

Ju Li

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- Experience**
- Massachusetts Institute of Technology* Cambridge, MA 02139
Full Professor (7/2011-present),
Department of Nuclear Science and Engineering and
Department of Materials Science and Engineering
- University of Pennsylvania* Philadelphia, PA 19104
Associate Professor (9/2007-6/2011),
Department of Materials Science and Engineering
- Ohio State University* Columbus, OH 43210
Assistant Professor (9/2002-9/2007),
Department of Materials Science and Engineering
- Massachusetts Institute of Technology* Cambridge, MA 02139
Research scientist (4/2002-9/2002), postdoctoral associate (9/2000-4/2002),
Departments of Nuclear Engineering and Materials Science and Engineering
- Honda R&D Co., Ltd. Wako Research Center* Wako-shi, Saitama, Japan
Visiting Scientist (1/13-2/14/2002)
- Ames Laboratory, USDOE* Ames, Iowa 50011
Visiting Scientist
(7/17-29/96, 6/11-7/3/97, 7/12-8/22/98, 12/19/00-1/19/01, 8/6-20/01, 12/17-24/02,
10/11-19/03, 7/14-23/05)
- Education**
- Massachusetts Institute of Technology* Cambridge, MA 02139
Department of Nuclear Engineering (1994-2000) Ph.D., Sept. 2000
- Cumulative GPA: 5.0/5.0 (618 graduate degree credits)
40 graduate-level courses offered by 8 MIT departments.
- University of Science and Technology of China* Hefei, Anhui 230026, P.R.C.
Special Class for Gifted Young (1990-1994) B.S. in Physics, 1994
- Awards**
- Chinese Ministry of Education and Li Ka Shing Foundation Chang Jiang Scholar Award (2009)
- TMS Robert Lansing Hardy Award (2009), for “a young person in the broad fields of metallurgy and materials science for exceptional promise of a successful career”

Technology Review TR35 award, for 35 “world’s top innovators” under age 35 (2007)

National Academy of Engineering U.S. Frontiers of Engineering Symposium (Microsoft Research, Sept. 24-26, 2007), “that brings together 100 of the nation’s outstanding young engineers (ages 30-45)”, and German-American Frontiers of Engineering Symposium (Oak Ridge, April 22-25, 2010) co-sponsored by the Alexander von Humboldt Foundation.

Materials Research Society (MRS) 2006 Outstanding Young Investigator Award, “to recognize outstanding, interdisciplinary scientific work in materials research by a young scientist or engineer”

Ohio State University College of Engineering 2006 Lumley Research Award

Presidential Early Career Award for Scientists and Engineers (PECASE) 2005, “the highest honor bestowed by the United States Government on scientists and engineers beginning their independent careers”

Outstanding Paper Award in the Fifth International Conference on Advanced Materials 1999, sponsored by the International Union of Materials Research Societies (IUMRS). (10 out of ~ 2,000 papers)

Materials Research Society (MRS) Graduate Student Silver Medalist in 1998.

Sole recipient of the 1996-1997 MIT Nuclear Engineering Department Manson Benedict Fellowship.

Two Letters of Commendation (1996,1997) from MIT Nuclear Engineering Department for outstanding academic performance.

**Advisee
Awards**

Best Poster Award, Gordon Research Conferences on Physical Metallurgy, August 2-7, 2009, Proctor Academy, Andover, NH: Erik Bitzek, William T. Cox, Sanket Sarkar, Thomas J. Lenosky, Yunzhi Wang, Ju Li, “Atomic-Scale Modeling of Diffusion-Driven Microstructure Evolution”

Teaching

Instructor, Penn *MSE440/540 Phase Transformations* (Spring Term, 2008, 2009, 2010, 2011)

Instructor, OSU *MSE730 Thermodynamics of Materials* (Wi Qtr., 2004,2005,2006,2007); Penn *MSE 530 Thermodynamics of Materials* (Fall Term, 2008, 2009, 2010)

Instructor (with Suliman Dregia and Yunzhi Wang), OSU *MSE894 Theoretical Methods in Materials Science* (Au Qtr., 2006)

Instructor, OSU *MSE695.01 Senior Design Project I* (Au Qtr., 2003,2004,2005,2006)

Instructor, OSU *MSE533 Modeling of Materials Processing Methods* (Sp Qtr., 2003,2004,2005,2006)

Instructor, OSU *MSE564 Mechanical Behavior and Material Microstructure* (Wi Qtr., 2003)

Instructor, OSU *MSE795 Graduate Seminar and Colloquium* (Au Qtr., 2004)

Instructor, MIT *22.51 Interactions of Radiation with Matter* (Fall 2001)

Course webpage: <http://web.mit.edu/22.51/www/>

Co-instructor, MIT *22.53 Statistical Processes and Atomistic Simulations*

(Fall 2000) Course webpage: <http://web.mit.edu/22.53/www/>

Instructor, GEM⁴ Summer School on Cell and Molecular Mechanics in BioMedicine, [with a focus on infectious diseases](#), August 7-18, 2006, MIT, gave four lectures. [with a focus on cancer](#), June 25 - July 6, 2007, National University of Singapore, gave three lectures.

