

Yongfeng Zhang, Ph.D

Contact information

Engineering Physics Department
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Research Interest

Computational nuclear materials, microstructure evolution, structure-property correlation, mechanical deformation, fracture

Education

Ph.D. (2009)	Mechanical Engineering	Rensselaer Polytechnic Institute
M. S. (2004)	Mechanical Engineering	University of Science and Technology of China
B. S. (2001)	Mechanical Engineering	University of Science and Technology of China

Professional experience

2019-present, Assistant Professor, Engineering Physics Department, University of Wisconsin
2015-2019: Computational Microstructure Science Group Lead, INL
2011-2019: Staff Scientist, Fuel Modeling and Simulation Department, INL
2010-2011: Postdoctoral Researcher, Fuel Modeling and Simulation Department, INL

Honors/Awards

- 2016: Laboratory Director's Award for Leadership, INL.
- 2016: Expanded Recognition Award, Nuclear Science & Technology Directorate, INL (group awarded as the lead).
- 2014, 2016, 2017 & 2018 (4 times): Exceptional Contribution Program Award, INL.
- Guanghua Scholarship, University of Science and Technology of China.
- Outstanding student scholarship (3 times), University of Science and Technology of China.

Teaching experience

- 2006: Teaching assistant, Introduction to Finite Elements, Rensselaer Polytechnic Institute
- 2006: Teaching assistant, Computer-Aided Design, Rensselaer Polytechnic Institute
- 2001: Substitute instructor, General Physics, University of Science and Technology of China

Project leadership

Principal investigators (PIs) of DOE programs (non-proposal-based)

- DOE NE NEAMS lower length-scale model development package (INL, FY15-FY19)
- DOE NE NEAMS ATF-HIP lower length-scale model development package (INL, FY16-17)
- DOE NNSA USHPRR microstructure level modeling work package (INL, FY16-FY18)

PIs of INL Laboratory directed research & development projects (LDRD, Proposal-based)

- 19A39-071FP: *Mitigating irradiation assisted stress corrosion cracking by rapid alloy design*, FY19-FY21

- 14-026: *Multiscale Modeling on Delayed Hydride Cracking in Zirconium: Hydrogen Transport and Hydride Nucleation*, FY14-FY16;
- 13-050, *Concurrent Atomistic to Macroscale Modeling of Materials under Irradiation Using the Phase Field Crystal Method*, FY14-FY15

Co-PIs of INL LDRDs

- 19A39-012FP: *Accelerated Nuclear Materials and Fuel Qualification by Adopting a First to Failure Approach*, (FY19-FY21; PI: Dr. Jeffery Aguiar)
- 17P11-007FP: *Coupling of Modeling and Experiment to Develop Predictive Models of the Mechanical Behavior of Nuclear Fuels and Materials* (FY18-FY20; PI: Dr. Cheng Sun)
- 16-010: *Development of a fully coupled radiation damage production and evolution simulation capability* (FY16-FY18; PI: Dr. Daniel Schwen)

Co-PIs of Office of Science, Basic Energy Science projects (proposal-based)

- Core program: *The Role of Anisotropy on the Self-Organization of Gas Bubble Superlattices* (FY17 – FY19); PI: Dr. Jian Gan.
- Energy Frontier Research Center: *Thermal Energy Transport under Irradiation* (FY19); PI: Dr. David Hurley.

Co-PIs of Nuclear Energy University Programs (NEUP, proposal-based)

- 16-10821: *Microstructure, Thermal, and Mechanical Properties Relationships in U and UZr Alloys* (PI: Dr. Maria Okuniewski, Purdue University)
- 16-10667: *A Coupled Experimental and Simulation Approach to Investigate the Impact of Grain Growth, Amorphization, and Grain Subdivision in Accident Tolerant U₃Si₂ Light Water Reactor Fuel* (PI: Dr. Michael Tonks, Pennsylvania State University)
- 16-10221: *Alloying agents to Stabilize Lanthanides Against Fuel Cladding Chemical Interaction: Tellurium and Antimony Studies* (PI: Dr. Jinsuo Zhang, Ohio State University)
- 16-10537: *Enhancing Irradiation Tolerance of Steels via Nanostructuring by Innovative Manufacturing Techniques* (PI: Dr. Haiming Wen, Idaho State University)
- 17- 12748: *Combined modeling and experiments to predict corrosion and embrittlement in dual-phase stainless steels within the MARMOT framework* (PI: Dr. Julie Tucker, Oregon State University)

