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6. AUTHORS
Jacob L. Jones

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The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT
Phase-transforming materials enable environmental sensing and interaction critical to several military functions such as surveillance, navigation, threat identification, target acquisition, and missile guidance. Domain wall motion, or the planar defects separating regions of spontaneous polarization and strain, underlies the origin and evolution of coupling behavior. This project characterizes domain wall motion and domain configurations under driving forces (e.g. changes in temperature and electric fields) in an effort to: 1) understand the underlying linkage between domain architectures and macroscopic properties, 2) explore new methods to control domain structures, and 3)

15. SUBJECT TERMS
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a. REPORT	b. ABSTRACT	c. THIS PAGE			Jacob Jones
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Report Title

Final Report: Domain Wall Evolution in Phase Transforming Oxides

ABSTRACT

Phase-transforming materials enable environmental sensing and interaction critical to several military functions such as surveillance, navigation, threat identification, target acquisition, and missile guidance. Domain wall motion, or the planar defects separating regions of spontaneous polarization and strain, underlies the origin and evolution of coupling behavior. This project characterizes domain wall motion and domain configurations under driving forces (e.g. changes in temperature and electric fields) in an effort to: 1) understand the underlying linkage between domain architectures and macroscopic properties, 2) explore new methods to control domain structures, and 3) identify unique domain configurations with novel properties. In the final year of this project, we have reported several new results related to the structure of lead-free materials based on Bi, Ba, Ca, Na and K. These results point towards local structures that are dramatically different than lead-based perovskites, the likely reason for lower effective properties. In PZT, we have used in situ diffraction measurements to help develop new constitutive models. We have also used in situ X-ray diffraction of PZT thin films in order to provide key insight into their synthesis and performance. Strong collaborations have continued with Argonne National Laboratories in X-ray scattering, as well as outreach and integration with the Army Research Laboratory.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
01/14/2015	39.00	Chris M. Fancher, Jacob L. Jones, Giovanni Esteves. In situ characterization of polycrystalline ferroelectrics using x-ray and neutron diffraction, Journal of Materials Research, (11 2014): 0. doi: 10.1557/jmr.2014.302
01/14/2015	49.00	Lili Zhao, Matthew Nelson, Henry Aldridge, Thanakorn Iamsasri, Chris M. Fancher, Jennifer S. Forrester, Toshikazu Nishida, Saeed Moghaddam, Jacob L. Jones. Crystal structure of Si-doped HfO2, Journal of Applied Physics, (01 2014): 34104. doi: 10.1063/1.4861733
01/14/2015	48.00	Z. Zhou, O. Obi, T. X. Nan, S. Beguhn, J. Lou, X. Yang, Y. Gao, M. Li, S. Rand, H. Lin, N. X. Sun, G. Esteves, K. Nittala, J. L. Jones, K. Mahalingam, M. Liu, G. J. Brown. Low-temperature spin spray deposited ferrite/piezoelectric thin film magnetoelectric heterostructures with strong magnetoelectric coupling, Journal of Materials Science: Materials in Electronics, (01 2014): 1188. doi: 10.1007/s10854-014-1707-7
01/14/2015	47.00	Robert Dittmer, Wook Jo, Kyle G. Webber, Jacob L. Jones, Jürgen Rödel. Local structure change evidenced by temperature-dependent elastic measurements: Case study on Bi1/2Na1/2TiO3-based lead-free relaxor piezoceramics, Journal of Applied Physics, (02 2014): 84108. doi: 10.1063/1.4866092
01/14/2015	46.00	Jared Carter, Elena Aksel, Thanakorn Iamsasri, Jennifer S. Forrester, Jun Chen, Jacob L. Jones. Structure and ferroelectricity of nonstoichiometric (Na0.5Bi0.5)TiO3, Applied Physics Letters, (03 2014): 112904. doi: 10.1063/1.4868109
01/14/2015	45.00	Goknur Tutuncu, Longlong Fan, Jun Chen, Xianran Xing, Jacob L. Jones. Extensive domain wall motion and deaging resistance in morphotropic 0.55Bi(Ni1/2Ti1/2)O3–0.45PbTiO3 polycrystalline ferroelectrics, Applied Physics Letters, (03 2014): 132907. doi: 10.1063/1.4870506
01/14/2015	44.00	Goknur Tutuncu, Binzhi Li, Keith Bowman, Jacob L. Jones. Domain wall motion and electromechanical strain in lead-free piezoelectrics: Insight from the model system (1 ? x)Ba(Zr0.2Ti0.8)O3–x(Ba0.7Ca0.3) TiO3 using in situ high-energy X-ray diffraction during application of electric fields, Journal of Applied Physics, (04 2014): 144104. doi: 10.1063/1.4870934
01/14/2015	43.00	Sungwook Mhin, Krishna Nittala, Jinhyung Lee, Douglas S. Robinson, Jon F. Ihlefeld, Geoff L. Brennecka, Luz M. Sanchez, Ronald G. Polcawich, Jacob L. Jones. Phase and Texture Evolution in Chemically Derived PZT Thin Films on Pt Substrates, Journal of the American Ceramic Society, (09 2014): 2973. doi: 10.1111/jace.13007
01/14/2015	42.00	Jacob L. Jones, Justin D. Starr, Jennifer S. Andrew. Anisotropy in magnetoelectric composites, Applied Physics Letters, (06 2014): 242901. doi: 10.1063/1.4883639
01/14/2015	41.00	Brian K. Voas, Tedi-Marie Usher, Xiaoming Liu, Shen Li, Jacob L. Jones, Xiaoli Tan, Valentino R. Cooper, Scott P. Beckman. Special quasirandom structures to study the <math xmlns="http://www.w3.org/1998/Math/MathML"><mo>(</mo><msub><mi mathvariant="normal" >K</mi><mn>0.5</mn></msub><msub><mi>Na</mi><mn>0.5</mn></msub><mo>) </mo><mi>Nb</mi><msub><mi mathvariant="normal">O</mi><mn>3</mn></msub></math> random alloy, Physical Review B, (07 2014): 24105. doi: 10.1103/PhysRevB.90.024105

