp capacitor applications, energy-harvesting devices etc.[1] Besides, it has associated problems like the hygroscopic nature of constituent alkali components which renders its physical properties sensitive to atmospheric conditions. Its moderate electromechanical properties, tendency of abnormal grain growth and narrow range of sintering temperature are issues of concern.[2] In order to overcome the above issues, many strategies have been taken into considerations e.g. addition of sintering aid, hot-plasma sintering, micro-wave sintering, spark-plasma sintering, chemical substitution and fabrication of solid solutions. Among these approaches, the fabrication of solid solutions, being the most effective one has been employed in this work. In the present study, we have synthesized the ferroelectric solid solution of KNN and $BiScO_3$. Bi^{3+} is isoelectronic with Pb^{2+} which can hybridize with O^{2-} to produce a lone pair leading to enhancement of piezoelectricity and other functional properties.[3]

The ferroelectric solid solutions with chemical formula: (1-x) $K_{0.5}Na_{0.5}NbO_3$-$x$$BiScO_3$, where x = 0.000, 0.005, 0.010, 0.015, 0.020, 0.030, 0.040, 0.050 are synthesized via conventional solid-state reaction method. A combination of X-ray powder diffraction (XRPD), SEM micrographs, Raman spectroscopy, and temperature-dependent dielectric and piezoelectric measurements were employed to gather data across diverse experimental conditions. XRPD patterns have confirmed the crystallization of the ceramic solid solution in a perovskite phase. Raman scattering spectra and Rietveld refinement analysis of the XRPD data provides deep down insights into the phase transitions driven by composition. Temperature dependent dielectric properties dielectric constant (ε_r) and dielectric loss (tan δ) at various frequencies offers perspective on the ferroelectric phase transition behaviour. The piezoelectric coefficient (d_{33}) for KNN has been significantly enhanced, with a maximum value of 154 pC/N at x = 0.015, highlighting the effectiveness of $BiScO_3$ in enhancing piezoelectric properties.

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Weak ferroelectric response in bulk polycrystalline Y_2O_3-$Hf_{0.5}Zr_{0.5}O_2$ ceramics

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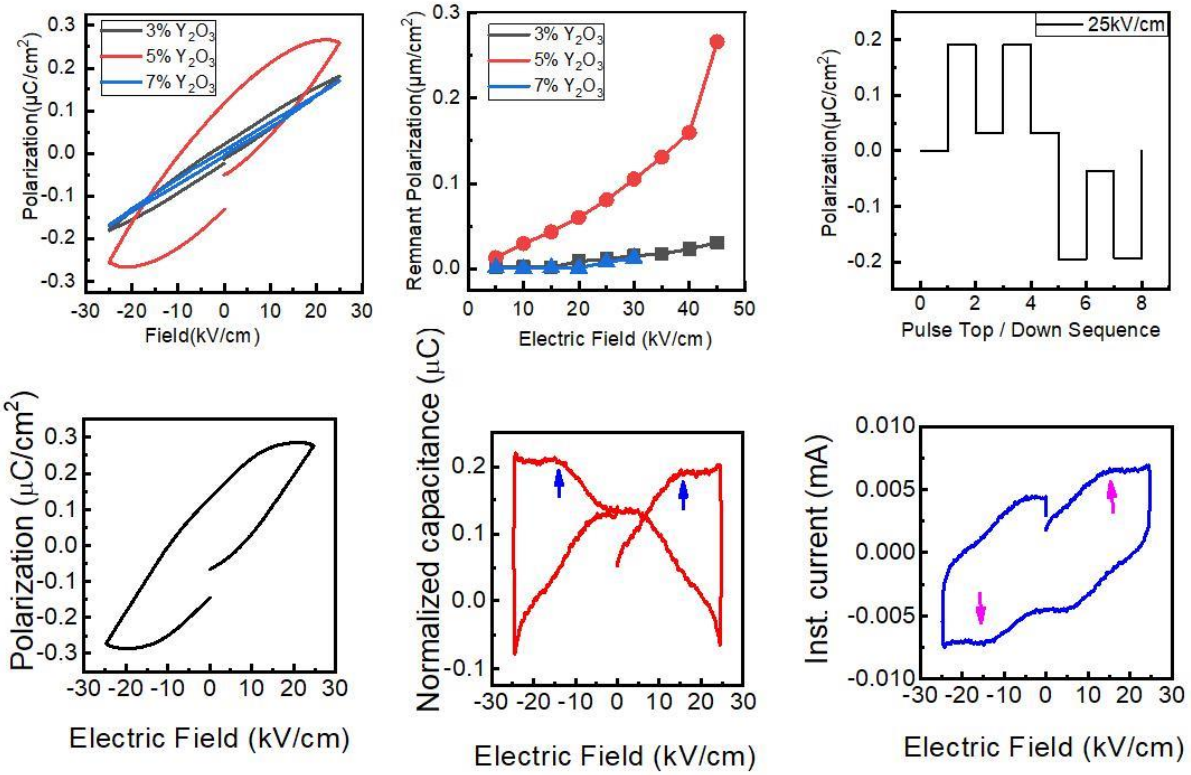
Abstract

The ferroelectric response in HfO_2-ZrO_2 has gained significant attention because of its numerous benefits in devices compared to conventional ferroelectrics. However, so far, ferroelectricity has been reported in thin films. Here, for the first time, a critical composition of polycrystalline Y_2O_3-$Hf_{0.5}Zr_{0.5}O_2$ ceramics has shown a weak ferroelectric response. Through a novel powder poling technique, its mechanism is deduced to be associated with the electric field-induced phase transformation from monoclinic to cubic via an intermediate orthorhombic phase.

Keywords: Ferroelectric, HfO_2, ZrO_2 .