Academic services

Proposal review: INL LDRD; DOE NEUP; DOE Small Business Innovation Research program

Journal review (over 25 journals): Nature Communications, Nature Scientific Reports, Proceedings of the National Academy of Science (PNAS), Physical Review Letters, Journal of Nuclear Materials, Acta Materialia, Physical Review B, Journal of Physical Chemistry, etc.

Conference symposiums and event organization

- TMS 2017 & TMS 2019, “Ceramic Materials for Nuclear Energy Research and Applications”
- Student Career Forum at TMS2017 Meeting
- MRS-Spring 2015, “Multiscale Modeling on The Microstructure Evolution in Nuclear Materials”
- Society of Engineering Science 2017 Meeting, “Radiation Damage and Defect Mechanics”

Publications

Journal publications (* as corresponding authors)

1. C. Sun, D. J. Sprouster, **Y. Zhang**, C. Di, Y. Wang, L. E. Ecker, and J. Gan, *Formation window of gas bubble superlattice in molybdenum under ion implantation*, Phys. Rev. Mat., in press.
2. W. Jiang, T. Hu, L. K. Aagesen and **Y. Zhang**, *Three-dimensional Phase-field Modeling of Porosity Dependent Intergranular Fracture in UO₂*, Computational Materials Science, in press.