Advising

PhD adviser of Dr. Liang Qi (Penn MSE, August 2009), Dr. Amit Samanta (Penn MSE, August 2009), Wei Liu (qualifying exam passed May 2008), Wenbin Li (qualifying exam passed May 2009).

Master's degree adviser of Liang Qi (OSU MSE, March 2007), Amit Samanta (OSU MSE, June 2007), Liu Cao (OSU MSE, September 2007), Zheng Li (Penn MSE, 2008), Wei Liu (Penn MSE, August 2009), Cheng-Wei Huang, Hsu-Chung Ko.

Postdoctoral adviser of Dr. James Jianguo Yu (8/2003-10/2004), Dr. Thomas J. Lenosky (8/2006-8/2007), Dr. Erik Bitzek (8/2008-12/2009), Dr. Ji Feng (2/2009-1/2011), Dr. Liang Qi (9/2009-), Dr. Yu Chieh Lo (11/2009-), Dr. Akihiro Kushima (4/2010-).

Host of visiting scholars: Prof. Shigenobu Ogata (Osaka University), Dr. Futoshi Shimizu (Japan Atomic Energy Agency), Joshua Fujiwara (Honda), Mitsumoto Kawai (Honda), Prof. ZhengPing Fu (University of Science and Technology of China), Prof. Shotaro Hara (University of Tokyo), Prof. Erik Bitzek (Universitat Erlangen-Nurnberg), Yvonne Ritter (Technische Universitat Darmstadt).

Host of visiting students: Hyoung Gyu Kim (Korea Advanced Institute of Science and Technology, 1-7/2005), JingShan Qi (Nanjing University of Aeronautics and Astronautics, 6/2009-9/2010), Yi-Gil Cho (Seoul National University, 7/2010-3/2011).

Presentations Keynote presentation, ASME McMat2011, symposium on Low Dimensional Carbon NanoMaterials: Properties and Applications, Chicago, May 31-June 2, 2011.

Invited talk, Electron Microscopy and Multiscale Modeling 2011, Granlibakken Conference Center and Lodge, May 22-27, 2011.

Invited talk, Pennergy Symposium "Materials Under Extremes," April 9, 2011, Philadelphia.

Invited talk, Harvard Applied Mechanics Colloquium, February 2, 2011.

Invited talk, MRS Fall Meeting, Boston, November 29 - December 3, 2010.

Microstructure Modelling symposium, MMM2010, the Fifth Conference on Multiscale Material Modelling, Freiburg, Germany, October 7, 2010.

Penn Department of Mechanical Engineering and Applied Mechanics Seminar Series, September 16, 2010.

Invited talk, Physics and Astronomy Colloquium Series at University of Southern California, August 30, 2010.

Invited talk, Department of Engineering Science and Mechanics, Pennsylvania State University, July 16, 2010.

Invited talk, 17th International Symposium on Metastable, Amorphous and Nanostructured Materials (ISMANAM 2010), Zurich, Switzerland, July 4 - 9, 2010.

Invited talk, Sixth International Conference on Materials Structure & Micromechanics of Fracture (MSMF6), Brno, Czech Republic, June 28 - 30, 2010.

Invited talk, Department Werkstoffwissenschaften, Lehrstuhl WWI: Allgemeine Werkstoffeigenschaften, Universitat Erlangen-Nurnberg, Germany, June 24, 2010.

Invited talk, International Workshop on Materials Behavior at Micro- and Nano-Scale, Xi'an, China, June 11, 2010.

Invited talk, International Conference on Mechanical Properties of Materials (ICMPM), Hangzhou, China, May 27, 2010.

Two invited talks, 2010 SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 23, 2010.

Invited talk, Materials Science and Engineering Seminar, University of Tennessee, Knoxville, April 26, 2010.

Invited talk, Materials Science and Engineering Seminar, Rensselaer Polytechnic Institute, Troy, April 7, 2010.

Invited talk, TMS 2010 Annual Meeting & Exhibition, Seattle, February 14-18, 2010.

Keynote talk (40 min), mini-symposium Finite Plasticity & Viscoplasticity of Conventional & Emerging Materials (In celebration of 65 Years of Akhtar Khan), Plasticity 2010, St. Kitts, West Indies, January 3-8, 2010.

Invited talk, MIT Center for Computational Engineering (CCE), December 2, 2009.

Invited talk, MRS Fall Meeting, symposium *Mechanical Behavior of Nanomaterials Experiments and Modeling*, Boston, November 30 - December 4, 2009.

Invited talk, Civil Infrastructure Seminar, School of Civil and Environmental Engineering, Cornell University, November 10, 2009.

Invited talk, Mechanical & Aerospace Engineering Seminar, The University of Texas at Arlington, September 4, 2009.

Invited talk, Department of Mechanical Engineering Seminar, University Of Houston, September 3, 2009.

Invited talk, *Workshop on Probing the Limits of Strength*, Lawrence Berkeley National Laboratory, Berkeley, California, August 11-12, 2009.

Invited talk, “In-situ Observation of Graphene Sublimation and Edge Reconstructions,” mini-symposium *Graphene growth and properties through experiments and simulations*, tenth U.S. National Congress on Computational Mechanics (US-NCCM X), Columbus, July 16-19, 2009.

Invited talk, School of Materials Science and Engineering, Shanghai Jiao Tong University, June 10, 2009.

