

Yijia Gu

ASSISTANT PROFESSOR · MISSOURI UNIVERSITY OF SCIENCE AND TECHNOLOGY

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Education

PH.D in Materials Science and Engineering (Minor: Computational Science)

PENNSYLVANIA STATE UNIVERSITY

University Park, PA

Aug. 2009 - Oct. 2014

- Advisor: Long-Qing Chen
- Dissertation: "Phase-Field Modeling of Flexoelectric Effect in Perovskite Ferroelectrics"

M.ENG in Materials Physics and Chemistry

SHANGHAI JIAO TONG UNIVERSITY

Shanghai, China

Sep. 2006 - Mar. 2009

- Advisor: Xuejung Jin
- Thesis: "The Ordering Transformations in Au-Cu-Al Alloys"

B.ENG in Materials Science and Engineering

SHANDONG UNIVERSITY

Jinan, China

Aug. 2002 - Jul. 2006

Employment History

Assistant Professor

MISSOURI UNIVERSITY OF SCIENCE AND TECHNOLOGY

Rolla, MO

Jan. 2019 - Present

Staff Engineer, Senior Engineer

ARCONIC TECHNOLOGY CENTER (PREVIOUSLY ALCOA TECHNICAL CENTER)

New Kensington, PA

Nov. 2014 - Nov. 2018

Student Internship

LAWRENCE LIVERMORE NATIONAL LABORATORY

Livermore, CA

Jun. 2011 - Aug. 2011

Research Interests

- Computational materials science (phase-field method, CALPHAD, and first-principles calculations)
- Additive manufacturing of metals and alloys
- Alloy design, microstructural modeling of metallurgical processes
- Phase-field modeling of domain switching of functional oxides, chemical reaction-driven phase transformations, and ionic transport in batteries and other energy materials

Honors & Awards

- 2017 **Finalist**, Global Impact Awards, Arconic Inc.
- 2014 **Chinese Government Award for Outstanding Students Abroad**, China Scholarship Council
- 2013 **Diamond Award**, Graduate Excellence in Materials Science, the American Ceramic Society
- 2013 **TMS Travel Grant**, Metals and Materials Society (TMS)
- 2012 **2nd Place**, Annual Departmental Graduate Poster Competition, Pennsylvania State University
- 2012 **Robert E. Newnham Award for Research Excellence**, Department of MatSE, Pennsylvania State University
- 2007 **Showa Denko Scholarship**, Shanghai Jiao Tong University
- 2005 **Chinese Academy of Sciences Scholarship**, Shandong University
- 2005 **1st-Class (top 5%) Scholarship**, Shandong University
- 2004 **General Group Scholarship**, Shandong University
- 2004 **1st-Class (top 5%) Scholarship**, Shandong University
- 2003 **General Group Scholarship**, Shandong University
- 2003 **1st-Class (top 5%) Scholarship**, Shandong University