Polarization Reversibility and Electrothermal Response in lead free Disordered Perovskite $0.9Ba_{0.6}Sr_{0.4}TiO_3$-$0.1Bi_{0.5}Na_{0.5}TiO_3$ system

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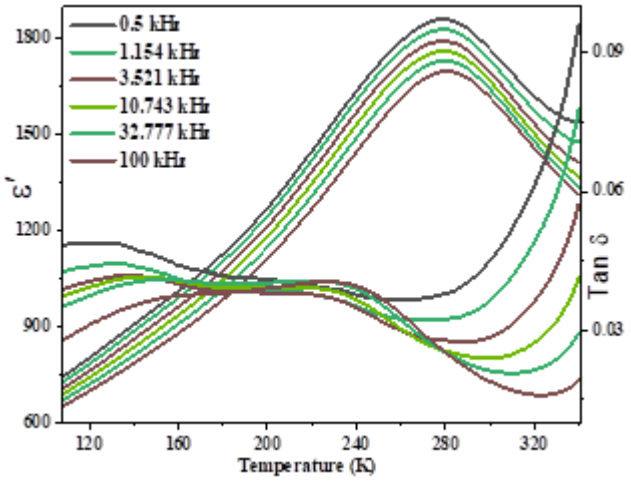
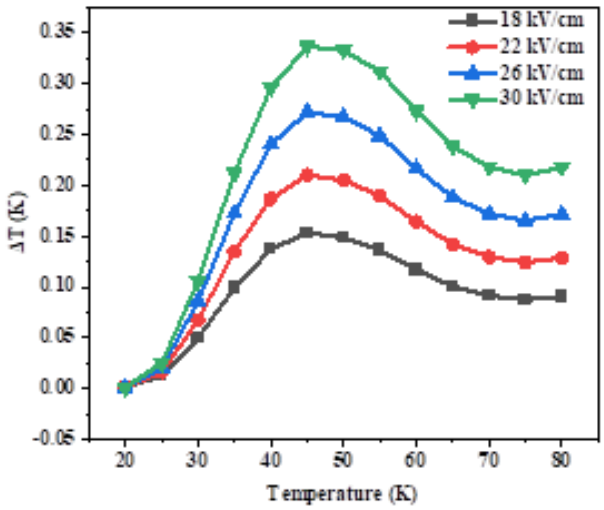
Abstract:

Electrocaloric effect (ECE) is significantly influenced by the phase transition and change in the polarization with respect to temperature. However, the practical implementation has been deeply limited due to the occurance of 1st order ferroelectric to para electric transition at higher temperature. Therefore, our goal orients towards achieving the phase transition near room temperature so as to achieve significant ECE values near room temperature. The present work primarily focuses on the structural, dielectric and ferroelectric properties along with energy storage and electrocaloric performances of the lead free $0.9Ba_{0.6}Sr_{0.4}TiO_3$-$0.1Bi_{0.5}Na_{0.5}TiO_3$ ferroelectric ceramic. Following the preparation of the ceramic using solid state reaction route, X-Ray diffraction has been used to understand the phase purity of the ceramic and Raman spectroscopy provides an insight into the vibrational modes present in the ceramic. The dielectric response shows that the system posseses the transition around a wide temperature range with negligible amount of dielectric loss. The energy storage and electrocaloric performances were investigated from the polarization-Electric field(P-E) loop measurement over a broad temperature range. From the thinner hysteresis loops, we have achieved a maximum energy storage density of 298 mJ/cm^3 with an efficiency of 87% at 68 kV/cm at room temperature. Meanwhile, a maximum EC temperature change (ΔT_{max}) of 0.34 K with an electrocaloric strength of ξ_{max} = 0.12 K mm/kV is obtained under 30 kV/cm at 318 K.





Influence of poling-field strength on the thermal restoration of antiferroelectric order in (Pb, La)(Zr, Sn, Ti)O_3 ceramics

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Lanthanum-modified Lead zirconate stannate titanate [(Pb, La)(Zr, Sn, Ti)O_3 (PLZST)]-based antiferroelectric (AFE) oxides are interesting ceramic materials for capacitors, sensors, and actuator applications. These applications make use of the development of electrical polarization and the change in the specific volume associated with the field-induced antiferroelectric-ferroelectric (FE) phase change.[1] However, in some PLZST compositions, the field-stabilized FE phase can be transformed back to the AFE phase by increasing the temperature to the depolarization temperature (T_d).[2,3] It is generally believed that the better the degree of ferroelectric order induced by the electric field, the more thermal energy is required to restore the antiferroelectric state. Recently, it has been reported that applying an electric field of reverse polarity triggers FE to AFE phase transformation at room temperature.[4] Given this scenario, an interesting question is: *how is the thermal restoration of the AFE phase influenced by the FE phase stabilized by poling the system in a different manner?* We have investigated this aspect on a representative AFE composition $Pb_{1-3x/2}La_x(Zr_{0.60}Sn_{0.30}Ti_{0.10})O_3$. We undertook a comparative study on two different types of samples: (i) samples which were pre-poled (by applying a DC field for 30 minutes at room temperature) and (ii) samples which were not pre-poled. The recovery of the AFE phase from the induced FE phase on heating was ascertained by monitoring the characteristic changes in the shapes of bipolar polarization-field and strain-field measurements. To better appreciate the thermal restoration of the AFE phase, depolarization current curves are recorded. We found that a lower temperature was required to restore the AFE phase in pre-poled specimens compared to non-pre-poled specimens. A plausible mechanism associated with this phenomenon is discussed.

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Role of A-site volatile Compensation and its influence on the Structural and Functional Properties of high T_C $BiScO_3$–$PbTiO_3$ Piezoceramics

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Abstract

The performance of $BiScO_3$–$PbTiO_3$ (BSPT) ceramics in high-temperature piezoelectric applications is critically influenced by the stoichiometry and microstructure, particularly due to Bi_2O_3 and PbO volatility during the high temperature sintering. In this study, a systematic investigation on the effects of excess Bi_2O_3 (0–3 mol%) combined with 1 mol% PbO addition on the structure, microstructure, dielectric behaviour, and ferro/piezoelectric performance of $0.36BiScO_3$–$0.64PbTiO_3$ ceramics synthesized via a solid-state route. Excess additions of Bi and Pb have significantly influenced phase fractions, grain size, and piezoelectric properties of BSPT ceramics. The 2 mol% Bi + 1 mol% Pb excess composition exhibited an optimal tetragonal–rhombohedral phase coexistence near the MPB, along with refined grains (~4.8 μm).Improved dielectric homogeneity and increased grain boundary resistance were confirmed by impedance analysis. Enhanced functional properties—P_r of 28.9 μC/cm², P_s of 36.6 μC/cm², and unipolar strain of 0.226%—reflects the optimized domain switching and stabilized structure. Overall, this work demonstrates how precise stoichiometric tuning of volatile A-site components governs phase evolution, grain structure, and dielectric behavior—establishing strong structure–property correlations for performance optimization in BSPT piezo ceramics.