Invited talk, International Workshop on Size Effect on Materials Mechanical Behavior, Beijing, May 24 - 26, 2009.

Invited talk, “The Coming of Age of Ultra-Strength Materials,” Center for Integrated Nanotechnologies (CINT), Sandia National Laboratories, Albuquerque, New Mexico, May 7, 2009.

Invited talk, Othmer-Jacobs Department of Chemical and Biological Engineering, Polytechnic Institute of NYU, Brooklyn, New York, May 4, 2009.

Invited talk, MRS Spring Meeting, symposium *Probing Mechanics at Nanoscale Dimensions*, San Francisco, April 13-17, 2009.

Invited talk, Shanghai Institute of Ceramics, March 10, 2009.

Invited talk, TMS 2009 Annual Meeting & Exhibition, San Francisco, February 15-19, 2009.

Keynote talk (40 min), “Tensile Ductility of Nanostructured Metals,” Plasticity 2009, St. Thomas, U.S. Virgin Islands, January 3-8, 2009.

Invited talk, Workshop on Mechanical Behaviors of Micro/Nano Materials, XiAn Jiao Tong University, December 30-31, 2008.

Two invited talks, National Sun Yat-sen University, Kaohsiung, Taiwan, December 13-21, 2008.

Invited talk, Georgia Institute of Technology Woodruff School of Mechanical Engineering Seminar, Oct. 23, 2008.

Invited talk, Dislocations 2008, Hong Kong, Oct. 13-17, 2008.

Invited talk, Brown University Joint Materials/Solid Mechanics Seminar, September 12, 2008.

Invited talk, “Plasticity in amorphous and nanocrystalline metals,” Gordon Research Conference on Thin Film & Small Scale Mechanical Behavior, Colby College, Maine, July 27 - August 1, 2008.

Two invited lectures, Workshop on Multi-Scale Modeling of Moving Interfaces in Materials, Katholieke Universiteit Leuven, Belgium, July 2-4, 2008.

Invited talk, 2nd International Conference on Heterogeneous Materials Mechanics (ICHMM-2008), HuangShan, China, June 3-8, 2008.

Invited talk, International Workshop on *in situ* Electron Microscopy in Advanced Materials Research, Beijing, May 31 - June 2, 2008.

Invited talk, NIST 2008 Diffusion Workshop, Gaithersburg, Maryland, May 12-13, 2008.

Invited talk, TMS 2008 Annual Meeting & Exhibition, New Orleans, March 9-13, 2008.

Invited talk, International Workshop on Small Scale Plasticity, Braunwald, Switzerland, September 5-8, 2007.

Keynote talk (45 min), “Cytoskeletal Dynamics Simulations of Red Blood Cell,” ninth U.S. National Congress on Computational Mechanics (USNCCM IX), San Francisco, July 22-26, 2007.

Invited seminar at Department of Aerospace and Mechanical Engineering, University of Notre Dame, March 20, 2007.

Los Alamos National Lab Physics & Theoretical Colloquium, March 15, 2007, 2007.

Invited talk, “Shear localization lengthscale in metallic glasses,” Center for Advanced Metallic and Ceramic Systems (CAMCS) Seminar, Johns Hopkins University, Baltimore, Maryland, January 3, 2007.

Invited talk, “[Yield Point of Metallic Glass](#),” Pacific Northwest National Laboratory, Richland, WA, September 15, 2006.

Invited talk, “Atomistic Modeling of Rate Dependence of Deformation and Fracture,” 232nd ACS National Meeting, San Francisco, September 10-14, 2006.

MRS OYI presentation, “The Mechanics and Physics of Defect Nucleation,” San Francisco, April 19, 2006.

Invited talk, “A minimal mesoscopic model of the self-assembly and micro-rheology of red blood cell cytoskeleton,” *First International Conference on Mechanics of Biomaterials & Tissues*, Waikoloa, Hawaii, December 11-15, 2005.

Invited talk, “Modified Frenkel model and ductility of solids,” *International Workshop on Nanomechanics*, Asilomar conference grounds, Pacific Grove, California, July 14-17, 2004.

Invited talk, “How bonds break in shear and why it matters,” Case Western Reserve University Materials Science and Engineering Departmental Colloquium, September 16, 2003.

Invited talk, AFOSR *Materials Engineering in Affordable New Systems (MEANS)* workshop, Boulder, Colorado, August 6-8, 2003.

Invited talk, “Coupling coarse variables to microscopic simulations,” *Workshop on Algorithm Refinement*, Los Alamos National Laboratory, April 22-24, 2002.

Invited talk, “Consequences of energy locality on atomistic calculations of defect mobility,” *Computational Materials Science Network Workshop on Microstructural Effects on the Mechanics of Materials*, Lawrence Berkeley National Laboratory, June 18-20, 2001.

Conference Fellowship, “Optimal particle controller for coupled continuum/MD fluid simulation,” *First MIT Conference on Computational Fluid and Solid Mechanics*, MIT, June 12-15, 2001.

Invited talk, “Nearly exact solution for coupled continuum/MD fluid simulation,” *NIST Workshop on Hybrid Computational Methods for Multiscale Modeling of Materials*, in Gaithersburg, Maryland, May 12-14, 1999.