Publications

- ORCID: 0000-0001-8036-6309
- ResearcherID: A-6418-2013
- Google Scholar

Peer-Reviewed Journal Articles

1. B. Wang, **Y. Gu**, S. Zhang and L. Q. Chen, "Flexoelectricity in solids: Progress, challenges and perspectives", *Progress of Materials Science* 106, 100570 (2019)
2. F. Xue, Y. Li, **Y. Gu**, J. Zhang and L. Q. Chen, "Strain phase separation: Formation of ferroelastic domain structures", *Physical Review B* 94, 220101(R) (2016)
3. N. F. Quackenbush, H. Paik, M. J. Wahila, S. Sallis, M. E. Holtz, X. Huang, A. Ganose, B. J. Morgan, D. O. Scanlon, **Y. Gu**, F. Xue, L. Q. Chen, G. E. Sterbinsky, C. Schlueter, T. L. Lee, J. C. Woicik, J. H. Guo, J. D. Brock, D. A. Muller, D. A. Arena, D. G. Schlom, L. F. J. Piper, "Stability of the M_2 phase of vanadium dioxide induced by coherent epitaxial strain", *Physical Review B* 94, 085105 (2016)
4. F. Xue, X. Wang, I. Socolenco, **Y. Gu**, L. Q. Chen and S. W. Cheong, "Evolution of statistical distribution of a topological defect network", *Scientific Reports* 5, 17057 (2015)
5. D. Lee, H. Lu, **Y. Gu**, S. Y. Choi, S. D. Li, S. Ryu, T. R. Paudel, K. Song, E. Mikheev, S. Lee, S. Stemmer, D. A. Tenne, S. H. Oh, E. Y. Tsybal, X. Wu, L. Q. Chen, A. Gruverman and C. B. Eom, "Emergence of room-temperature ferroelectricity at reduced dimensions", *Science* 349 (6254), 1314-1317 (2015)
6. **Y. Gu**, N. Wang, F. Xue and L. Q. Chen, "Origin of interfacial polar order in incipient ferroelectrics", *Physical Review B* 91, 174103 (2015)
7. M. D. Biegalski, L. Qiao, **Y. Gu**, A. Mehta, Q. He, Y. Takamura, A. Y. Borisevich and L. Q. Chen, "Impact of symmetry on the ferroelectric properties of CaTiO_3 thin films", *Applied Physics Letters* 106, 162904 (2015)
8. L. Jiang, Y. Zhou, Y. Zhang, Q. Yang, **Y. Gu** and L. Q. Chen, "Polarization switching of the incommensurate phase induced by flexoelectric coupling in ferroelectric thin films", *Acta Materialia* 90, 344-354 (2015)
9. **Y. Gu**, Z. Hong, J. Britson and L. Q. Chen, "Nanoscale mechanical switching of ferroelectric polarization via flexoelectricity", *Applied Physics Letters* 106, 022904 (2015)
10. F. Xue, L. Liang, **Y. Gu**, I. Takeuchi, S. V. Kalinin, and L. Q. Chen, "Composition- and pressure-induced ferroelectric to antiferroelectric phase transitions in Sm-doped BiFeO_3 system", *Applied Physics Letters* 106, 012903 (2015)
11. F. Xue, **Y. Gu**, L. Liang, Y. Wang and L. Q. Chen, "Orientations of low-energy domain walls in perovskites with oxygen octahedral tilts", *Physical Review B* 90, 220101(R) (2014)
12. M. Li, **Y. Gu**, Y. Wang, L. Q. Chen and W. Duan, "First-principles study of 180° domain walls in BaTiO_3 : Mixed Bloch-Néel-Ising character", *Physical Review B* 90, 054106 (2014)
13. **Y. Gu**, F. Xue, S. Lei, T. T. A. Lummen, J. Wang, V. Gopalan and L. Q. Chen, "Monoclinic phases arising across thermal inter-ferroelectric phase transitions", *Physical Review B* 90, 024104 (2014)
14. **Y. Gu**, M. Li, A. N. Morozovska, Y. Wang, E. Eliseev, V. Gopalan and L. Q. Chen, "Flexoelectricity and ferroelectric domain wall structures: Phase-field modeling and DFT calculations", *Physical Review B* 89, 174111 (2014)
15. T. Favaloro, J. Suh, B. Vermeersch, K. Liu, **Y. Gu**, L. Q. Chen, K. X. Wang, J. Wu and A. Shakouri, "Direct observation of nanoscale Peltier and Joule effects at metal-insulator domain walls in vanadium dioxide nanobeams", *Nano Letters* 14, 2394-2400 (2014)
16. M. D. Maya, E. A. Eliseev, **Y. Gu**, L. Q. Chen, V. Gopalan and A. N. Morozovska, "Electric-field induced ferromagnetic phase induced in paraelectric antiferromagnets", *Physical Review B* 89, 014112 (2014)
17. T. T. A. Lummen, **Y. Gu**, J. Wang, S. Lei, F. Xue, A. Kumar, A. T. Barnes, E. Barnes, S. Denev, A. Belianinov, M. Holt, A. N. Morozovska, S. V. Kalinin, L. Q. Chen and V. Gopalan, "Thermotropic phase boundaries in classic ferroelectrics", *Nature Communications* 5, 3172 (2014)
18. E. A. Eliseev, S. V. Kalinin, **Y. Gu**, M. D. Glinchuk, V. Khist, A. Borisevich, V. Gopalan, L. Q. Chen and A. N. Morozovska, "Universal emergence of spatially modulated structures induced by flexo-antiferrodistortive coupling in multiferroics", *Physical Review B* 88, 224105 (2013)
19. A. N. Morozovska, **Y. Gu**, V. V. Khist, M. D. Glinchuk, L. Q. Chen, V. Gopalan and E. A. Eliseev, "Low-symmetry monoclinic ferroelectric phase stabilized by oxygen octahedra rotations in strained $\text{Eu}_x\text{Sr}_{1-x}\text{TiO}_3$ thin films", *Physical Review B* 87, 134102 (2013)
20. **Y. Gu**, L. Q. Chen, T. W. Heo, L. Sandoval, J. F. Belak, "Phase field model of deformation twinning in tantalum: Parameterization via molecular dynamics", *Scripta Materialia* 68 (7), 451-454 (2013)
21. D. J. Franzbach, **Y. Gu**, L. Q. Chen and K. G. Webber, "Electric field-induced tetragonal to orthorhombic phase transitions in $[110]_c$ -oriented BaTiO_3 single crystals", *Applied Physics Letters* 101, 232904 (2012)
22. E. A. Eliseev, A. N. Morozovska, **Y. Gu**, A. Y. Borisevich, L. Q. Chen, V. Gopalan and S. V. Kalinin, "Conductivity of twin-domain-wall/surface junctions in ferroelastics: Interplay of deformation potential, octahedral rotations, improper ferroelectricity, and flexoelectric coupling", *Physical Review B* 86, 085416 (2012)
23. **Y. Gu**, K. Rabe, E. Bousquet, V. Gopalan and L. Q. Chen, "Phenomenological thermodynamic potential for CaTiO_3 single crystals", *Physical Review B* 85, 064117 (2012)
24. C. T. Nelson, P. Gao, J. R. Jokisaari, C. Heikes, C. Adamo, A. Melville, S. H. Baek, C. M. Folkman, B. Winchester, **Y. Gu**, Y. Liu, K. Zhang, E. Wang, J. Li, L. Q. Chen, C. B. Eom, D. G. Schlom and X. Pan, "Domain dynamics during ferroelectric switching", *Science* 334 (6058), 968-971 (2011)
25. W. Fan, J. Cao, J. Seidel, **Y. Gu**, J. Yim, C. Barrett, K. Yu, J. Ji, R. Ramesh, L. Q. Chen, J. Wu, "Large kinetic asymmetry in the metal-insulator transition nucleated at localized and extended defects", *Physical Review B* 83, 235102 (2011) (Editor's Choice)
26. J. Cao, **Y. Gu**, W. Fan, L. Q. Chen, D. F. Ogletree, K. Chen, N. Tamura, M. Kunz, C. Barrett, J. Seidel and J. Wu, "Extended mapping and exploration of the vanadium dioxide stress-temperature phase diagram", *Nano Letters* 10, 2667-2673 (2010)
27. **Y. Gu**, J. Cao, J. Wu and L. Q. Chen, "Thermodynamics of strained vanadium dioxide single crystals", *Journal of Applied Physics* 108, 083517