3. M. G. Abdoelatef, F. Badry, D. Schwen, C. Permann, **Y. Zhang**, and K. Ahmed, *Mesoscale Modeling of High Burn-Up Structure Formation and Evolution in UO₂*, JOM, in press.
4. B. Beeler, D. Andersson, M. W. Cooper and **Y. Zhang**, *A molecular dynamics study of the behavior of Xe in U₃Si₂*, Journal of Nuclear Materials 523, 413-420 (2019).
5. Y. Gao*, **Y. Zhang***, D. Schwen, C. Jiang and J. Gan, *Bifurcation and Pattern Symmetry Selection in Reaction-Diffusion Systems with Kinetic Anisotropy*, Scientific Reports 9(1),7835 (2019).
6. D.J. Sprouster, C. Sun, **Y. Zhang**, S.N. Chodankar, J. Gan and L.E. Ecker, *Irradiation-Dependent Helium Gas Bubble Superlattice in Tungsten*, Scientific reports 9 (1), 2277 (2019).
7. Y. Zhang, D. Schwen, **Y. Zhang**, X.-M. Bai, *Effects of oversized tungsten on the primary damage behavior in Fe-W alloys*, Journal of Alloys and Compounds 794, 482-490 (2019).
8. B. J. Heuser, T. R. Prisk, J.-L. Lin, T. J. Dax, and **Y. Zhang**, *Direct measurement of hydrogen diffusivity and solubility limits in Zircaloy 2 (formula unit of ZrH_{0.0153}) using incoherent quasi-elastic neutron scattering*, Journal of Nuclear Materials 518, 177-189 (2019).
9. L. K. Agesen, D. Schwen, M. R. Tonks, and **Y. Zhang**, *Phase-field modeling of fission gas bubble growth on grain boundaries and triple junctions in UO₂ nuclear fuel*, Computational Materials Science 161, 35-45 (2019).
10. B. Beeler, M. Baskes, D. Andersson, M. W.D. Cooper, and **Y. Zhang**, *Molecular dynamics investigation of grain boundaries and surfaces in U₃Si₂*, Journal of Nuclear Materials, 514, 290-298 (2019).
11. Y. Gao, Y. Wang and **Y. Zhang**, *Deformation Pathway and Defect Generation in Crystals: A Combined Group Theory and Graph Theory Description*, IUCrJ, 6, 99-104 (2019).
12. Y. Gao, **Y. Zhang***, D. Schwen, C. Jiang and J. Gan, *Formation and Self-organization of Void Superlattices under Irradiation: A Phase Field Study*, Materialia 1, 77-88 (2018).
13. Y. Gao, **Y. Zhang***, D. Schwen, C. Jiang, C. Sun, J. Gan, and X.M. Bai, *Self-organization of void superlattice under irradiation*, Scientific Reports 8, 6629 (2018).
14. Y. Gao, **Y. Zhang**, B. W. Beeler, Y. Wang, *Self-organized multi-grain patterning with special grain boundaries produced by phase transformation cycling*, Physical Review Materials 2, 073402 (2018).
15. B. Beeler, **Y. Zhang**, and Y. Gao, *An atomistic study of grain boundaries and surfaces in γ U-Mo*, Journal of Nuclear Materials 507, 207-211 (2018).
16. B. Beeler, **Y. Zhang**, M. Okuniewski, C. Deo, *Calculation of the displacement energy of α and γ uranium*, Journal of Nuclear Materials 508, 181-194 (2018).
17. C. Jiang, **Y. Zhang**, Y. Gao and J. Gan, *Ab initio theory of noble gas atoms in bcc transition metals*, Phys. Chem. Chem. Phys. 20, 17048-17058 (2018).
18. D.J. Antonio, K. Shrestha, J.M. Harp, C.A. Adkins, **Y. Zhang**, J. Carmack et al., *Thermal and transport properties of U₃Si₂*, Journal of Nuclear Materials 508, 154-158 (2018).
19. C. Sun, D. J. Sprouster, K. Hattar, L. E. Ecker, L. He, Y. Gao, **Y. Zhang** and J. Gan, *Formation of tetragonal gas bubble superlattice in bulk molybdenum under helium ion implantation*, Scripta Materialia 149, 26-30 (2018).
20. S. R. Phillpot, A. C. Antony, L. Shi, M. L. Fullarton, T. Liang, S. B. Sinnott, **Y. Zhang** and S. B. Biner, *Charge Optimized Many Body (COMB) Potentials for Simulation of Nuclear Fuel and Clad*, Computational Materials Science 148, 231-241(2018).
21. J. Gan, C. Sun, L. He, **Y. Zhang**, C. Jiang, and Y. Gao, *Thermal Stability of Helium Bubble Superlattice under TEM in-situ Heating*, Journal of Nuclear Materials 505, 207-211 (2018).
22. S. Novascone, P. Medvedev, J.W. Peterson, **Y. Zhang**, J. Hales, *Modeling porosity migration in LWR and fast reactor MOX fuel using the finite element method*, Journal of Nuclear Materials 508, 226-236 (2018).
23. I. Greenquist, M. R. Tonks, **Y. Zhang**, *Review of Sintering and Densification in Nuclear Fuels: Physical Mechanisms, Experimental Results, and Computational Models*, Journal of Nuclear Materials 507, 381-395 (2018).
24. **Y. Zhang***, C. Jiang, and X. Bai, *Anisotropic hydrogen diffusion in α -Zr and Zircaloy predicted by accelerated kinetic Monte Carlo simulations*, Scientific Reports 7, 41033 (2017).
25. M. R. Tonks, D. Andersson, S. R. Phillpot, **Y. Zhang**, R. Williamson, C. R. Stanek, B. P. Uberuaga, S. L. Hayes, *Mechanistic materials modeling for nuclear fuel performance*, Annals of Nuclear Energy 105, 11-24 (2017).

