

Dr. Guofeng Wang
Assistant Professor of Mechanical Engineering
Indiana University-Purdue University Indianapolis (IUPUI)

Education

- 2002, Ph.D., Materials Science, California Institute of Technology, Pasadena, California.
- 1999, M.S., Materials Science, California Institute of Technology, Pasadena, California.
- 1997, M.E., Materials Science and Engineering, Tsinghua University, Beijing, China.
- 1995, B.E., Material Science and Engineering, Tsinghua University, Beijing, China.

Positions Held at IUPUI

- 2007-Present, Assistant Professor of Mechanical Engineering.

Other Related Experience

- 2006-2007, Research Assistant Professor, Department of Chemistry and Physics, University of South Carolina Aiken.
- 2005-2006, Research Associate, Department of Chemical Engineering, Texas A&M University.
- 2002-2005, Postdoctoral Fellow, Division of Materials Sciences, Lawrence Berkeley National Laboratory.

Teaching Interests

Atomistic materials simulations, computational methods, material mechanics, and material science.

Courses Taught at IUPUI

ME 262 Mechanical Design I

ME 272 Mechanics of Materials

Research Interests

Computational materials science, multiscale modeling approach, parallel computing, density functional theory, molecular dynamics, Monte Carlo method, catalysts for renewable energy technology, mechanical properties of nanomaterials.

General Summary

Dr. Wang has been focusing his research interest on investigating material properties using multi-scale simulation approaches and novel simulation algorithms. His Ph.D. thesis work was devoted to *First Principles Based Multi-scale Modeling of Single*

Crystal Plasticity: Application to BCC Tantalum (Ta). Part of the Accelerated Strategic Computing Initiative (ASCI) program, he contributed to the development a quantitative multiscale approach of describing material plasticity based on dislocation mechanism. From 2002 to 2005, he worked at Lawrence Berkeley National Laboratory as a postdoctoral fellow and developed a multiscale simulation approach to designing Pt alloys for their application as fuel cell catalysts. He has also developed and applied the novel direct Monte Carlo (MC) method to modeling the structure of various dendritic polymer systems, studied the thermoelectric properties of semiconductor superlattices, and investigated the size-dependent elastic modulus of nanomaterials. He has published many research articles (include one invited review paper) and presented lectures at various national and international conferences.

Current Projects

1. Design fuel cell catalysts from first-principles multiscale computations.
2. Investigation of the size-dependent elastic properties of one-dimensional wurtzite nanostructures.
3. Study the mechanism of the whisker growth in Sn.

Principal Publications (recent)

Journal Papers

1. M.I. Baskes, S.Y. Hu, S.M. Valone, G. Wang, and A.C. Lawson, “Atomistic simulations of Ga atom ordering in Pu 5 at.% Ga alloys”, *Journal of Computer-Aided Materials Design*, **14**, 379-388 (2007).
2. G. Wang and T. Cagin, “Electronic structure of thermoelectric materials Bi₂Te₃ and Sb₂Te₃ from first-principles calculations”, *Physical Review B*, **76**, 075201 (2007).
3. V.R. Stamenkovic, B.S. Mun, K.J.J. Mayrhofer, C.A. Lucas, G. Wang, P.N. Ross, and N.M. Markovic, “Trends in electrocatalysis: from extended to nanoscale surfaces”, *Nature Materials*, **6**, 241 (2007).
4. V.R. Stamenkovic, B. Fowler, B.S. Mun, G. Wang, P.N. Ross, C.A. Lucas, and N.M. Markovic, “Improved oxygen reduction activity on Pt₃Ni(111) via increased surface site availability”, *Science*, **315**, 493 (2007).
5. G. Wang and T. Cagin, “Investigation of effective mass of carriers in Bi₂Te₃/Sb₂Te₃ superlattices via electronic structure studies on its component materials”, *Applied Physics Letters*, **89**, 152101 (2006).
6. R.S. Lillard, G. Wang, and M.I. Baskes, “The role of metallic bonding in the crystallographic pitting of Magnesium”, *Journal of The Electrochemical Society*, **153**, B358-B364 (2006).
7. G. Wang, M.A. Van Hove, P.N. Ross, and M.I. Baskes, “Quantitative prediction of surface segregation in bimetallic Pt-M alloy nanoparticles (M=Ni, Re, Mo)”, *Progress in Surface Science*, **79**, 28-45 (2005).
8. G. Wang, M.A. Van Hove, P.N. Ross, and M.I. Baskes, “Surface structures of cubo-octahedral Pt-Mo catalyst nanoparticles from Monte Carlo simulations”, *The Journal of Physical Chemistry B*, **109**, 11683 (2005).