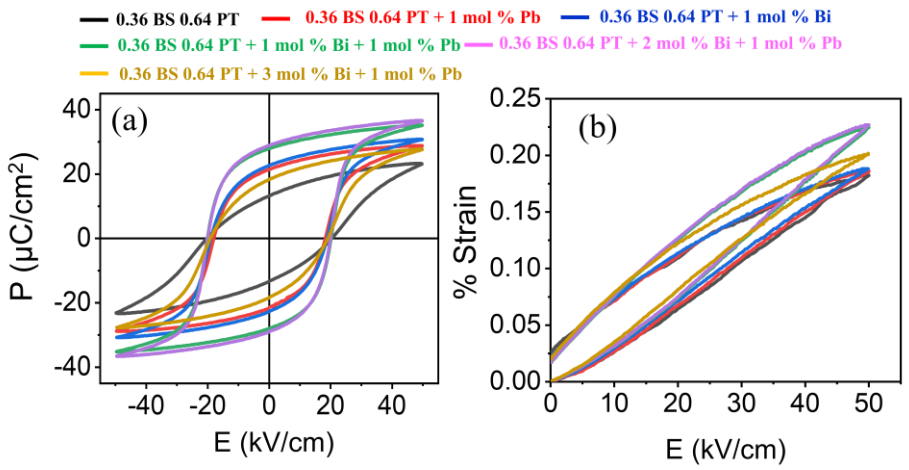

Fig. fig1.*Ferroelectric properties of BSPT ceramics with varying Bi_2O_3 and PbO addition:(a) Polarization–electric field (P–E) loops (b) Unipolar S–E curves.*

Enhanced energy density in the low electric field region via hybrid polarization mechanism in BNT-based relaxors

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Abstract

Dielectric electrostatic capacitors have emerged as a promising solution to the current environmental pollution and energy crisis owing to their quick charge/discharge rates (<1 μs), highest power densities (~10^8 W/kg), highest operational voltage, and exceptional stability/lifetime [1,2]. Although substantial advancements have been made in achieving ultrahigh energy densities in ceramic materials, the energy storage output of the state-of-the art dielectrics remains low, especially under low electric fields, limiting further miniaturization of pulsed power devices. In the present study, the above challenge of enhancing the energy density output at low electric fields in capacitive energy storage was addressed through the development of $(1-x)Bi_{0.35}Na_{0.35}Sr_{0.3}TiO_3$-$xBaZr_{0.15}Ti_{0.85}O_3$ [written as (1−x)BNST-xBZT; $0 \leq x \leq 0.15$] materials employing a solid-state reaction process. Impressive energy storage characteristics of a large recoverable energy density (W_{rec}) of 4.49 J/cm^3, a large efficiency (η) of 86.22 %, and a giant coefficient of energy storage (W_{rec}/E_b) of 0.02401 μC/cm^2 were attained in the 0.88BNST − 0.12BZT sample at a low external field of ~187 kV/cm through a synergistic composition design strategy. The optimized ceramics also displayed outstanding thermal (25 to 140 °C) and frequency (20 to 200 Hz) stability and excellent retention of ferroelectric properties even after 1,00,000 hysteresis cycles. The results demonstrate that 0.88BNST−0.12BZT is a strong alternative for excellent energy storage characteristics, especially in low electric field environments, and this study will guide the further development of miniature, lightweight, and low-cost electrical power systems.

Keywords: Relaxor ferroelectric, BNT-based, Polar nano-regions, Low electric field, Ceramic energy storage.

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Enhancing the Energy Storage performance in (Ba, Ca)(Zr, Ti)O_3 Ceramics via Cerium Oxide Doping

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Abstract: Dielectric ceramic capacitors are necessary in modern electronics, primarily due to their exceptional power density, which highly suitable for pulsed power applications. Among various lead-free ceramic systems, (Ba,Ca)(Zr,Ti)O_3 (BCZT) ceramics have garnered significant attention due to their outstanding dielectric characteristics—namely, high permittivity, superior breakdown strength, and minimal dielectric loss. These qualities make BCZT ceramics as promising candidates for advanced energy storage technologies. This investigation systematically examines the influence of Ce^{4+} ion doping on the energy storage capabilities of BCZT ceramics. Ce^{4+} was incorporated into the BCZT matrix via a cost-effective solid-state reaction route. This study evaluates the resultant modifications in dielectric behaviour, breakdown strength, and energy storage density. Key findings demonstrate that optimally doped Ce^{4+} BCZT ceramics exhibit a markedly enhanced recoverable energy storage density (U_{rec}) of 0.484 J/cm³, accompanied by an efficiency of 86%. In addition, undoped BCZT ceramics display a U_{rec} of 0.25 J/cm³ with an efficiency of 77.8%. The improvement in energy storage performance is attributed to Ce^{4+} which enhance the energy storage capacity. These results underscore the potential of Ce^{4+}-doped BCZT ceramics as advanced dielectric materials for high energy storage density capacitor applications.