01/14/2015 40.00 Astri Bjørnetun Haugen, Gerhard Henning Olsen, Francesco Madaro, Maxim I. Morozov, Goknur Tutuncu, Jacob L. Jones, Tor Grande, Mari-Ann Einarsrud, D. Johnson. Piezoelectric K0.5Na0.5NbO3 ceramics textured using needle-like K0.5Na0.5NbO3 templates,
Journal of the American Ceramic Society, (12 2014): 3818. doi: 10.1111/jace.13223

02/19/2014 37.00 Dipankar Ghosh, Akito Sakata, Jared Carter, Pam A. Thomas, Hyuksu Han, Juan C. Nino, Jacob L. Jones. Domain Wall Displacement is the Origin of Superior Permittivity and Piezoelectricity in BaTiO,
Advanced Functional Materials, (02 2014): 0. doi: 10.1002/adfm.201301913

02/19/2014 38.00 Humberto Foronda, Marco Deluca, Elena Aksel, Jennifer S. Forrester, Jacob L. Jones. Thermally-induced loss of piezoelectricity in ferroelectric Na0.5Bi0.5TiO3–BaTiO3,
Materials Letters, (01 2014): 0. doi: 10.1016/j.matlet.2013.10.041

08/06/2012 24.00 Anderson D. Prewitt, Jacob L. Jones. Effects of the Poling Process on Piezoelectric Properties in Lead Zirconate Titanate Ceramics,
Ferroelectrics, (01 2011): 0. doi: 10.1080/00150193.2011.594725

08/06/2012 22.00 Jennifer Forrester, Elena Aksel, Benjamin Kowalski, Marco Deluca, Dragan Damjanovic, Jacob Jones. Structure and properties of Fe-modified Na_{0.5}Bi_{0.5}TiO_{3} at ambient and elevated temperature,
Physical Review B, (01 2012): 24121. doi: 10.1103/PhysRevB.85.024121

08/06/2012 21.00 Dipankar Ghosh, Hyuksu Han, Juan C. Nino, Ghatu Subhash, Jacob L. Jones, S. Trolier-McKinstry. Synthesis of BaTiO3-20wt%CoFe2O4 Nanocomposites via Spark Plasma Sintering,
Journal of the American Ceramic Society, (08 2012): 2504. doi: 10.1111/j.1551-2916.2012.05221.x