9. G. Wang, M.A. Van Hove, P.N. Ross, and M.I. Baskes, “Monte Carlo simulations of segregation in Pt-Ni catalyst nanoparticles”, *Journal of Chemical Physics*, **122**, 024706 (2005).
10. G. Wang, M.A. Van Hove, P.N. Ross, and M.I. Baskes, “Monte Carlo simulations of segregation in Pt-Re catalyst nanoparticles”, *Journal of Chemical Physics*, **121**, 5410-5422 (2004).
11. P. K. Maiti, T. Cagin, G. Wang, and W. A. Goddard, III, “Structure of PAMAM dendrimers: Generation 1 through 11”, *Macromolecules*, **37**, 6236-6254 (2004).
12. G. Wang, A. Strachan, T. Cagin, and W.A. Goddard, III, “Calculating the Peierls energy barrier and Peierls stress from atomistic simulations of screw dislocation dynamics: application to bcc Tantalum”, *Modelling and Simulation in Materials Science and Engineering*, **12**, S371-S389 (2004).
13. G. Wang, A. Strachan, T. Cagin, and W.A. Goddard, III, “Atomistic simulations of kinks in $1/2a\langle 111 \rangle$ screw dislocations in Tantalum”, *Physical Review B*, **68**, 224101 (2003).
14. G. Wang, A. Strachan, T. Cagin, and W.A. Goddard, III, “Role of core polarization curvature of screw dislocations in determining the Peierls stress in bcc Ta – a new criterion for designing high performance materials”, *Physical Review B*, **67**, 140101(R) (2003).
15. G. Wang, A. Strachan, T. Cagin, and W.A. Goddard, III, “Kinks in the $a/2\langle 111 \rangle$ screw dislocation in Ta”, *Journal of Computer-Aided Materials Design*, **8**, 117-125 (2001).
16. A.M. Cuitino, L. Stainier, G. Wang, A. Strachan, T. Cagin, W.A. Goddard, III, and M. Ortiz, “A multiscale approach for modeling crystalline solids”, *Journal of Computer-Aided Materials Design*, **8**, 127-149 (2001).
17. T. Cagin, G. Wang, R. Martin, G. Zamanakos, N. Vaidehi, D.T. Mainz, and W.A. Goddard, III, “Multiscale modeling and simulation methods with applications to dendritic polymers”, *Computational and Theoretical Polymer Science*, **11**, 345-356 (2001).
18. G. Wang, A. Strachan, T. Cagin, and W.A. Goddard, III, “Molecular dynamic simulations of $a/2\langle 111 \rangle$ screw dislocations in Ta”, *Materials Science and Engineering: A*, **Vol 309-310**, 133-137 (2001).
19. T. Cagin, G. Wang, R. Martin, N. Breen, and W.A. Goddard, III, “Molecular modelling of dendrimers for nanoscale applications”, *Nanotechnology*, **11**, 77-84 (2000).

Conference Proceedings/Book Chapters

1. G. Wang, M.A. Van Hove, P.N. Ross, and M.I. Baskes, “Atomistic simulations of fcc $Pt_{75}Ni_{25}$ and $Pt_{75}Re_{25}$ cubo-octahedral nanoparticles”, in ***Nanoparticles and Nanowire Building Blocks-Synthesis, Processing, Characterization, and Theory***, Eds. O. Glembocki, C. Hunt, C. Murray, and G. Galli, (2004).
2. G. Wang, A. Strachan, T. Cagin, and W.A. Goddard, III, “Atomistic simulation of kinks for $1/2a\langle 111 \rangle$ screw dislocation in Ta”, in ***Advances in Materials Theory and Modeling--Bridging Over Multi-Length and Time Scales***, Eds. V. Bulatov, F. Cleri, L. Colombo, L. Lewis, and N. Mousseau, (2001).
3. T. Cagin, P.J. Miklis, G. Wang, G. Zamanakos, R. Martin, H. Li, D.T. Mainz, N. Vaidehi, and W.A. Goddard, III, “Recent advances in simulation of dendritic

- polymers”, in *Dynamics in Small Confining Systems V* Eds. J.M. Drake, G.S. Grest, J. Klafter, and R. Kopelman, (1999).
4. X. Chen, G. Wang, T. Gao, and H. Chen, “The strength and wear resistance of metal reinforced carbon matrix composite”, in *Proceedings of The First Asia International Conference on Tribology*, V2, (1998).

Invited Lectures

1. “Toward the nanoscale design of catalysts for fuel cells: A computational approach”, *233rd American Chemical Society National Meeting*, March 25-29, 2007, Chicago, Illinois.

Membership in Scientific and Professional Societies

1. Member, American Physical Society (APS).
2. Member, Materials Research Society (MRS).

Honors and Awards

1. 2002, Graduate Student Award, MRS.

Significant Professional Service (recent)

Journal Reviews

1. Journal of Chemical Physics.
2. Journal of Physical Chemistry.
3. Nanotechnology.
4. Modelling and Simulation in Materials Science and Engineering.
5. Journal of Physics: Condensed Matter.
6. New Journal of Physics
7. Semiconductor Science and Technology.

Others

1. Proposal review for the International Research Fellowship Program of National Science Foundation (NSF).