Service

Faculty Advisor to Chinese Students and Scholars Association at Penn (CSSAP, 1/2009-present)

Penn MSE Graduate Group Chair (7/1/2009-6/30/2011)

Penn MSE Colloquium Organizer (9/2008-6/2009)

Penn MSE Faculty Search Committee (9/2008-6/2009)

OSU MSE Faculty Meeting Secretary (9/2002-8/2005)

OSU MSE Library and Computing Committee (9/2004-8/2006, 4/2007-9/2007)

OSU MSE Graduate Studies Committee (1/2005-8/2006)

OSU MSE Faculty Search Committee (2/2006-1/2007)

OSU MSE Undergraduate Studies Committee (9/2006-9/2007)

OSE MSE Student Relations Committee (9/2006-4/2007)

OSE MSE Ad Hoc Committee on Undergraduate Curriculum Adjustments (9/2006-2/2007)

Ph.D. candidacy exam committee of: Eunha Lee (OSU MSE 2002), Sudhakar Mahajanam (OSU MSE 2003), James M. Nash (OSU MSE 2004), Mala Seth (OSU MSE 2004), Matthew C. Brandes (OSU MSE 2005), Jonathan P. Blank (OSU MSE 2005), Barbara N. Padgett (OSU MSE 2005), Liang Qi (OSU MSE 2005), Amy M. Hayes (Chemistry 2005), Michael Rauscher (OSU MSE 2005), Lanlin Zhang (OSU MSE 2006), Amit Samanta (OSU MSE 2006), Sungwoo Ahn (OSU Mathematics 2007), Weiqi Luo (OSU MSE 2007); Jae Hong Choi (Penn MSE, 2008)

Ph.D. thesis committee of: Yao Shen (OSU MSE 2004), Tao Liang (OSU MSE 2005), Shanhu Li (OSU MechE 2005), Libor Kovarik (OSU MSE 2006), Carmen M. Carney (OSU MSE 2006); XueLian Zhu (Penn MSE, 2010), Ivan Sergeyevich Baldychev (Penn CBE, 2011), Tingting Qi (Penn Chemistry, 2011), Miguel Angel Mendez Polanco (Penn Chemistry), Kevin Bakhmutsky (Penn CBE), John Mark Martirez (Penn Chemistry), Tevis Jacobs (Penn MEAM), Vicky Doan-Nguyen (Penn MSE), Matthew A. Caporizzo (Penn MSE), Rubal Dua (Penn CBE)

Senior project advisor of: Jaumale L. Daniels (OSU MSE 2005), Danelle Violet (OSU MSE 2006), Joseph Lydon and Arthur Spector, "Building efficiency modeling and materials selection" (Penn MSE 2010).

Undergraduate Research Opportunities (REU) Program advisor of: Miten Mistry (Penn MSE, Jan 2009 -), Jonathan Rosen (Penn Nano-Bio Interface Center, June 2009 -)

American Chemical Society Project SEED High School Summer Research Experience: Manohjah Blackmanhe

Lead organizer of AFOSR [Workshop on Modeling Materials in Extreme Environment](#), Sept. 24-25, 2005, Washington D.C.

Panel member, [Basic Research Needs for Advanced Nuclear Energy Systems](#) (panel 6: Predictive Modeling and Simulation), July 31 - August 2, 2006, Washington, D.C., sponsored by the Office of Basic Energy Sciences, Department of Energy.

Panel member, [Advanced High-Strength Steels: Fundamental Research Issues](#) (panel A: Models versus Experiments), October 22-23, 2006, Washington, D.C., sponsored by the National Science Foundation, Department of Energy, and the Auto/Steel Partnership.

Member of DOE-BES Site Review Committee of the BES/Division of Materials Science & Engineering core program at Sandia National Laboratories, Albuquerque, March 22-25, 2010.

Member of Scientific Committee, Third International Conference of Heterogeneous Materials Mechanics (ICHMM 2011), ChongMing Island, China, May 22-26, 2011.

Co-organizer (with Zhiwei Shan, Xiaodong Li and Jun Sun), 4th International Workshop on Materials Behavior at Micro- and Nano-Scale, Xi'an, China, May 19-21, 2011.

Co-organizer (with Erik van der Giessen and Marc G.D. Geers) of symposium "Micromechanics" in MMM2010, the Fifth Conference on Multiscale Material Modelling, Freiburg, Germany, October 4-8, 2010.

Co-organizer (with Sulin Zhang, Gang Bao, Huajian Gao, K. Jimmy Hsia) of symposium "Molecular and Cellular Biomechanics: Adhesion, Cell-ECM Interaction, and Mechanotransduction," 16th US National Congress of Theoretical and Applied Mechanics (USNCTAM), Pennsylvania State University, State College, PA 16801, June 27 - July 2, 2010.

Co-organizer (with Zhiwei Shan, Jun Sun and Evan Ma), International Workshop on Materials Behavior at Micro- and Nano-Scale, Xi'an, China, June 8-11, 2010.

Co-organizer (with Peter M. Derlet, Mike D. Uchic, Daniel Weygand, Eric Le Bourhis) of Symposium "GG: Plasticity in Confined Volumes - Modeling and Experiments", MRS Fall Meeting, Boston, November 30 - December 4, 2009.