(2010)

28. M. Jin, **Y. Gu** and X. Jin, "Characterization of ordering transitions in Au-Cu-Al alloys", *Materials Characterization* 60, 1395-1399 (2009)
29. **Y. Gu**, M. Jin and X. Jin, "A2 $\rightarrow$ B2 $\rightarrow$ L2₁ ordering transitions in Au-Cu-Al alloys", *Intermetallics* 17, 704-707 (2009)
30. M. Jin, **Y. Gu** and X. Jin, "Internal friction analysis of transformations in AuCuAl alloy", *Journal of Shanghai Jiaotong University* 44, 609-612 (2010) (in Chinese)
31. **Y. Gu**, M. Jin and X. Jin, "Martensitic transformation in Au-Cu-Al alloy system", *Journal of Shanghai Jiaotong University* 44, 36-40 (2010) (in Chinese)

Book Chapters

1. L. Q. Chen and **Y. Gu**, "Chapter 27: Computational Metallurgy" in *Physical Metallurgy* (5th Edition), 2807-2835 (2014), edited by D. E. Laughlin and K. Hono

Conference Proceedings

1. C. T. Nelson, P. Gao, J. P. Jokisaar, X. Pan, C. Heikes, C. Adamo, A. Melville, D. G. Scholm, S. Beak, C. M. Folkman, C. Eom, B. Winchester, **Y. Gu**, L. Q. Chen, Y. Liu, and J. Li, "Interface effects on static and dynamic properties of multiferroic BiFeO₃", *Microscopy and Microanalysis* 18 (S2: Proceedings of Microscopy & Microanalysis 2012), 320-321 (2012)
2. M. Jin, H. Ding, **Y. Gu** and X. Jin, "Precipitation in Fe-Ni-Co-Ti ferromagnetic shape memory alloy", *International Journal of Modern Physics B* 24, 2363-2368 (2010)
3. M. Jin, **Y. Gu** and X. Jin, "Precipitation during austempering and composition design for ferromagnetic shape memory effect of Fe-Ni-Co-Ti alloys", *International Conference on Martensitic Transformations (ICOMAT)*, 601-606 (2008)
4. N. Min, **Y. Gu** and X. Jin, "Strain aging of heavily drawn pearlitic steel wires", *Advanced Materials Research* 26-28, 1299-1302 (2007)