26. K. Ahmed, M. R. Tonks, **Y. Zhang**, B. Biner, A. El-Azab, *Particle-grain boundary interactions: A phase field study*, Comp. Mater. Sci. 134, 25-37 (2017).
27. W. Z. Xu, **Y. Zhang**, G. M. Cheng, S.N. Mathaudhu, R.O. Scattergood, C.C. Koch, E. J. Lavernia, Y. T. Zhu, *On the origin and behavior of irradiation-induced c-component dislocation loops in magnesium*, Acta Mater. 131, 457-466 (2017).
28. X. M. Bai, H. Ke, **Y. Zhang**, B. W. Spencer, *Modeling copper precipitation hardening and embrittlement in a dilute Fe-0.3at.%Cu alloy under neutron irradiation*, Journal of Nuclear Materials 495, 442-454 (2017).
29. B. Beeler, M. Baskes, D. Andersson, M.W.D. Cooper, **Y Zhang**, *A modified Embedded-Atom Method interatomic potential for uranium-silicide*, Journal of Nuclear Materials 495, 267-276 (2017).
30. **Y. Zhang***, X. M. Bai, J. Yu, M. R. Tonks, M. J. Noordhoek and S. R. Phillpot, *Homogeneous hydride formation path in α -Zr: molecular dynamics simulations with the charge-optimized manybody potential*, Acta Mater. 111, 357-365 (2016).
31. X. M. Bai, M. R. Tonks, **Y. Zhang** and J. D. Hales, *Multiscale modeling of thermal conductivity of high burnup structures in UO_2 fuels*, J. Nucl. Mater. 470, 208 (2016).
32. P. Chakraborty, **Y. Zhang** and M. R. Tonks, *Multi-scale modeling of microstructure dependent intergranular brittle fracture using a quantitative phase-field based method*, Comp. Mater. Sci. 113, 38-52 (2016).
33. S. B. Biner, W. Rao and **Y. Zhang**, *The stability of precipitates and the role of lattice defects in Fe-1% Cu1% Ni1% Mn alloy: A phase-field model study*, Journal of Nuclear Materials 468, 9-16 (2016).
34. **Y. Zhang***, X. M. Bai, M. R. Tonks and S. B. Biner, *Formation of prismatic loops from $C15$ Laves phase interstitial clusters in body-centered cubic iron*, Scripta Mater. 98, 5 (2015).
35. **Y. Zhang***, P. C. Millett, M. R. Tonks, X. M. Bai and S. B. Biner, *Preferential Cu precipitation at extended defects in bcc Fe: An atomistic study*, Comp. Mater. Sci. 101, 181-188 (2015).
36. X. M. Bai, **Y. Zhang** and M. R. Tonks, *Testing thermal gradient driving force for grain boundary migration using molecular dynamics simulations*, Acta Mater. 85, 95 (2015).
37. M. R. Tonks, **Y. Zhang**, A. Butterfield and X. M. Bai, *Development of a grain boundary pinning model that considers particle size distribution using the phase field method*, Modelling Simul. Mater. Sci. Eng. 23, 045009, (2015).
38. W. Z. Xu, **Y. Zhang**, G. M. Cheng, W. W. Jian, P. C. Millett, C. C. Koch, S. N. Mathaudhu and Y. T. Zhu, *Dynamic Void Growth and Shrinkage in Mg under Electron Irradiation*, Mater. Res. Letts. 2, 176 (2014)
39. **Y. Zhang***, P. C. Millett, M. R. Tonks, X. M. Bai, S. B. Biner, *Molecular dynamics simulations of intergranular fracture in UO_2 with nine empirical interatomic potentials*, J. Nucl. Mater. 452, 296 (2014).
40. **Y. Zhang***, L. G. Zhou and H. C. Huang, *Size dependence of twin formation energy of metallic*, Inter. J. Smart and Nano Mater. 4, 112 (2013).
41. M. R. Tonks, **Y. Zhang**, X. M. Bai and P. C. Millett, *Demonstrating the Temperature Gradient Impact on Grain Growth in UO_2 Using the Phase Field Method*, Mater. Res. Letts. 2, 23 (2014).
42. G. M. Cheng, W. Xu, W. W. Jian, H. Yuan, M. Tsai, Y. T. Zhu, **Y. Zhang** and P. C. Millett, *Dislocation with edge component in nanocrystalline body-centered-cubic Mo*, J. Mater. Research 28, 1820 (2013).
43. M. R. Tonks, **Y. Zhang**, S. B. Biner, P. C. Millett and X. M. Bai, *Guidance to Design Grain Boundary Mobility Experiments with Quantitative Phase-Field Modeling*, Acta Mater. 61, 1373 (2013).
44. P. C. Millett, M. R. Tonks, K. Chockalingam, **Y. Zhang** and S. B. Biner, *Three Dimensional Calculations of the Effective Kapitza Resistance of UO_2 Grain Boundaries Containing Intergranular Bubbles*, J. Nucl. Mater. 439, 117 (2013).
45. P. C. Millett, **Y. Zhang**, M. Tonks and S. B. Biner, *Consideration of Grain Size Distribution in the Diffusion of Fission Gas to Grain Boundaries*, J. Nucl. Mater. 440, 435 (2013).