08/06/2012 20.00 Goknur Tutuncu, Yunfei Chang, Stephen Poterala, Gary L. Messing, Jacob L. Jones, J. Roedel. In Situ Observations of Templated Grain Growth in (Na0.5K0.5)0.98Li0.02NbO3 Piezoceramics: Texture Development and Template-Matrix Interactions,
Journal of the American Ceramic Society, (08 2012): 2653. doi: 10.1111/j.1551-2916.2012.05268.x

08/06/2012 19.00 Eva-Maria Anton, Ljubomira Ana Schmitt, Manuel Hinterstein, Joe Trodahl, Ben Kowalski, Wook Jo, Hans-Joachim Kleebe, Jürgen Rödel, Jacob L. Jones. Structure and temperature-dependent phase transitions of lead-free Bi1/2Na1/2TiO3–Bi1/2K1/2TiO3–K0.5Na0.5NbO3 piezoceramics,
Journal of Materials Research, (07 2012): 0. doi: 10.1557/jmr.2012.195

08/06/2012 18.00 Goknur Tutuncu, Dragan Damjanovic, Jun Chen, Jacob Jones. Deaging and Asymmetric Energy Landscapes in Electrically Biased Ferroelectrics,
Physical Review Letters, (04 2012): 177601. doi: 10.1103/PhysRevLett.108.177601

08/06/2012 17.00 Elena Aksel, Goknur Tutuncu, Jacob Jones, Tedi-Marie Usher, Jun Chen, Xianran Xing, Andrew Studer. Domain wall and interphase boundary motion in a two-phase morphotropic phase boundary ferroelectric: Frequency dispersion and contribution to piezoelectric and dielectric properties,
Physical Review B, (07 2012): 24104. doi: 10.1103/PhysRevB.86.024104

08/06/2012 23.00 Elena Aksel, Jennifer Forrester, Benjamin Kowalski, Jacob Jones, Pam Thomas. Phase transition sequence in sodium bismuth titanate observed using high-resolution x-ray diffraction,
Applied Physics Letters, (12 2011): 222901. doi: 10.1063/1.3664393

08/10/2012 26.00 Elena Aksel, Jennifer Forrester, , Humberto Foronda, Robert Dittmer, Dragan Damjanovic, Jacob L. Jones. Structure and Properties of La-modified Na0.5Bi0.5TiO3 at Ambient and Elevated Temperatures,
Journal of Applied Physics, (08 2012): 0. doi:

08/28/2011 8.00 Jennifer S. Forrester, Jacob L. Jones, Jinxia Deng, Ranbo Yu, Xianran Xing, Krishna Nittala, Jun Chen. The Role of Spontaneous Polarization in the Negative Thermal Expansion of Tetragonal PbTiO,
Journal of the American Chemical Society, (07 2011): 0. doi: 10.1021/ja2046292

08/28/2011 16.00 Thorsten Leist, Kyle G. Webber, Wook Jo, Emil Aulbach, Jürgen Rödel, Anderson D. Prewitt, Jacob L. Jones, Josh Schmidlin, Camden R. Hubbard. Stress-induced structural changes in La-doped BiFeO3–PbTiO3 high-temperature piezoceramics,
Acta Materialia, (10 2010): 0. doi: 10.1016/j.actamat.2010.07.012

08/28/2011 15.00 Wook Jo, John E. Daniels, Jacob L. Jones, Xiaoli Tan, Pamela A. Thomas, Dragan Damjanovic, Ju?rgen Ro?del. Evolving morphotropic phase boundary in lead-free (Bi[sub 1/2]Na[sub 1/2])TiO[sub 3]–BaTiO [sub 3] piezoceramics,
Journal of Applied Physics, (01 2011): 0. doi: 10.1063/1.3530737

08/28/2011 14.00 Abhijit Pramanick, Dragan Damjanovic, John E. Daniels, Juan C. Nino, Jacob L. Jones. Origins of Electro-Mechanical Coupling in Polycrystalline Ferroelectrics During Subcoercive Electrical Loading,
Journal of the American Ceramic Society, (02 2011): 0. doi: 10.1111/j.1551-2916.2010.04240.x