Keywords: Dielectric ceramic capacitor, lead-free ceramics, relaxor ferroelectric, energy storage density

Influence of Local Polarization and Octahedral tilt on the specific volume of the ferroelectric alloy system $SrTiO_3$-$Na_{0.5}Bi_{0.5}TiO_3$

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We investigated the associated mechanism with the intriguing phenomenon when the incipient ferroelectric $SrTiO_3$ (ST) is alloyed with $Na_{0.5}Bi_{0.5}TiO_3$ (NBT, a non-ergodic relaxor ferroelectric), the composition dependence of the specific volume of the alloy (1-x)ST-(x)NBT follows a non-monotonic trend giving maximum at $x \sim 0.35$. We found that despite the smaller-size ion combination $Na^{+1}_{0.5}Bi^{+3}_{0.5}$ replacing Sr^{+2} in the host ST matrix, the electrostriction caused by the polar nano regions far overwhelms the size effect and increases the specific volume. This trend ceases when octahedral tilt instability sets in above the critical concentration resulting in a sharp decline in the specific volume.

Key Words: Relaxor Ferroelectric, Octahedral Tilt, X-ray Diffraction, Neutron Diffraction

Influence of defect engineering on electrocaloric behaviour in non-stoichiometric lead-free $BaTiO_3$-based system

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Abstract

Solid-state refrigeration based on the electrocaloric effect (ECE) has recently emerged as a prominent research focus. The ECE is characterised by an adiabatic temperature change (ΔT) in response to the application or removal of an electric field in a ferroelectric material. In the $BaTiO_3$ system, site-engineering through the simultaneous substitution of a heterovalent ion at the Ba-site and an isovalent ion at the Ti-site has emerged as a promising strategy. This dual-site doping approach tunes defect concentrations and dilutes ferroelectric ordering, promoting relaxor-like behaviour. Consequently, the phase transition is broadened across a wide temperature range, allowing the system to sustain a consistent electrocaloric response (ΔT). In this context, the ECE was examined in $Ba_{1-x}La_{2x/3}Ti_{1-y}Zr_yO_3$ ($x = 0.05$; $y = 0.00$, 0.01, 0.03, 0.05, and 0.07) samples synthesised via the solid-state method. The X-ray diffraction data, after Rietveld refinement, revealed the existence of both tetragonal and cubic phases in all samples. For $x = 0.05$, $y = 0.00$, 0.01, and 0.03, the tetragonal phase dominates over the cubic phase, while for $x = 0.05$, $y = 0.05$, and 0.07, the cubic phase dominates over the tetragonal phase. Raman spectroscopy investigations demonstrated the presence of locally generated vibrational modes caused by vacancies at the higher wavelength side, which arise to offset the total charge in the perovskite. The local structural characterisation of the samples by electron paramagnetic resonance (EPR) spectroscopy and X-ray photoelectron spectroscopy (XPS) reveals the existence of cationic vacancies. Temperature-dependent dielectric measurements revealed a decrease in T_C and an increase in the degree of diffuseness (γ) parameters with increased incorporation of Zr. Temperature-dependent pyroelectric current measurement displays three distinct transitions corresponding to the transition from defects, structural transition and lower structural transition. The EC responses estimated using Maxwell's thermodynamic relations from the Pyroelectric current measurement display three distinct EC responses (ΔT_{spike}, ΔT_s and ΔT_f) over three distinct transitions within the operational temperature window, contributing to maximise the ΔT_{span} with the incorporation of Zr. The superior temperature stability of ΔT in these samples makes them potentially suitable for efficient cooling applications.

Keywords: ferroelectric, pyroelectric current, phase transition, vacancy, degree of diffuseness

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Simultaneous enhancement of d_{33} and depolarization temperature of the morphotropic phase boundary composition of the Pb-free piezoceramic $Na_{1/2}Bi_{1/2}TiO_3$–$BaTiO_3$

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Abstract

Piezoceramics are used in wide ranging applications as sensors, actuators and transducers. We investigate the influence of oxygen deficient modifier $BaAlO_{2.5}$ (BAO) on the structure, depolarization temperature, dielectric, and piezoelectric properties of the morphotropic phase boundary composition $Na_{1/2}Bi_{1/2}TiO_3$-6.5$BaTiO_3$ (NBT-6.5BT) of the lead-free piezoceramic solid solution. For practical applications it is desirable that the piezoelectric material exhibit large weak signal longitudinal piezoelectric coefficient (d_{33}) and depolarization temperature (T_d). The d_{33} and T_d of the NBT-6.5BT piezoceramic is ~150 pC/N and 90 ℃, respectively. In general, chemical modification strategies which enhances d_{33} of NBT-BT reduces the depolarization temperature. In contrast to this trend, here we show it is possible to improve both the d_{33} and T_d of NBT-6.5BT ceramic. We found that merely 1 mole percent of BAO increases the d_{33} to 205 pC/N. This is accompanied by a remarkable increase in the T_d to 160 ℃.

Keywords: Pb-free piezoceramic; depolarization temperature; morphotropic phase boundary

Microstructure and ferroelectric studies of aliovalent doped lead-free (K,Na)NbO_3 ceramics

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Abstract:

Lead-free piezoelectric potassium sodium niobate ((K,Na)NbO_3 (KNN)) based perovskite ceramics with the multielement composition $((K_{0.5}Na_{0.5})_{0.975}Li_{0.005}Ba_{0.02}Nb_{0.94-x}Sb_{0.03}Ta_xZr_{0.03}O_3$, x=0.01,0.02,0.03) were synthesized via the conventional solid-state reaction method with double calcination process. Microstructural evolution and secondary phase formation were investigated using scanning electron microscopy (SEM) and X-ray diffraction (XRD). Temperature-dependent dielectric studies from room temperature to 450℃ revealed a crystal structure transition influenced by Ta content. Variation in Ta composition also affected the grain size and tetragonal-cubic transition temperature(T_C). The ferroelectric properties were evaluated using polarization -electric field (P−E) hysteresis loop.

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Influence of A-Site Samarium Substitution on the Dielectric Behaviour of $Ba_{0.6}Sr_{0.4}TiO_3$

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Abstract

Barium strontium titanate ($Ba_{0.6}Sr_{0.4}TiO_3$, BST) is a promising tunable dielectric material, widely explored for microwave and RF phase shifter applications due to its high permittivity and electric field-dependent properties. However, its practical use is limited by high leakage current and moderate dielectric constant, which constrain its tunability and efficiency. To address these issues, Sm^{3+} doping is employed to modify the A-site of the perovskite lattice, where Sm^{3+} partially substitutes Ba^{2+}/Sr^{2+}, inducing local lattice distortions and influencing polarization behaviour. This substitution enhances dipolar interactions by increasing TiO_6 octahedral distortion, resulting in improved dielectric constant and reduced dielectric losses.