Patents

1. J. Lin, Z. Tang, A. Kulovits, **Y. Gu**, and L. Karabin, "Additively manufactured alloy products and methods of making the same", International Application No. PCT/US2018/050843, Publication NO. WO/2019/055630
2. J. Lin, Z. Tang, A. Kulovits, **Y. Gu**, and L. Karabin, "Aluminum alloy products, and methods of making the same", International Application No. PCT/US2018/050835, Publication NO. WO/2019/055623
3. D. Heard, J. Lin, L. Karabin, C. Yanar, **Y. Gu**, A. Askin, Z. Tang, A. Kulovits, "Aluminum alloys having iron and rare earth elements", International Application No. PCT/US2018/027622, Publication No. WO/2018/191695
4. T. Borchers, **Y. Gu**, J. Lin, K. Williams, J. Williams, and J. McMichael, "Aluminum alloy compositions, products and methods of making the same", International Application No. PCT/US2018/020031, Publication No. WO/2018/157159
5. L. Karabin, D. Heard, Z. Tang, **Y. Gu**, M. Chu, J. Lin, and A. Kulovits, "Aluminum alloy products having fine eutectic-type structures, and methods for making the same", International Application No. PCT/US2017/067979, Publication WO/2018/119283
6. Z. Tang, L. Karabin, **Y. Gu**, C. Yanar, W. Wang, R. Nguyen-Dinh, and D. Sauza, "Nickel-iron-aluminum-chromium based alloys, and products made therefrom", International Application No. PCT/US2017/054559, Publication No. WO/2018/097901
7. H. Ding, X. Jin, M. Jin, **Y. Gu**, Y. Gao, "Ferro-nickel-cobalt-titanium alloy with room-temperature sheet martensitic structure and preparation method thereof", Chinese Patent, CN 101560630 A
8. X. Jin, X. Zhang, R. Wang, D. Zhu, J. Chen, W. Zhang, M. Jin, and **Y. Gu**, "A gold alloy with 18k span effect and preparation method thereof", Chinese Patent, CN 101565783 B

Presentations

1. L. Karabin, J. Lin, **Y. Gu**, and A. Kulovits, "Development of Novel Alloys for Additive Manufacturing Applications", **MS&T Meeting**, Pittsburgh, PA, October, 2017 (Contributed)
2. **Y. Gu**, F. Xue, S. Lei, T. T. Lummen, J. Wang, V. Gopalan, and L. Q. Chen, "Monoclinic phases arising across thermal inter-ferroelectric phase transitions", **MRS Fall Meeting**, Boston, MA, December, 2014 (Oral)
3. **Y. Gu**, and L. Q. Chen, "Thermodynamics of strained VO₂ single crystals", **MRSEC IRG2 Seminar**, Pennsylvania State University, University Park, PA, October, 2014 (Oral)
4. **Y. Gu**, M. Li, J. Britson, Y. Wang, V. Gopalan, and L. Q. Chen, "Phase-field modeling of flexoelectric effect in perovskite ferroelectrics", **MRSEC IRG1 Seminar**, Pennsylvania State University, University Park, PA, October, 2014 (Oral)
5. **Y. Gu**, M. Li, A. N. Morozovska, Y. Wang, J. Britson, E. A. Eliseev, A. Gruverman, V. Gopalan, and L. Q. Chen, "Phase-field modeling of flexoelectric effect in ferroelectrics", **Workshop on Multifunctional Interface Materials**, Madison, WI, August 2014 (Oral)
6. **Y. Gu**, M. Li, A. N. Morozovska, Y. Wang, J. Britson, E. A. Eliseev, A. Gruverman, V. Gopalan, and L. Q. Chen, "Phase-field modeling of flexoelectric effect in ferroelectrics", **the Third International Symposium on Phase-Field Method**, State College, PA, August, 2014 (Poster)
7. **Y. Gu**, M. Li, A. N. Morozovska, Y. Wang, J. Britson, E. A. Eliseev, A. Gruverman, V. Gopalan, and L. Q. Chen, "Phase-field modeling of flexoelectric effect in ferroelectrics", **IEEE ISAF Workshop**, State College, PA, May, 2014 (Oral)
8. **Y. Gu**, M. Li, A. N. Morozovska, Y. Wang, E. A. Eliseev, V. Gopalan, and L. Q. Chen, "Non-Ising character of a ferroelectric wall arises from a flexoelectric effect", **Workshop on the Fundamental Physics of Ferroelectrics and Related Materials**, Washington, DC, January, 2014 (Poster)
9. **Y. Gu**, M. Li, Y. Wang, V. Gopalan, L. Q. Chen, A. N. Morozovska, and E. A. Eliseev, "Flexoelectricity and ferroelectric domain wall structures: Phase-field model", **MRS Fall Meeting**, Boston, MA, December, 2013 (Oral)