08/28/2011 13.00 Mie Marsilius, Torsten Granzow, Jacob L Jones. Effect of electrical and mechanical poling history on domain orientation and piezoelectric properties of soft and hard PZT ceramics,
Science and Technology of Advanced Materials, (02 2011): 0. doi: 10.1088/1468-6996/12/1/015002

08/28/2011 12.00 Alp Sehirlioglu, Ali Sayir, Fred Dynys, Krishna Nittala, Jacob Jones. Structure and Piezoelectric Properties Near the Bismuth Scandium Oxide-Lead Zirconate-Lead Titanate Ternary Morphotropic Phase Boundary,
Journal of the American Ceramic Society, (03 2011): 0. doi: 10.1111/j.1551-2916.2010.04142.x

08/28/2011 11.00 Mie Marsilius, Torsten Granzow, Jacob L. Jones. Quantitative comparison between the degree of domain orientation and nonlinear properties of a PZT ceramic during electrical and mechanical loading,
Journal of Materials Research, (4 2011): 0. doi: 10.1557/jmr.2011.40

08/28/2011 10.00 Jennifer S. Forrester, Elena Aksel, Jacob L. Jones, Pam A. Thomas, Katharine Page, Matthew R. Suchomel. Monoclinic crystal structure of polycrystalline Na[sub 0.5]Bi[sub 0.5]TiO[sub 3],
Applied Physics Letters, (04 2011): 0. doi: 10.1063/1.3573826

08/28/2011 9.00 Matthew Davies, Elena Aksel, Jacob L. Jones. Enhanced High-Temperature Piezoelectric Coefficients and Thermal Stability of Fe- and Mn-Substituted Na0.5Bi0.5TiO3 Ceramics,
Journal of the American Ceramic Society, (05 2011): 0. doi: 10.1111/j.1551-2916.2011.04441.x

08/31/2010 1.00 John E. Daniels, Wook Jo, Jürgen Rödel, V. Honkimäki, Jacob L. Jones. Electric-field-induced phase change behavior in (Bi0.5Na0.5)TiO3 - BaTiO3 - (K0.5Na0.5)NbO3: A combinatorial investigation,
Acta Materialia, (11 2009): . doi:

08/31/2010 2.00 Elena Aksel, Jacob L. Jones. Advances in Lead-Free Piezoelectric Materials for Sensors and Actuators,
Sensors, (03 2010): . doi:

08/31/2010 3.00 Thorsten Leist, Kyle G. Webber, Wook Jo, Emil Aulbach, Jürgen Rödel, Anderson D. Prewitt, Jacob L. Jones, Joshua Schmidlin, Cambden Hubbard. Stress induced structural changes in La-doped BiFeO3-PbTiO3 high temperature piezoceramics,
Acta Materialia, (07 2010): . doi:

08/31/2013 27.00 Sungwook Mhin, Clayton Cozzan, Krishna Nittala, Patrick Wanninkhof, Jon F. Ihlefeld, Geoff L. Brennecka, Jacob L. Jones. Effect of Switching Atmospheric Conditions during Crystallization on the Phase Evolution of Solution-Derived Lead Zirconate Titanate Thin Films,
Journal of the American Ceramic Society, (08 2013): 0. doi: 10.1111/jace.12522

08/31/2013 28.00 Goknur Tutuncu, Thanakorn Iamsasri, Chunmanus Uthaisar, Soodkhet Pojprapai, Jacob L. Jones. Analysis methods for characterizing ferroelectric/ferroelastic domain reorientation in orthorhombic perovskite materials and application to Li-doped Na0.5K0.5NbO3,
Journal of Materials Science, (06 2013): 6905. doi: 10.1007/s10853-013-7495-2

08/31/2013 29.00 Elena Aksel, Jennifer S. Forrester, Juan C. Nino, Katharine Page, Daniel P. Shoemaker, Jacob L. Jones. Local atomic structure deviation from average structure of Na_{0.5}Bi_{0.5}TiO_{3}: Combined x-ray and neutron total scattering study,
Physical Review B, (03 2013): 104113. doi: 10.1103/PhysRevB.87.104113

08/31/2013 30.00 Yo-Han Seo, Daniel J. Franzbach, Jurij Koruza, Andreja Bencan, Barbara Malic, Marija Kosec, Jacob L. Jones, Kyle G. Webber. Nonlinear stress-strain behavior and stress-induced phase transitions in soft Pb (Zr(1-x)Tix)O3 at the morphotropic phase boundary,
Physical Review B, (03 2013): 94116. doi: 10.1103/PhysRevB.87.094116