46. W. Z. Xu, **Y. Zhang**, G. M. Cheng, W. W. Jian, P. C. Millett, C. C. Koch, S. N. Mathaudhu and Y. T. Zhu, *In-situ atomic-scale observation of irradiation-induced void formation*, Nature Communications 4, 2288 (2013).
47. X. M. Bai, **Y. Zhang** and M. R. Tonks, *Strain effects on oxygen transport in tetragonal zirconium dioxide*, Phys. Chem. Chem. Phys. 15, 19438 (2013).
48. **Y. Zhang***, P. C. Millett, M. Tonks and B. Biner, *Deformation-twin-induced grain boundary failure*, Scripta Mater. 66, 117 (2012).
49. **Y. Zhang***, H. C. Huang, P. C. Millett, M. Tonks, D. Wolf and S. Phillpot, *Atomistic study of grain boundary sink strength under prolonged electron irradiations*, J. Nucl. Mater. 422, 69 (2012).
50. **Y. Zhang***, X. Y. Liu, P. C. Millett, M. Tonks, D. A. Andersson and B. Biner, *Crack tip plasticity in single crystal UO₂: Atomistic simulations*, J. Nucl. Mater. 430, 96 (2012).
51. **Y. Zhang***, P. C. Millett, M. Tonks, L. Zhang and B. Biner, *Molecular dynamics simulations of He bubble nucleation at grain boundaries*, J. Phys.: Condens. Matter 24, 305005 (2012).
52. **Y. Zhang***, P. C. Millett, M. Tonks and B. Biner, *Deformation-twin in nanocrystalline BCC Mo as predicted by molecular dynamics simulations*, Acta Mater. 60, 6241 (2012).
53. **Y. Zhang** and H. C. Huang, *Design of twin structure in SiC nanowires*, J. Comp. Theoretical Nanoscience 9, 1(2012).
54. P. C. Millett, M. Tonks, S. Biner, L. Zhang, K. Chockalingam, **Y. Zhang**, *Phase-field simulation of intergranular bubble growth and percolation in bicrystals*. J. Nucl. Mater. 425, 130 (2012).
55. L. Zhang, M. Tonks, P. C. Millett, **Y. Zhang**, K. Chockalingam, and B. Biner, *Phase-Field modeling of low thermal conductivity pores in nuclear fuels due to Soret effect*, Comp. Mater. Sci. 56, 161 (2012).
56. P. C. Millett, **Y. Zhang**, D. A. Andersson, Michael Tonks, S. Biner, *Random-Walk Monte Carlo Simulation of Intergranular Gas Bubble Nucleation in UO₂ Fuel*. J. Nucl. Mater. 430, 44 (2012).
57. **Y. Zhang***, P. C. Millett and M. Tonks, *Energetics and diffusional properties of He in BCC Mo: An empirical potential for molecular dynamics simulations*, Comp. Mater. Sci. 50, 3224 (2011).
58. **Y. Zhang** and H. C. Huang, *Controllable introduction of twin boundaries into nanowires*. J. Appl. Phys. 108, 1 (2010).
59. **Y. Zhang** and H. C. Huang, *Do twin boundaries always strengthen metal nanowires?* Nanoscale Research Lett. 4, 34 (2009).
60. **Y. Zhang** and H. C. Huang, *Twin Cu nanowires using energetic beams*. Appl. Phys. Lett. 95, 111914 (2009).
61. **Y. Zhang** and H. C. Huang, *Stability of single-wall silicon carbide nanotubes – molecular dynamics simulations*. Comp. Mater. Sci. 29, 664 (2008).
62. **Y. Zhang** and H. C. Huang, *Size dependence of twin formation energy in cubic SiC at the nanoscale*. Appl. Phys. Lett. 92, 261908 (2008).
63. H. W. Shim, **Y. Zhang** and H. C. Huang, *Twin formation during SiC nanowire synthesis*. J. Appl. Phys. 104, 063511 (2008).
64. **Y. Zhang**, H. C. Huang and S. N. Atluri, *Strength asymmetry of twinned copper nanowires under tension and compression*. CMES 35, 215 (2008).