10. **Y. Gu**, J. Britson, L. Q. Chen, H. Lu, and A. Gruverman, "Mechanical switching via flexoelectricity: Phase-field simulation", **MRS Fall Meeting**, Boston, MA, December, 2013 (Oral)
11. **Y. Gu**, M. Li, Y. Wang, V. Gopalan, L. Q. Chen, A. N. Morozovska, and E. A. Eliseev, "Flexoelectricity induced charged domain walls: Phase-field model", **MS&T Meeting**, Montreal, QC, Canada, October, 2013 (Oral, **Invited**)
12. **Y. Gu**, L. Sandoval, T. W. Heo, J. F. Belak, and L. Q. Chen, "A phase field model of deformation twinning in tantalum: Parameterization via molecular dynamics", **Graduate Exhibition**, Pennsylvania State University, University Park, PA, March, 2013 (Poster)
13. **Y. Gu**, T. T. Lummen, F. Xue, V. Gopalan, and L. Q. Chen, "The polarization rotation mechanism in ferroelectric phase transitions", **MRS Fall Meeting**, Boston, MA, November, 2012 (Poster)
14. **Y. Gu**, V. Gopalan, L. Q. Chen, A. N. Morozovska, and E. A. Eliseev, "Phase-field modeling of flexoelectricity in perovskite ferroelectrics", **MS&T Meeting**, Pittsburgh, PA, October, 2012 (Oral)
15. **Y. Gu**, F. Xue, and L. Q. Chen, "Mesoscale domain structures of complex oxides: Phase-field method", **Materials Day**, Pennsylvania State University, University Park, PA, April, 2012 (Poster)
16. **Y. Gu**, J. Cao, J. Wu and L. Q. Chen, "A phase-field model for the structural transition of vanadium dioxide single crystals", **MRS Fall Meeting**, Boston, MA, November, 2011 (Poster)
17. **Y. Gu**, K. Rabe, E. Bousquet, V. Gopalan and L. Q. Chen, "A phenomenological thermodynamic potential for CaTiO_3 single crystals", **MS&T Meeting**, Columbus, OH, October, 2011 (Poster)
18. **Y. Gu**, K. Rabe, E. Bousquet, V. Gopalan and L. Q. Chen, "A phenomenological potential for CaTiO_3 single crystals", **MRSEC Seminar**, Pennsylvania State University, University Park, PA, March, 2011 (Oral)
19. **Y. Gu**, J. Cao, J. Wu and L. Q. Chen, "Thermodynamics of strained vanadium dioxide single crystals", **MRS Fall Meeting**, Boston, MA, December, 2010 (Poster)

Teaching Experience

Missouri University of Science and Technology

- MET 4637: Material Selection, Fabrication and Failure, Fall 2019

Pennsylvania State University (Teaching Assistant)

- MatSE 503: Kinetics of Materials Processes, Spring 2013
- MatSE 401: Thermodynamics of Materials, Fall 2011

Professional Activities

NSF Panel Review Member

- CMMI Advanced Manufacturing (5/2016)

Journal Reviewer

- Acta Materialia
- Applied Physics Letters
- Computational Materials Science
- International Journal of Mechanics and Materials in Design
- International Journal of Modern Physics B
- JOM (Journal of The Minerals, Metals & Materials Society)
- Journal of Applied Physics
- Materials Letters
- Modeling and Simulation in Materials Science and Engineering
- Modern Physics Letters B
- Nanotechnology
- Science and Technology of Advanced Materials

Professional Affiliations

- TMS (member)