08/31/2013 31.00 I. M. Reaney, E-M. Anton, Wook Jo, I. Levin, J. Rödel, J. Pokorny, L. A. Schmitt, H-J. Kleebe, M. Hinterstein, J. L. Jones. Local structure, pseudosymmetry, and phase transitions in Na_{1/2}Bi_{1/2}TiO_{3}–K_{1/2}Bi_{1/2}TiO_{3} ceramics,
Physical Review B, (01 2013): 24113. doi: 10.1103/PhysRevB.87.024113

08/31/2013 32.00 Jennifer S. Forrester, Dragan Damjanovic, Binzhi Li, Keith J. Bowman, Jacob L. Jones, Astri Bjo?rnetun Haugen. Structure and phase transitions in 0.5(Ba0.7Ca0.3TiO3)-0.5(BaZr0.2Ti0.8O3) from -100°C to 150°C,
Journal of Applied Physics, (01 2013): 14103. doi: 10.1063/1.4772741

08/31/2013 33.00 A. Pramanick, J. L. Jones, G. Tutuncu, D. Ghosh, A. D. Stoica, K. An. Strain incompatibility and residual strains in ferroelectric single crystals,
Scientific Reports, (12 2012): 929. doi: 10.1038/srep00929

08/31/2013 34.00 J. S. Forrester, C. R. dela Cruz, J. L. Jones, T.-M. Usher. Crystal structure of 0.96(Na0.5Bi0.5TiO3)–0.04 (BaTiO3) from combined refinement of x-ray and neutron diffraction patterns,
Applied Physics Letters, (10 2012): 152906. doi: 10.1063/1.4759117

08/31/2013 35.00 Abhijit Pramanick, Anderson D. Prewitt, Jennifer S. Forrester, Jacob L. Jones. Domains, Domain Walls and Defects in Perovskite Ferroelectric Oxides: A Review of Present Understanding and Recent Contributions,
Critical Reviews in Solid State and Materials Sciences, (12 2012): 243. doi: 10.1080/10408436.2012.686891

08/31/2013 36.00 Dipankar Ghosh,, Akito Sakata, Jared Carter, Pam A. Thomas, Hyuksu Han, Juan C. Nino, Jacob L. Jones. Domain wall displacement is the origin of superior permittivity and piezoelectricity in BaTiO3 at intermediate grain sizes,
Advanced Functional Materials, (09 2013): 0. doi:

TOTAL: 44

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

INVITED departmental seminars and INVITED meeting presentations by the PI that acknowledged ARO support:

- "Mechanics of Smart Materials: Origins of Property Coefficients from in situ X-ray and Neutron Scattering," J. L. Jones, University of California San Diego, Department of NanoEngineering, Departmental Seminar, November 1, 2012.
- "In situ X-ray and neutron diffraction tools in materials science," J. L. Jones,* K. Nittala, G. Tutuncu, and A. Pramanick, 24th Annual Kavli Frontiers of Science Symposium, National Academy of Sciences, Arnold and Mabel Beckman Center, Irvine, California, November 4, 2012.
- "Origins of Piezoelectric, Dielectric, and Elastic Property Coefficients from in situ X-ray and Neutron Scattering," J. L. Jones, Departmental Seminar, Department of Materials Science and Engineering, North Carolina State University, Raleigh, NC, September 21, 2012.
- "Diffraction of ferroelectrics during electric field application: Comprehensive results of lattice strain, domain wall and interphase boundary motion in traditional and emerging compositions," J. L. Jones, Conference on Smart Materials, ASME Adaptive Structures & Intelligent Systems (SMASIS), Stone Mountain, GA, September 19, 2012.
- "Mechanics of Smart Materials: Origins of Property Coefficients from in situ X-ray and Neutron Scattering," J. L. Jones, College of Engineering Structural Mechanics Seminar Series, Georgia Institute of Technology, Atlanta, GA, September 18, 2012.