Conference Proceedings

1. J. Yu, C. Jiang and **Y. Zhang**, *Influence of alloying elements and effect of stress on anisotropic hydrogen diffusion in Zr-based alloys predicted by accelerated kinetic Monte Carlo simulations*, Proceedings of Environmental Degradation 2017. Portland, USA, (2017).
2. J. Yu, **Y. Zhang**, and J. Hales. *Development of molecular dynamics potential for uranium silicide fuels*, Proceedings of Top Fuel 2016. Boise, USA, (2016).
3. **Y. Zhang***, P. C. Millett, M. R. Tonks, X. M. Bai and S. B. Biner, *Intergranular fracture in UO₂: derivation of traction-separation law from atomistic simulations*, ANS Global 2013 Meeting, Salt Lake City UT, OCT 2013

Invited talks

Conferences (9 invited, over 30 total talks)

1. **Y. Zhang**, D. Andersson, and M. Tonks, *Microstructure based modeling of in-reactor behavior of oxide nuclear fuels*, 43rd International Conference and Exposition on Advanced Ceramics and Composites - ICACC2019, Daytona Beach, FL USA.
2. **Y. Zhang**, D. Schwen, D. Andersson, M. Tonks, S. Novascone, K. Ahmed and B. Beeler, *Introduction of the Meso-Scale Fuel Performance Modeling Code MARMOT*, NFSM-2018 embedded meeting at ANS 2018 Meeting, Philadelphia, PA USA.
3. **Y. Zhang** and D. A. Andersson, *Atomic to Mesoscale Research and Development for U3Si2 Accident Tolerant Fuel*, TMS 2018 Meeting, Phoenix AZ, USA.
4. **Y. Zhang**, C. Jiang and B. Biner, *Multiscale modeling of hydride formation in Zr and Zircalloys*, MRS-Spring 2017, Phoenix AZ, USA.
5. **Y. Zhang**, C. Jiang, X. Bai, J. Yu, S. R. Phillpot, M. Fullarton and M. Noordhoek, *Understanding Hydride Formation in Alpha-Zr at the Atomic Scale*, 2016 MST Annual Meeting, Salt Lake City, UT, USA.
6. **Y. Zhang**, D. Schwen, M. Tonks and D. A. Andersson, *Meso-scale fuel performance modeling using the MARMOT code*, NFSM-2016 embedded meeting at ANS 2016 Meeting, New Orleans LA, USA.
7. **Y. Zhang**, P. Chakraborty, D. Schwen, X. M. Bai, and B. Spencer, *Multiscale Modeling of solute precipitation in Reactor Pressure Vessels*, MRS-Spring 2016, Phoenix, AZ, USA.
8. **Y. Zhang**, P. Chakraborty, D. Schwen, X. M. Bai, M. R. Tonks and B. Spencer, *Multiscale Modeling of Microstructure Evolution and Property Degradation in Reactor Pressure Vessels*, 2015 MST Annual Meeting, Columbus, OH, USA.
9. **Y. Zhang**, X. Y. Liu, P. C. Millett, M. Tonks, D. A. Andersson and B. Biner, *Intra- and intergranular fracture behavior in UO₂*, 3rd Symposium on Predictive Science and Technology in Mechanics and Materials, Mississippi State University, MS, USA. 2012

Student Seminar

1. **Y. Zhang**, Y. Gao, C. Jiang, D. Schwen, Cheng Sun and J. Gan, *Void Superlattice Self-organization by Chemical Freezing of Phase Separation*, North Carolina State University, December 2018.
2. **Y. Zhang**, Y. Gao, C. Jiang, D. Schwen and J. Gan, *Self-organization of nanoscale void superlattice under radiation*, Oregon State University, November 2017.
3. **Y. Zhang**, D. Schwen, M. Tonks and D. A. Andersson, *A Microstructure Based Mesoscale Fuel Performance Tool: MARMOT*, Brigham Young University – Idaho, February 2016.
4. **Y. Zhang**, P. Chakraborty, D. Schwen, X. M. Bai and B. Spencer, *Multiscale modeling of microstructure evolution in reactor pressure vessel steels*, Rensselaer Polytechnic Institute, October 2015.