In this study, Sm-doped BST ceramics were synthesized via the sol–gel method, enabling fine compositional control and uniform microstructure at lower processing temperatures. X-ray diffraction (XRD) confirmed single-phase perovskite formation with systematic peak shifts, indicating successful Sm incorporation. Rietveld refinement showed a consistent reduction in lattice parameters with increasing Sm content, supporting A-site substitution. Dielectric measurements revealed enhanced permittivity, reduced loss tangent, and improved tunability, contributing to a higher figure of merit (FOM). These results highlight Sm-doped BST as a promising material for tunable components in advanced microwave and RF systems.

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Dimension dependence electrodeformation behavior ($K_{0.5}Na_{0.5}$)NbO_3 -based Pb-free piezoceramics

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Abstract

Recently, there has been series of reports showing ultrahigh strain (~ 1 % or higher) in Pb-free piezoceramics wherein creation of defect dipoles is argued to play a key role in enabling such large strain values. We examine this phenomenon on differently modified ($K_{0.5}Na_{0.5}$)NbO_3 (KNN) piezoceramics. We synthesized solid solutions of KNN with off-stoichiometric compositions such as Sr-modified KNN to deliberately create defect dipoles, and also stoichiometric compositions like KNN-$SrTiO_3$ and Li-modified KNN. We performed thickness dependent electrostrain measurement on disc shaped specimens (10-12 mm in diameter) of these piezoceramics using an electrostrain measurement setup with flat bottom electroded and a movable top cylindrical electrode. We found that in all cases, as the specimen was thinned below 1.0 mm, the bipolar strain loop displayed increasing asymmetry with large strain in one (positive) half cycle and negligible strain in the other (negative) half cycle. We performed x-ray diffraction in-situ with field and found negligible reversible switching of the ferroelectric-ferroelastic domains. Consistent with this result, the true longitudinal strain of these piezoceramics is found to be small (<0.3 %). We confirm that the display of such asymmetric bipolar strain-field loops is not intrinsic longitudinal strain of the piezoceramic material but a manifestation of bending, the magnitude of which increases with decreasing thickness and increasing field.

Superior Piezoelectric Properties in $BiGaO_3$-Modified $BiFeO_3$–$BaTiO_3$ Ceramics: Insights from Phase Stability and Defect Engineering

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$BiFeO_3$–$BaTiO_3$ (BF–BT) lead-free piezoelectric ceramics demonstrate considerable potential for high-temperature applications due to their favorable piezoelectric properties and elevated Curie temperature (T_C). However, the existence of mixed-valence Fe ions (Fe^{2+}/Fe^{3+}) and the volatilization of Bi^{3+} during sintering contribute to the formation of secondary phases ($Bi_{25}FeO_{40}$, $Bi_2Fe_4O_9$) and oxygen vacancies, which substantially impair electrical insulation, which is a critical factor for effective poling. To mitigate this issue, this study examines the effect of $BiGaO_3$ (BG) modification on improving both the insulation and piezoelectric performance of 0.7BF-0.3BT ceramics, thereby facilitating their optimization for high-temperature electromechanical applications. The impact of BG content on phase structure, microstructure, and electrical properties including insulation resistance, dielectric response, ferroelectric polarization, and piezoelectric behavior was thoroughly investigated. The addition of BG stabilizes Fe valence states and reduces oxygen vacancy concentration, leading to a significant enhancement in insulation resistance, with leakage current decreasing to approximately 4×10^{-8} A·cm^{-2}. Furthermore, the optimal coexistence of rhombohedral (R) and pseudo-cubic (PC) phases in 0.7BF-(0.3-x)BT-xBG (x = 0.001–0.005) ceramics results in superior piezoelectric performance, achieving a high piezoelectric coefficient $d_{33} = 242\ pC/N$ and $d_{33}^{*} = 384\ pm/V$, large-signal piezoelectric strain $S\% = 0.25\%$, and an elevated $T_C = 502°C$. The improved thermal stability is attributed to the stabilized R-PC domain structure and its high-temperature switching behavior, which minimizes property degradation under thermal stress. This work confirms that BG modification is an effective approach for enhancing the high-temperature piezoelectric properties of BF–BT ceramics, reinforcing their viability for advanced electromechanical applications.

Keywords: Lead-free piezoelectric ceramics, BF-BT, Defect engineering

Compositional Control and Phase Evolution in NBT-KBT Single Crystals Near the Morphotropic Phase Boundary

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Piezoelectric materials enable energy conversion between mechanical and electrical forms, making them essential for sensors, actuators, and memory devices. The most widely used piezoelectric materials, like PZT, are lead based & offer excellent performance. Due to lead toxicity in conventional materials like PZT, lead-free alternatives such as NBT-BT exhibiting strong piezoelectricity near its morphotropic phase boundary are gaining prominence. The growth of high-quality $(Na_{(1-x)}K_xBi)_{0.5}TiO_3$ single crystals (Figure 1 (a)) using the high-temperature solution growth (self-flux) method is hindered by the preferential segregation of potassium ions. In this study, potassium incorporation was systematically investigated by varying the initial K content in the growth solution. Elemental analysis revealed a consistently low incorporation efficiency of potassium in the resulting crystals. A correlation between the starting Na/K ratio and the final crystal composition was established, offering insights into the segregation behavior.

Structural and piezoelectric properties of the crystals were further analysed as a function of potassium content. X-ray line profile analysis and Rietveld refinement revealed a structural transition with increasing K concentration, with rhombohedral and tetragonal phase coexistence emerging near the morphotropic phase boundary (MPB). Notably, compositions near the MPB exhibited enhanced piezoelectric charge coefficients shown in Figure 1 (b). These findings highlight the critical role of compositional control in optimizing both the structure and functional properties of NBT-KBT single crystals and provide a pathway for tailoring their growth toward targeted applications.