Presentations given by students, postdocs, or other collaborators that acknowledged ARO support:

- "Domain wall motion and electric?field?induced strains in NBT?xBT solid solutions from in situ neutron diffraction," T.-M. Usher,* J. S. Forrester, E. Aksel, A. J. Studer, and J. L. Jones, Electronic Materials and Applications 2013, Orlando, FL, January 23-25, 2013. (Usher received the annual best student oral presentation award at EMA 2013 from the Electronics Division of the American Ceramic Society)
- "Crystallographic refinement yields point defect and lattice changes in PZT as a result of neutron irradiation," J. S. Forrester,* A. Henriques, S. B. Seshadri, D. Brown, J. T. Graham, S. Landsberger, J. Ihlefeld, G. L. Brennecka, and J. L. Jones, Electronic Materials and Applications 2013, Orlando, FL, January 23-25, 2013.
- "In situ diffraction reveals the dependence of domain wall motion on BaTiO3 grain size and relation to macroscopic properties," D. Ghosh,* A. Sakata, J. Carter, P. A. Thomas, H. Han, J. C. Nino, and J. L. Jones, Electronic Materials and Applications 2013, Orlando, FL, January 23-25, 2013.
- "Crystallographic and Electrical Properties of (Na0.5?xBi0.5+x)TiO3±?, where (?0.01?x?0.01)," J. J. Carter,* E. Aksel, J. S. Forrester, and J. L. Jones, Electronic Materials and Applications 2013, Orlando, FL, January 23-25, 2013.
- "Mechanical Depoling and Piezoelectricity Loss in the Region of the Morphotropic Phase Boundary of NBT?BT," L. M. Denis,* J. Glaum, M. Hoffman, J. Forrester, and J. L. Jones, Electronic Materials and Applications 2013, Orlando, FL, January 23-25, 2013.
- "Structural Changes in Lead Zirconate Titanate due to High Neutron Radiation Exposure," A. Henriques,* J. S. Forrester, S. B. Seshadri, D. Brown, J. T. Graham, J. Ihelfeld, G. L. Brennecka, and J. L. Jones, Electronic Materials and Applications 2013, Orlando, FL, January 23-25, 2013. (2nd place winner of overall student poster competition)
- "Crystallographic changes in lead zirconate titanate due to high neutron radiation exposure," A. Henriques,* J. Forrester, S. Seshadri, J. Graham, S. Landsberger, J. Ihlefeld, G. Brennecka, D. Brown, and J. L. Jones, International Workshop on Scattering Techniques for Nuclear Materials, Berkeley, CA, October 17-19, 2012.

Number of Presentations: 12.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received	Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received	Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received	Paper
08/06/2012 25.00	Abhijit Pramanick, Anderson Prewitt, Jennifer Forrester, Jacob Jones. Domains, domain walls and defects in perovskite ferroelectric oxides: A review of present understanding and recent contributions, Critical Reviews in Solid State and Materials Sciences (04 2011)
08/31/2010 4.00	Alp Sehirlioglu, Krishna Nittala, Jacob L. Jones, and A. Sayir. Structure and Piezoelectric Properties near the Bismuth Scandium Oxide-Lead Zirconate-Lead Titanate Ternary Morphotropic Phase Boundary, Journal of the American Ceramic Society (07 2010)
08/31/2010 5.00	Mie Marsilius, Torsten Granzow, Jacob L. Jones. Influence of electrical and mechanical poling history on domain orientation and piezoelectric properties of soft and hard PZT ceramics, Acta Materialia (08 2010)
08/31/2010 6.00	• Abhijit Pramanick, Dragan Damjanovic, John E. Daniels, Juan C. Nino, Jacob L. Jones. Origins of electro-mechanical coupling in polycrystalline ferroelectrics during subcoercive electrical loading, Journal of the American Ceramic Society (08 2010)
08/31/2010 7.00	Anderson D. Prewitt, Jacob L. Jones. Effects of the Poling Process on Piezoelectric Properties in Lead Zirconate Titanate Ceramics, Ferroelectrics (08 2010)