Organizer (with Wei Cai, Ting Zhu, Diana Farkas, Jacob Eapen, Krystyn J. Van Vliet) of symposium "1.1 Multiphysics Materials Modeling from Atoms to Continuum: A Symposium in Honor of Professor Sidney Yip", tenth U.S. National Congress on Computational Mechanics (USNCCM X), July 16-19, 2009.

Local Organizing Committee, tenth U.S. National Congress on Computational Mechanics (USNCCM X), Columbus, Ohio, July 16-19, 2009.

Co-organizer (with George Lykotrafitis, Sulin Zhang, Greg Huber and Ming Dao) of symposium "Mechanics of Biomembranes", 2009 Joint ASCE-ASME-SES Conference on Mechanics and Materials, Blacksburg, VA, June 24-27, 2009.

Co-organizer (with Shaofan Li and Sukky Jun) of symposium "Recent Developments in Nanoscale Simulations: From Quantum to Coarse-Grained Modeling", ninth U.S. National Congress on Computational Mechanics (USNCCM IX), San Francisco, July 22-26, 2007.

Member of Editorial Board of *Modelling and Simulation in Materials Science and Engineering* (Feb. 2008-), *Nano Research* (Mar. 2008-), *Scientific Modeling and Simulation* (Jan. 2008-).

Co-editor of *Mechanical Behavior at Small Scales - Experiments and Modeling*, Materials Research Society Symposium Proceedings volume 1224, eds. Jun Lou, Erica Lilleodden, Brad Boyce, Lei Lu, Peter M. Derlet, Daniel Weygand, Ju Li, Michael Uchic, and Eric Le Bourhis (Materials Research Society, Warrendale, Pennsylvania, 2010). Symposia FF/GG held on November 30 - December 3, 2009, Boston, USA. ISBN 978-1-60511-197-1.

3-Member Executive Board (Oct. 2010-present) and International Advisory Board (Aug. 2009-present) of Multiscale Materials Modeling (MMM) conference series.

Materials Research Society Awards Committee (2007-present).

Miscellaneous Listed in *Nanobiomechanics*, one of 10 Emerging Technologies in 2006 according to *Technology Review*.

“New muscles: faster, lighter, better?” on CNN web site.

Author of free molecular visualization software *AtomEye*:
<http://www.google.com/search?q=AtomEye>

Ab initio tight-binding analysis with quasiatomic orbitals (with Xiaofeng Qian):
<http://mt.seas.upenn.edu/Archive/QO/>

Builder of
12-CPU 64-bit Beowulf PC cluster at OSU (May 2005): <http://164.107.78.193/>
14-CPU Gigabit Beowulf PC cluster at OSU (April 2003): <http://164.107.78.220/>
12-CPU Beowulf PC cluster at MIT (March 2002): <http://wulf.mit.edu/>

Peer-Reviewed Papers¹

126. X.H. Liu, L. Zhong, L.Q. Zhang, A. Kushima, S.X. Mao, J. Li, Z.Z. Ye, J.P. Sullivan and J.Y. Huang, “Lithium fiber growth on the anode in a nanowire lithium ion battery during charging,” *Appl. Phys. Lett.* **98** (2011) 183107.
125. N. Zhou, C. Shen, M. J. Mills, J. Li and Y.Z. Wang, “Modeling displacive-diffusional coupled dislocation shearing of gamma prime precipitates in Ni-base superalloys,” *Acta Mater.* **59** (2011) 3484-3497.
124. J. Li, A. Kushima, J. Eapen, X. Lin, X.F. Qian, J. C. Mauro, P. Diep and S. Yip, “Computing the Viscosity of Supercooled Liquids: Markov Network Model,” *PLoS ONE* **6** (2011) e17909.

¹ ResearcherID: A-2993-2008 ISI Web of Knowledge search keywords: “Li J” in Author and “nucl same engn same 02139 or mat same 43210 or mat same Univ Penn or 2041 same Columbus” in Address.