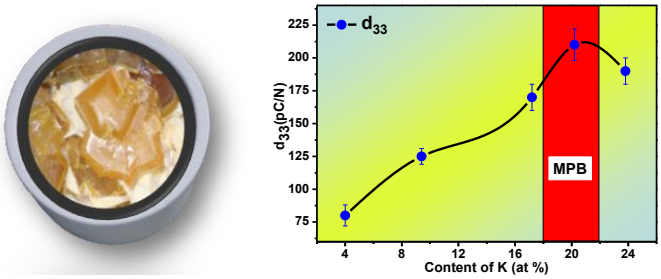

Figure 1: (a) Grown crystals in crucible, (b) Variation of d_{33} coefficient with K content in NBT-KBT

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High-Performance Lead-Free Piezoelectric Ceramics for Sensors and Actuators via Phase Boundary Engineering in KNN-Based Systems

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ABSTRACT

With the growing demand for eco-friendly alternatives to lead-based piezoelectrics, lead-free perovskite ceramics have emerged as promising candidates for applications in actuators, transducers, energy harvesters, and microelectromechanical systems (MEMS). Among these, KNN-based systems have garnered significant attention due to their favorable piezoelectric characteristics and high Curie temperatures. In this study, we investigate a compositionally tuned lead-free ceramic system:

(1-x)$K_{0.4}Na_{0.6}Nb_{0.90}Sb_{0.05}Ta_{0.05}O_3$−x$(Bi_{0.45}Sm_{0.05})Na_{0.5}ZrO_3$(x=0.01–0.04) designed to optimize dielectric, piezoelectric and ferroelectric performance through phase boundary engineering.X-ray diffraction analysis revealed a composition-driven phase evolution: a pure rhombohedral **R3c** structure for x=0.01 and 0.020, a **coexistence of rhombohedral (R3c) and tetragonal (P4mm)** phases at x=0.03, and a **mixed rhombohedral (R3c) and monoclinic (Pm)** phase for x=0.04. The emergence of this **phase coexistence near x=0.03** is associated with a **morphotropic phase boundary (MPB)**-like behavior, resulting in a remarkable enhancement of piezoelectric response.

The piezoelectric charge coefficient d_{33} peaks at 341 pC/N for x=0.03, accompanied by a large dielectric constant (7185 at 1 kHz), and saturated polarization (19.77 μC/cm²), with a moderate coercive field of 7.99 kV/cm. The enhancement is attributed to increased polarization rotation and domain wall motion enabled by the structural instability at the phase boundary. A further increase to x=0.04 leads to a decline in d_{33}, likely due to the stabilization of the monoclinic phase and reduced domain mobility.The dielectric constant increased with x up to 0.03, then declined, while the Curie temperature ranged from 193.3 °C to 216.2 °C, indicating thermal reliability for practical applications. The enhancement in dielectric and piezoelectric properties near the MPB is attributed to increased domain wall mobility and polarization rotation facilitated by structural instability.

These results highlight the potential of this KNN-based system for use in high-performance lead-free piezoelectric devices, particularly in sensors, precision actuators, and energy harvesting systems.

Keywords: Lead-free piezoelectrics, morphotropic phase boundary, KNN ceramics, dielectric constant, actuator materials

Rare-Earth-Driven Structural Engineering for enhanced Piezoelectricity and high Curie temperature in MPB based $Pb_{(1-x)}Sm_{(x)}(Mg_{0.05}Nb_{0.1}Zr_{0.43}Ti_{0.42})$ Ceramics.

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Abstract-

A well-recognized challenge in the design of ferroelectric ceramics is the trade-off between Curie temperature and piezoelectric performance—enhancing one often leads to the compromise of the other. As a result, achieving high piezoelectricity typically lowers the Curie temperature, limiting the material's effectiveness across broad temperature ranges. However, by revisiting the thermal and compositional stability, more advanced and technologically promising phases can be accessed through the design of ternary morphotropic phase boundary (MPB) compositions. Local structure heterogeneity is a generic route towards optimization of the piezoelectric performance via rare earth doping, as rare-earth doping introduces the local structural distortions. To enhance piezoelectric response, we adopt rare earth Sm^{3+} doping into ternary based MPB $Pb_{(1-x)}Sm_{(x)}(Mg_{0.05}Nb_{0.1}Zr_{0.43}Ti_{0.42})$ (x = 0% and 1%) (PMN-PZT) ceramics. The effect of Sm^{3+} doping on the structure, dielectric, ferroelectric and piezoelectric properties of PMN-PZT were investigated. Dielectric spectroscopy and order parameter analysis collectively reveal that the free energy landscape of MPB is further softened via local structural heterogeneity, enabled via rare earth doping. As a result of free energy flattening, dielectric and piezoelectric responses of Sm^{3+} doped system are significantly enhanced with high value of $T_c \sim 300°C$. Piezoelectric voltage coefficient (d^*_{33}) increases from 400 pm/V (x = 0%) to 805 pm/V (x = 1%) with Sm^{3+} doping**.** Observed results suggest that the piezoelectric and ferroic performances of MPB based PMN-PZT can further be improved by hetero-structural tuning via optimized rare earth doping.

Keywords: morphotropic based boundary; piezoelectricity; PZT

Magnetoelectric Performance and Stability of Epoxy-Modulated Ni/PZT Composites: Quasi-Static, Dynamic, and Fatigue Characterization