TOTAL: **5**

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT SUPPORTED	Discipline
Giovanni Esteves	1.00	
Tedi-Marie Usher	1.00	
FTE Equivalent:	**2.00**	
Total Number:	**2**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Jennifer Forrester	0.50
Chris Fancher	0.20
FTE Equivalent:	**0.70**
Total Number:	**2**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Jacob Jones	0.08	
FTE Equivalent:	**0.08**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED	Discipline
Jared Carter	1.00	Materials Science and Engineering
Lyndsey Denis	1.00	Materials Science and Engineering
FTE Equivalent:	**2.00**	
Total Number:	**2**	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 2.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 2.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 2.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 2.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 2.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME
Total Number:

Names of other research staff

NAME	PERCENT SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

Major scientific results and accomplishments are highlighted in the ten (14) peer-reviewed papers that have been published within the past project year. The experimental and theoretical work on these publications spanned the present reporting year and the prior project year at the University of Florida. A brief summary of the most impactful results are provided here:

1. Magnetoelectric Coupling: We considered the innate anisotropy of piezoelectric and magnetostrictive materials to determine the ideal directions and orientation relationships for which the maximum magnetoelectric response may be observed in a composite or heterostructure of these constituent materials. We introduced a formalism for the magnetoelectric effect that takes into account the independent anisotropy of the piezoelectric and magnetostrictive phases and their relative orientation. A maximum magnetoelectric effect was predicted in orientations that have not yet been synthesized experimentally, suggesting a need for the development of new routes to synthesize and fabricate designed composite materials with enhanced magnetoelectric response. This work was published in Applied Physics Letters in 2014.

2. Domain Wall Motion: Many of our prior domain wall motion studies have involved lead zirconate titanate (PZT) and lead-free compositions Na0.5K0.5NbO3 (NKN) and Na0.5Bi0.5TiO3 (NBT). This past year, we reported results on piezoelectric compositions (1-x)Ba(Zr0.2Ti0.8)O3–x(Ba0.7Ca0.3)TiO3 (BZT-xBCT) and 0.55Bi(Ni1/2Ti1/2)O3 – 0.45PbTiO3 (BNT-45PT) that provide further fundamental insight into domain wall motion in ferroelectrics. BZT-xBCT spans a model lead-free morphotropic phase boundary (MPB) between room temperature rhombohedral and tetragonal phases at approximately x=0.5. In this system, in situ X-ray diffraction measurements during electric field application were used to elucidate the origin of electromechanical strain in several compositions spanning the tetragonal compositional range $0.6 \leq x \leq 0.9$. As BCT concentration decreases towards the MPB, the tetragonal distortion (given by c/a-1) decreased concomitantly with an increase in 90° degree domain wall motion. The increase in observed macroscopic strain is predominantly attributed to the increased contribution from 90° domain wall motion. The results demonstrate that domain wall motion is a significant factor in achieving high strain and piezoelectric coefficients in lead-free polycrystalline piezoelectrics. We then reported similar measurements in the ferroelectric morphotropic phase boundary composition BNT-45PT. After application of strong electric fields, two phases were shown to coexist. In the tetragonal phase of this material, the extent of 90° domain wall motion is significant and the domain alignment is nearly saturated. Weak (subswitching) cyclic electric fields were then shown to induce domain wall motion. Deaging, or the progressive loss of preferred domain orientation during sequentially increasing field amplitudes, is notably low in these materials, showing that the initial domain alignment is strongly stabilized. Overall, the in situ measurements on these two compositions bring useful fundamental structure-property relations to the field of electroactive materials and reinforces the importance of understanding domain wall motion contributions to the physical properties of ferroelectrics. This work was published in Applied Physics Letters and Journal of Applied Physics.

3. Designed Atmospheric Changes During Crystallization of Films: The crystallization behavior of solution-derived lead zirconate titanate (PZT) thin films in different atmospheric environments was first studied using in situ X-ray diffraction. The stability of the transient intermetallic Pt3Pb phase and perovskite PZT was found to be dependent on oxygen partial pressure during crystallization. Based on the relationship between oxygen partial pressure and the resultant phase stability of intermediate phases, a new route to produce PZT thin films was developed. The new route involves switching atmospheres during crystallization and is shown to mitigate the formation of the transient intermetallic Pt3Pb phase and to promote the perovskite PZT phase. The route evidences a new and significant variable controlling film synthesis and film microstructure. This work was published in Journal of the American Ceramic Society.

Technology Transfer

The PI interacts with Dr. Ron Polcawich at the ARL Adelphi site on topics related to PZT thin films.