123. J. Y. Huang, L. Zhong, C. M. Wang, J. P. Sullivan, W. Xu, L. Q. Zhang, S. X. Mao, N. S. Hudak, X. H. Liu, A. Subramanian, H. Y. Fan, L. Qi, A. Kushima and J. Li, “[In situ observation of the electrochemical lithiation of a single SnO₂ nanowire electrode](#),” *Science* **330** (2010) 1515.
122. S.Z. Li, X.D. Ding, J.K. Deng, T. Lookman, J. Li, X.B. Ren, J. Sun and A. Saxena, “[Superelasticity in BCC nanowires by a reversible twinning mechanism](#),” *Phys. Rev. B* **82** (2010) 205435.
121. X.F. Qian, J. Li and S. Yip, “[Calculating phase-coherent quantum transport in nanoelectronics with ab initio quasiatomic orbital basis set](#),” *Phys. Rev. B* **82** (2010) 195442.
120. S. Hara and J. Li, “[Adaptive strain-boost hyperdynamics simulations of stress-driven atomic processes](#),” *Phys. Rev. B* **82** (2010) 184114.
119. P. A. Gordon, T. Neeraj, Y. Li and J. Li, “[Screw dislocation mobility in BCC metals: the role of the compact core on double-kink nucleation](#),” *Modelling Simul. Mater. Sci. Eng.* **18** (2010) 085008.
118. H.Y. Yuan, J. Li, G. Bao and S.L. Zhang, “[Variable Nanoparticle-Cell Adhesion Strength Regulates Cellular Uptake](#),” *Phys. Rev. Lett.* **105** (2010) 138101.
117. S. I. White, R. M. Mutiso, P. M. Vora, D. Jahnke, S. Hsu, J. M. Kikkawa, J. Li, J. E. Fischer and K. I. Winey, “[Electrical percolation behavior in silver nanowire-polystyrene composites: simulation and experiment](#),” *Adv. Funct. Mater.* **20** (2010) 2709-2716.
116. C. Zheng, P. Liu, J. Li and Y-W. Zhang, “[Phase Diagrams for Multi-Component Membrane Vesicles: A Coarse-Grained Modeling Study](#),” *Langmuir* **26** (2010) 12659-12666.
115. H.Y. Yuan, C.J. Huang, J. Li, G. Lykotrafitis and S.L. Zhang, “[One-particle-thick, solvent-free, coarse-grained model for biological and biomimetic fluid membranes](#),” *Phys. Rev. E* **82** (2010) 011905.
114. S. Z. Li, X. D. Ding, J. Li, X. B. Ren, J. Sun, E. Ma and T. Lookman, “[Inverse martensitic transformation in Zr nanowires](#),” *Phys. Rev. B* **81** (2010) 245433.
113. T. Zhu and J. Li, “[Ultra-strength materials](#),” *Progress in Materials Science* **55** (2010) 710-757.
112. J-Y. Zhang, G. Liu, R. H. Wang, J. Li, J. Sun and E. Ma, “[Double-inverse grain size dependence of deformation twinning in nanocrystalline Cu](#),” *Phys. Rev. B* **81** (2010) 172104.
111. S. Z. Li, X. D. Ding, J. Li, X. B. Ren, J. Sun and E. Ma, “[High-efficiency mechanical energy storage and retrieval using interfaces in nanowires](#),” *Nano Letters* **10** (2010) 1774-1779.
110. L. Qi, J.Y. Huang, J. Feng and J. Li, “[In situ observations of the nucleation and growth of atomically sharp graphene bilayer edges](#),” *Carbon* **48** (2010) 2354-2360.
109. Q. Yu, Z.-W. Shan, J. Li, X.X. Huang, L. Xiao, J. Sun and E. Ma, “[Strong crystal size effect on deformation twinning](#),” *Nature* **463** (2010) 335-338.

108. J. Y. Huang, L. Qi and J. Li, “*In situ* imaging of layer-by-layer sublimation of suspended graphene,” *Nano Research* **3** (2010) 43-50.
107. Y. Wang and J. Li, “Phase field modeling of defects and deformation,” *Acta Mater.* **58** (2010) 1212-1235. Overview No. 150.
106. Y. Mishin, M. Asta and J. Li, “Atomistic modeling of interfaces and their impact on microstructure and properties,” *Acta Mater.* **58** (2010) 1117-1151. Overview No. 148.
105. X.H. Liu, J.F. Gu, Y. Shen, J. Li and C.F. Chen, “Lattice dynamical finite-element method,” *Acta Mater.* **58** (2010) 510-523.
104. S. Ogata and J. Li, “Toughness scale from first principles”, *J. Appl. Phys.* **106** (2009) 113534.
103. A. Kushima, X. Lin, J. Li, X-F. Qian, J. Eapen, J. C. Mauro, P. Diep and S. Yip, “Computing the viscosity of supercooled liquids. II. Silica and strong-fragile crossover behavior,” *J. Chem. Phys.* **131** (2009) 164505.
102. J. Feng, L. Qi, J. Y. Huang and J. Li, “Geometric and electronic structure of graphene bilayer edges,” *Phys. Rev. B* **80** (2009) 165407.
101. P. Liu, J. Li and Y-W. Zhang, “Pressure-temperature phase diagram for shapes of vesicles: A coarse-grained molecular dynamics study,” *Appl. Phys. Lett.* **95** (2009) 143104.
100. J. Y. Huang, F. Ding, B. I. Yakobson, P. Lu, L. Qi and J. Li, “In situ observation of graphene sublimation and multi-layer edge reconstructions,” *PNAS* **106** (2009) 10103-10108.
99. L. Kovarik, R.R. Unocic, J. Li, P. Sarosi, C. Shen, Y. Wang and M.J. Mills, “Microtwinning and other shearing mechanisms at intermediate temperatures in Ni-based superalloys,” *Progress in Materials Science* **54** (2009) 839-873.
98. A. Kushima, X. Lin, J. Li, J. Eapen, J. C. Mauro, X.F. Qian, P. Diep and S. Yip, “Computing the viscosity of supercooled liquids,” *J. Chem. Phys.* **130** (2009) 224504.
97. L. Lu, M. Dao, T. Zhu and J. Li, “Size dependence of rate-controlling deformation mechanisms in nanotwinned copper,” *Scripta Mater.* **60** (2009) 1062-1066.
96. T. Zhu, J. Li, S. Ogata and S. Yip, “Mechanics of Ultra-Strength Materials,” *MRS Bulletin* **34** (March 2009) 167-172.
95. P.M. Derlet, P. Gumbsch, R. Hoagland, J. Li, D.L. McDowell, H. van Swygenhoven and J. Wang, “Atomistic Simulations of Dislocations in Confined Volumes,” *MRS Bulletin* **34** (March 2009) 184-189.
94. L. Kovarik, R. R. Unocic, J. Li and M. J. Mills, “The Intermediate Temperature Deformation of Ni-Based Superalloys: Importance of Reordering,” *JOM* **61** (2009) 42-48.
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5. J. Li, “Atomistic visualization,” Chap. 2.31 in *Handbook of Materials Modeling*, ed. S. Yip (Springer, Dordrecht, 2005), pp. 1051-1068. ISBN: 1402032870. Mistake free version at <http://alum.mit.edu/www/liju99/Papers/05/Li05-2.31.pdf>
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Research Grants