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Abstract: Magnetoelectric (ME) composites have gained significant interest due to their multifunctional capabilities, making them suitable for applications in sensors, energy harvesters, power converters, and biomedical devices. Effective characterization of these composites is essential for optimizing their performance. This study presents the quasi-static, dynamic, and fatigue characterization of low-cost epoxy-modulated Ni/PZT composites. The effect of PZT distribution within Ni on the composites performance was investigated by increasing the number of PZT discs from one to four while keeping the volume fraction constant. The composites were fabricated using vacuum bagging techniques. A significant enhancement in ME response was observed in the distributed Ni/PZT composites, with both single- and multi-disc configurations exhibiting a self-biased effect at room temperature. Under quasi-static conditions, the four-disc composite achieved an ME coefficient of 2.32 V/cm·Oe, representing a 163% improvement compared to the single-disc configuration. Additionally, the ME coefficient was decrease by approximately 22% in the single-disc and approximately 16% in the four-disc composite at elevated temperatures 75 °C. Furthermore, dynamic characterization revealed maximum ME coefficients of 12 V/cm·Oe and 13.1 V/cm·Oe for the single-disc and four-disc composites, respectively. Fatigue characterization demonstrated that exposure to 10^5 cycles of a DC magnetic field did not degrade the composite performance, confirming the stability of these self-biased composites for various applications.
Keywords: *Magnetoelectric composite, Magnetostriction, Nickel, PZT, Self-biased effect*

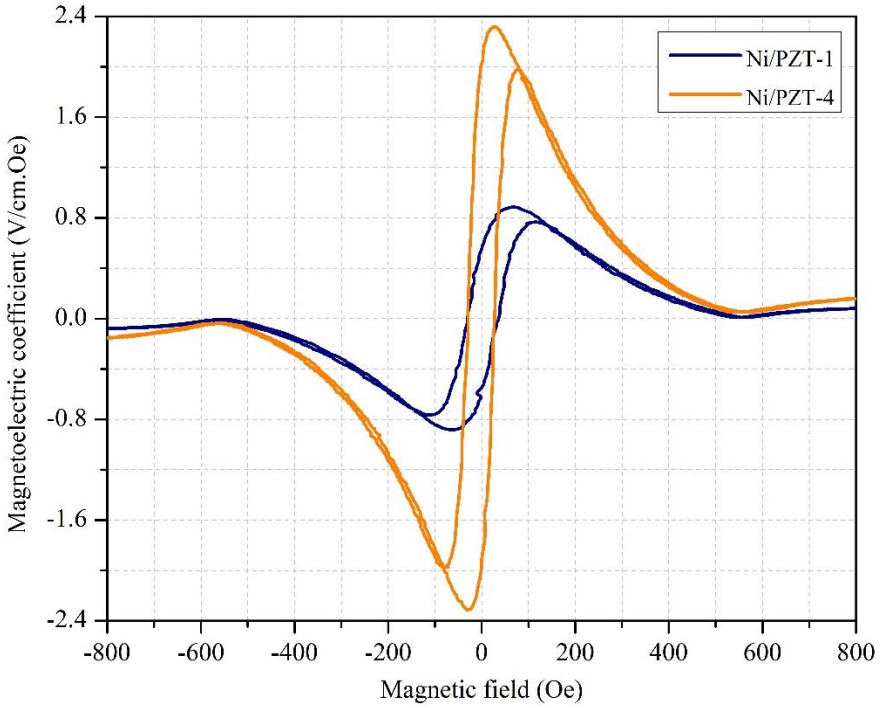

Figure: Variation of magnetoelectric coefficient with biased magnetic field for epoxy-bonded single disc and four discs Ni/PZT composite

Study of anomalous phase transition in modified barium titanate system via structural, electrical and local analysis

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Relaxors are characterised by a diffuse phase transition marked by a broad temperature range over which the transition occurs rather than a sharp first-order transition. In aliovalent systems like (1-x)$BaTiO_3$-$x$$BiScO_3$, weakly interacting nanopolar regions follow Vogel–Fulcher dynamics, limiting long-range dipole order, whereas in the well-studied NBT-BT system, relaxor nature is attributed to strain effects rather than chemical disorder. Le Zang *et al*. reported dual relaxor transitions in lead-free ferroelectrics, attributed to a percolating electric-dipole network (PEDN) formed by acceptor-donor interactions. Diffuse transitions and relaxor behavior in ferroelectrics arise from complex mechanisms, including compositional disorder, polar nanoregions (PNRs), and random fields. In this context, we reported one such exceptional transition in (1-x)$BaTiO_3$-$x$$LiNbO_3$ system. The system shows broad peaks in the dielectric spectra for $x \geq 0.04$, and there is a significant drop in dielectric permittivity. Dielectric spectra for $x \geq 0.04$ suggest that the two temperatures correspond to distinct types of special transitions. The V-F fitting across T_m suggests enhanced dynamic disorder and stronger local interactions among PNRs, indicative of a transition toward more pronounced relaxor behavior. The appearance of additional modes in Raman spectra indicates the disorder present in the system. Temperature-dependent Raman spectra confirm the local structural change occurring in the system from cubic to tetragonal to orthorhombic to rhombohedral upon cooling, although no structural changes are observed in temperature-dependent XRD. This suggests that, despite the average structure remaining unchanged upon cooling, local phase transitions are occurring within the system. Further, the ferroelectric measurement combined with Raman measurement indicates the breaking of long-range symmetry and disorder present in the system. This work helps to understand the mechanism driving the anomalous behaviour of the system and may accelerate the development of the design of future ferroelectric materials.

Keywords: ferroelectrics, relaxors, polar nano regions, barium titanate-based system, phase transition.

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Grain Boundary Engineering via Microwave Sintering in Lead-Free $Na_{0.5}Bi_{0.5}TiO_3$-based Ceramics for Enhanced Dielectric and Energy Storage Applications

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Abstract

Advanced synthesis and characterization techniques in materials science empirically open new avenues for realizing superior physical properties. The implementation of grain boundary engineering technique enhances dielectric strength and promotes relaxor-like characteristics. In this study, we synthesize lead free $0.94(Na_{0.5}Bi_{0.5})_{0.75}Sr_{0.25}TiO_3$-$0.06BaTiO_3$]-xwt%$Li_2CO_3$ via solid state reaction route employing microwave sintering as well as conventional sintering approaches. The microwave-sintered ceramic composition $0.94(Na_{0.5}Bi_{0.5})_{0.75}Sr_{0.25}TiO_3$–$0.06BaTiO_3$–3 wt% Li_2CO_3 demonstrated a high dielectric constant of $4278 \pm 15\%$ across an extended temperature range (96–330°C) as a result of grain boundary engineering. With a fine grain size, microwave-assisted ceramics demonstrate impressive energy storage characteristics, W_r ~1.00 J/cm³ and η ~74.46% for NBST-BT-3Li ceramic sample. Moreover, the microwave sintered samples demonstrated excellent thermal stability in their physical properties across a wide temperature range of 30°C to 180°C. The scaling behavior of the hysteresis loop area provides insight into the complex field-dependent mechanisms governing the material's response. Our study underscores the pivotal role of microwave sintering as an advanced processing technique in the fabrication of high-performance ceramics, particularly for energy storage applications. By enabling refined micro-structural control and grain boundary engineering, microwave sintering significantly contributes to the realization of lead-free ferroelectric ceramics with superior dielectric properties, thermal stability, and energy storage capabilities.

Keywords: Energy storage, $Na_{0.5}Bi_{0.5}TiO_3$, temperature stable, ferroelectrics

Influence of defect engineering on electrocaloric behaviour in non-stoichiometric lead-free $BaTiO_3$-based system

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Abstract

Solid-state refrigeration based on the electrocaloric effect (ECE) has recently emerged as a prominent research focus. The ECE is characterised by an adiabatic temperature change (ΔT) in response to the application or removal of an electric field in a ferroelectric material. In the $BaTiO_3$ system, site-engineering through the simultaneous substitution of a heterovalent ion at the Ba-site and an isovalent ion at the Ti-site has emerged as a promising strategy. This dual-site doping approach tunes defect concentrations and dilutes ferroelectric ordering, promoting relaxor-like behaviour. Consequently, the phase transition is broadened across a wide temperature range, allowing the system to sustain a consistent electrocaloric response (ΔT). In this context, the ECE was examined in $Ba_{1-x}La_{2x/3}Ti_{1-y}Zr_yO_3$ ($x = 0.05$; $y = 0.00$, 0.01, 0.03, 0.05, and 0.07) samples synthesised via the solid-state method. The X-ray diffraction data, after Rietveld refinement, revealed the existence of both tetragonal and cubic phases in all samples. For $x = 0.05$, $y = 0.00$, 0.01, and 0.03, the tetragonal phase dominates over the cubic phase, while for $x = 0.05$, $y = 0.05$, and 0.07, the cubic phase dominates over the tetragonal phase. Raman spectroscopy investigations demonstrated the presence of locally generated vibrational modes caused by vacancies at the higher wavelength side, which arise to offset the total charge in the perovskite. The local structural characterisation of the samples by electron paramagnetic resonance (EPR) spectroscopy and X-ray photoelectron spectroscopy (XPS) reveals the existence of cationic vacancies. Temperature-dependent dielectric measurements revealed a decrease in T_C and an increase in the degree of diffuseness (γ) parameters with increased incorporation of Zr. Temperature-dependent pyroelectric current measurement displays three distinct transitions corresponding to the transition from defects, structural transition and lower structural transition. The EC responses estimated using Maxwell's thermodynamic relations from the Pyroelectric current measurement display three distinct EC responses (ΔT_{spike}, ΔT_s and ΔT_f) over three distinct transitions within the operational temperature window, contributing to maximise the ΔT_{span} with the incorporation of Zr. The superior temperature stability of ΔT in these samples makes them potentially suitable for efficient cooling applications.

Keywords: ferroelectric, pyroelectric current, phase transition, vacancy, degree of diffuseness

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Effect of multipoles on the band structure of $MnSiN_2$

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The asymmetry and anisotropy of charge and magnetization densities, described by charge and magnetic multipoles, significantly influence the fine details of electronic bands. Recent studies have identified rank-3 magnetic octupoles as the lowest-order ferroic magnetic multipoles in inversion-symmetric antiferromagnets, where they give rise to non-relativistic spin splitting (NRSS) with characteristic d-wave symmetry [1]. However, in systems lacking inversion symmetry, magnetoelectric multipoles can emerge as the dominant ferroic components, raising questions about their role in NRSS. In this work, we investigate $MnSiN_2$, a representative material that hosts ferroic ordering of both magnetoelectric multipoles and magnetic octupoles. Our first-principles calculations reveal that magnetic octupoles are responsible for NRSS, while magnetoelectric multipoles introduce band asymmetry via spin-orbit coupling. We further explore the combined influence of these multipoles by analyzing structural and magnetic domains, and demonstrate the coexistence of NRSS with Rashba-type spin splitting arising from the electric dipole moment. Our work highlights the potential of multipolar engineering for tailoring band structures.

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Emergence of polar monoclinic phase in ferroelectric $CsGeX_3$ (X = Cl, Br, I)

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Inorganic halide perovskite of the form ABX_3 (A = Cs, Rb, Molecule; B = Ge, Sn, Pb; X = Cl, Br, I) are known for light absorbing material in optoelectronic devices[1]. The Ge-based halide perovskites have garnered significant attention recently because of their spontaneous polarization of about 12-20$\mu C/cm^2$[2]. The $CsGeX_3$ halide perovskites crystallise in a polar phase R3m at room temperature and undergoes a phase transition to a non-polar phase at high temperature $Pm^{-}3m$. From the effective Hamiltonian study, it is established that under the uniaxial and biaxial strain, the polar phase exhibits the monoclinic phase Cm. In the current, we explore the chemical routes to unravel such polar monoclinic phase, which is a commonly used method in experiments.

We used first-principle-based density functional theory (DFT) simulations as implemented in the Vienna Ab-initio Simulation package (VASP)[3][4][5]. We employed the Perdew-burke-Ernzerhof's (PBE) exchange correlation functional within projected-augmented-wave (PAW) pseudopotential. We carried out the structural relaxation of $CsGeX_3$, with halogens Cl, Br and I, in 2:1 form. The ground state structures exhibit a monoclinic phase with the Cm space group. These chemically tuned structures exhibit polarization larger than their pure form. In addition, the electronic band structure exhibits spin-splitting of 250 meV in the conduction bands. The chemically tuned structures exhibit persistent spin textures (PST), which are coupled to polarization direction. We believe the multifunctional property of these halide perovskites may find application in spintronics and quantum computing.

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