25. “Modeling Creep-Fatigue-Environment Interactions in Steam Turbine Rotor Materials for Advanced Ultrasupercritical Coal Power Plants,” Department of Energy, 12/1/2010-11/30/2013, \$220,000 (PI: Liang Jiang, General Electric Global Research, project total: \$1,199,940 + \$299,988 GE cost share).
24. “Materials World Network: Collaborative Research: Modeling Ferroelastic Strain Glasses,” DMR-1008349 (\$309,000, Yunzhi Wang) and DMR-1008104 (\$288,000, Ju Li), Condensed Matter and Materials Theory (CMMT), National Science Foundation, 9/15/2010-9/14/2013.
23. “Modeling Microscopic Damage in Hydrogen Embrittlement,” ExxonMobil Research & Engineering Company, 5/15/2010-5/14/2011, \$155,000.
22. “Modeling Nanowire Growth and Electrical Conduction,” Honda R&D Co., Ltd., Japan, 04/15/2010-04/14/2013, \$450,000.
21. Penn MRSEC (Materials Research Science and Engineering Center) seed grant, 1/1/2010, \$7,500 (PI: Arjun Yodh, University of Pennsylvania, \$20,052,603, DMR-0520020, 10/1/2005 - 9/30/2011).
20. “Metamaterials: a computational alchemy approach,” Honda Research Institute of America, 1/1/2008-12/31/2010, \$341,609.
19. “Modeling-assisted new catalyst discovery - phase III,” Honda Research Institute of America, 1/1/2008-12/31/2010, \$436,774.
18. “AHSS: Multi-scale Modeling of Deformation Mechanism for Design of New Generation of Steels,” NSF CMMI - Mechanics & Structure of Materials (award number CMMI-0728069), 6/1/2008-5/31/2012, \$430,000. (PI: Ju Li, \$215,000; Co-PI: Yunzhi Wang, Ohio State University, \$215,000).
17. “Atomistic and First-Principles Modeling of Materials under Extreme Environments,” Idaho National Laboratory LDRD (award number TM105), 12/26/06-12/27/09, \$254,850 (PI: Paul Meakin, Idaho National Laboratory, project total: \$405,000).
16. “First-principles modeling of mechanics and chemistry of materials,” Presidential Early Career Award for Scientists and Engineers (PECASE), Department of Defense / Air Force Office of Scientific Research (award number FA9550-07-1-0007, FA9550-08-1-0325), 12/01/06 - 11/30/11, \$500,000.

15. "First-principles modeling of phonon heat conduction in nanoscale crystalline structures," Department of Energy Basic Energy Sciences (award number DE-FG02-06ER46330), 9/1/06-08/31/09, approximately \$150,000 (PI: Sandip Mazumder, Department of Mechanical Engineering, OSU, project total: \$330,000).
14. "University computational materials consortium - ab-initio and atomistic modeling of solute and impurity effects on the fracture toughness of Ni-Fe alloys," Department of Energy National Energy Technology Laboratory DE-AM26-04NT41817, 1/9/06-12/31/06, \$68,500 (PI: David S. Sholl, Carnegie Mellon University, project total: \$342,500).
13. "Metallurgical Research Fund (MRF)," ExxonMobil Research & Engineering Company, \$15,000 (12/15/05) + \$15,000 (01/25/06) + \$25,000 (03/19/08) + \$20,000 (04/29/09).
12. "Multi-scale Analysis of Cellular Force Transmission and Biochemical Activation," National Institutes of Health (award number 1-R01-GM-076689-01), 09/01/05-08/31/08, consultant charging 1-month summer salary (PI: Roger D. Kamm, MIT, project total: \$1,098,263).
11. "Ab-initio modeling of metal-organic frameworks," Honda R&D Co., Ltd., Japan, 04/15/05-04/14/06, \$22,219.
10. "Nanomeso: A NSF-EC Cooperative Activity in Computational Research to Study Nano/Meso Length Scale Effects on Crystal Plasticity," National Science Foundation (award number DMR-0502711), 06/15/05-06/14/08, approximately \$140,000 (PI: Peter M. Anderson, OSU, project total: \$546,000).
9. "Modeling-assisted new catalyst discovery - phase II," Honda Research Institute of America, 01/01/05-12/31/07, \$547,801.
8. "Defense University Research Initiative on NanoTechnology (DURINT): Damage-resistant and failure-resistant nanostructures and interfacial materials," Office of Naval Research, \$15,000 administrated by Nitin P. Padture, 05/01/05- (PI: Subra Suresh, MIT).
7. "Experimental and Computational Tools for the Digital Representation and Prediction of Microstructure and its Incorporation in the Designer's Knowledge Base," Office of Naval Research (award number N00014-05-1-0504), 05/01/05-04/30/10, approximately \$400,000 (PI: Hamish L. Fraser, OSU, project total: \$5,553,111).
6. "Materials Engineering for Affordable New Systems II (MEANS2): Development of Microstructure- and Micromechanism-Sensitive Property Models and Their Integration Into the Design of Advanced Disk and Blade Systems", Air Force Office of Scientific Research (award number FA9550-05-1-0135), 02/15/05-10/31/07, approximately \$100,000 (PI: Michael J. Mills, OSU, project total: \$1,100,000).
5. "Molecular Modeling of High-Temperature Oxidation of Refractory Borides", Air Force Office of Scientific Research (award number FA9550-05-1-0026), 11/15/04-11/14/07, \$256,268.
4. "NER: Hydrogen in Carbon Nanotubes - NMR and Multiscale Simulations," National Science Foundation (award number 0403809), 07/01/04-06/30/05, \$15,000 (PI: David Cory, MIT, project total: \$100,000).

3. "MOF Modeling Fund (MMF)," Honda Research Institute USA, Inc., 06/01/04-12/31/04, \$20,000.
2. "Computational Research Fund (CRF)," Honda Research Institute USA, Inc., \$50,000 (05/01/04) + \$52,199 (03/18/05) + \$20,000 (03/22/06) + \$20,000 (06/07/06) + \$40,000 (09/26/2008).
1. "Modeling-assisted new catalyst discovery - phase I," Honda R&D Co., Ltd., Japan, 01/01/03-12/31/04, \$298,418.

Other Grants

8. Department of Energy user proposal "Patterning Multiple Layers of Graphene", with Dr. Jianyu Huang, Center for Integrated Nanotechnologies (CINT) operated by Los Alamos National Laboratory and Sandia National Laboratories, Albuquerque, New Mexico (CINT User project number RA2009A029 and C2010B1042), Aug. 27, 2009 - June 30, 2012.
7. \$17,036 from National Science Foundation (award number 0714540) to organize an International Workshop on Strength and Plasticity at Nanometer and Sub-Micron Scales, Braunschweig, Switzerland; September 4-7, 2007. (PI: Peter M. Anderson).
6. \$1,000 NSF travel grant to attend 210th Meeting of The Electrochemical Society in Cancun, Mexico, October 29-November 3, 2006.
5. Major Grant of 30,000 RUs (Nov. 14, 2005) + 30,000 RUs (July 13, 2007) + 30,000 RUs (June 1, 2009) (1 Resource Unit = 20 dedicated CPU hours on 2.4 GHz Xeon, cash equivalent: \$5) from Ohio Supercomputer Center (award number PAS0167), "Materials Design for Aero-Propulsion, Fuel Cells and Advanced Energy Storage".
4. \$27,044 from Air Force Office of Scientific Research (award number FA9550-05-1-0446) to organize a Workshop on Modeling Materials in Extreme Environment, Sept. 24-25, 2005, Washington D.C.
3. Travel grant from American Chemical Society Petroleum Research Fund to attend the Time-Dependent Density-Functional Theory and the Dynamics of Complex Systems (TDDFT 2004) Summer School in Santa Fe, NM, June 5-10, 2004.
2. Initiated and mediated a \$25,000 donation (03/01/04) from Honda Research Institute USA, Inc. to establish the HRI-USA Scholarship at Dept. Materials Science and Engineering.
1. With W. Windl and Y. Wang: "Highly parallel multiscale modeling suite for the simulation of real materials," 52-CPU Myrinet Beowulf cluster (Cluster Ohio Rev. 3) equipment grant from Ohio Supercomputer Center, hardware worth ~\$100,000, Feb. 4, 2004.

Projects Participated as Graduate Student and Post-doc at MIT

9. Modeling molecular actuation in conducting polymers (2002-2004, sponsored by Honda R&D, Inc.)
8. Theoretical analysis of conductance of molecular junctions (2002-2004, sponsored by the Office of Naval Research / Defense Advanced Research Projects Agency).
7. Defense University Research Initiative on NanoTechnology (DURINT): Damage-resistant and failure-resistant nanostructures and interfacial materials (2001-2005, sponsored by the Office of Naval Research).
6. First-principles theoretical evaluation of hydrogen storage capacity of carbon nanotubes (2000-2002, sponsored by the Honda Motor Company).
5. Construction of a many-body interatomic potential for ZrC_x starting from first principles, then compute its thermal conductivity (1999-2000, sponsored by the Knolls Atomic Power Laboratory).
4. Strengths of crystalline/amorphous/nanocrystalline materials with applications to SiC fiber matrix composites (1996-2002, sponsored by the Air Force Office of Scientific Research).
3. Multiscale techniques to couple continuum PDE with molecular dynamics in MEMS micro-channel flow modeling (1996-1998, sponsored by the Sandia National Laboratory).
2. Calculation of the lattice thermal conductivity of SiC before and after irradiation (1995-1997, sponsored by the Knolls Atomic Power Laboratory).
1. Molecular dynamics study of water and ice (1994-1995, sponsored by the American Chemical Society Petroleum Research Fund).