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Women in NSE
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Education

Ph.D., Department of Nuclear Engineering, Massachusetts Institute of Technology, 2000.
B.S., Special Class for Gifted Young and Department of Modern Physics, University of Science and Technology of China, 1994.

Research Interests

Overcoming Timescale Challenges in Atomistic Simulations

Atomistic and first-principles modeling, which describe the world as assembly of atoms and electrons, provide the most fundamental answer to problems of materials. However, they also suffer the most severe timescale limitations. For instance, in molecular dynamics (MD) simulations, in order to resolve atomic vibrations, the integration time step is limited to hundredth of a picosecond, and therefore the simulation duration is limited to sub-microsecond due to computational cost. Although a nanosecond simulation is often enough (surprisingly) for many physical and chemical properties, it is usually insufficient for predicting microstructural evolution and thermo-mechanical properties of materials. There is clearly a timescale barrier between science-based simulations and practical demands such as understanding plant reliability and nuclear waste storage.

Energy Storage and Conversion

A close coupling of *in situ* experimental observations with modeling has proven to be a powerful paradigm for understanding materials behavior [*Science* 330 (2010) 1515; *Nature* 463 (2010) 335]. Based on such fundamental understandings, we are developing novel nanostructured materials for energy storage and conversion, in applications such as batteries, fuel cells and hydrogen-embrittlement resistant steels.

Materials in Extreme Environments and Far from Equilibrium

Materials in nuclear fission and fusion applications often involve exceptionally high stresses, high temperature and high radiation flux. We study the effects of radiation on microstructure and thermal, electrical and mass transport properties. The concept of fictive temperature(s) that characterize out-of-equilibrium materials is an intriguing statistical mechanics problem, with applications in glasses and even in soft biological materials.

Recent Publications

1. Nanowire Liquid Pumps, J.Y. Huang, Y-C. Lo, J.J. Niu, A. Kushima, X.F. Qian, L. Zhong, S.X. Mao and J. Li, *Nature Nanotechnology* (2013) 8 (2013) 277-281.
2. A Transforming Metal Nanocomposite with Large Elastic Strain, Low Modulus, and High Strength, S.J. Hao, L.S. Cui, D.Q. Jiang, X.D. Han, Y. Ren, J. Jiang, Y.N. Liu, Z.Y. Liu, S.C. Mao, Y.D. Wang, Y. Li, X.B. Ren, X.D. Ding, S. Wang, C. Yu, X.B. Shi, M.S. Du, F. Yang, Y.J. Zheng, Z. Zhang, X.D. Li, D.E. Brown and J. Li, *Science* 339 (2013) 1191-1194.
3. Heterogeneously randomized STZ model of metallic glasses: Softening and extreme value statistics during deformation, P.Y. Zhao, J. Li and Y.Z. Wang, *Int. J. Plasticity* 40 (2013) 1-22.

Recent News

Strain can alter materials' properties

Watching fluid flow at nanometer scales

Funneling the sun's energy

Exploring new nanomaterials

Understanding and predicting materials behavior: NSE takes an interdisciplinary approach

New NSE Faculty Drive Curriculum Expansion Into Computational Science and Engineering

Atomic insights for new materials development

Labs + Groups

Li Group

Video

Research Thumbnail :: Ju Li

Elastic Strain Engineering

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4. Strain-engineered artificial atom as a broad-spectrum solar energy funnel, J. Feng, X-F. Qian, C-W. Huang and J. Li, *Nature Photonics* 6 (2012) 866-872.
5. Quantitative fracture strength and plasticity measurements of lithiated silicon nanowires by in situ TEM tensile experiments, A. Kushima, J.Y. Huang and J. Li, *ACS Nano* 6 (2012) 9425-9432.
6. Adsorbate interactions on surface lead to a flattened Sabatier volcano plot in reduction of oxygen, Liang Qi and Ju Li, *Journal of Catalysis* 295 (2012) 59-69.
7. Slip corona surrounding bilayer graphene nanopore, Liang Qi, Yunwei Mao and Ju Li, *Nanoscale* 4 (2012) 5989-5997.
8. Hydrogen embrittlement of ferritic steels: Observations on deformation microstructure, nanoscale dimples and failure by nanovoiding, Thirumalai Neeraj, Rajagopalan Srinivasan and Ju Li, *Acta Materialia* 60 (2012) 5160-5171.
9. In situ transmission electron microscopy of electrochemical lithiation, delithiation and deformation of individual graphene nanoribbons, Xiao Hua Liu, Jiang Wei Wang, Yang Liu, He Zheng, Akihiro Kushima, Shan Huang, Ting Zhu, Scott X. Mao, Ju Li, Sulin Zhang, Wei Lu, James M. Tour and Jian Yu Huang, *Carbon* 50 (2012) 3836-3844.
10. Finding activation pathway of coupled displacive-diffusional defect processes in atomistics: Dislocation climb in fcc copper, Sanket Sarkar, Ju Li, William T. Cox, Erik Bitzek, Thomas J. Lenosky and Yunzhi Wang, *Physical Review B* 86 (2012) 014115.
11. Patterning of graphene, Ji Feng, Wenbin Li, Xiaofeng Qian, Jingshan Qi, Liang Qi and Ju Li, *Nanoscale* 4 (2012) 4883-4899.
12. Sample size matters for Al88Fe7Gd5 metallic glass: Smaller is stronger, Cheng-Cai Wang, Jun Ding, Yong-Qiang Cheng, Jing-Chun Wan, Lin Tian, Jun Sun, Zhi-Wei Shan, Ju Li, Evan Ma, *Acta Materialia* 60 (2012) 5370-5379.
13. In Situ TEM Experiments of Electrochemical Lithiation and Delithiation of Individual Nanostructures, Xiao Hua Liu, Yang Liu, Akihiro Kushima, Sulin Zhang, Ting Zhu, Ju Li and Jian Yu Huang, *Advanced Energy Materials* 2 (2012) 722-741.
14. Icosahedral Platinum Alloy Nanocrystals with Enhanced Electrocatalytic Activities, Jianbo Wu, Liang Qi, Hongjun You, Adam Gross, Ju Li and Hong Yang, *Journal of the American Chemical Society* 134 (2012) 11880-11883.
15. Electrical Wind Force-Driven and Dislocation-Templated Amorphization in Phase-Change Nanowires, Sung-Wook Nam, Hee-Suk Chung, Yu Chieh Lo, Liang Qi, Ju Li, Ye Lu, A.T. Charlie Johnson, Yeonwoong Jung, Pavan Nukala, Ritesh Agarwal, *Science* 336 (2012) 1561-1566.

Full publication list

Recent Awards

- TMS Robert Lansing Hardy Award (2009)
- MRS Outstanding Young Investigator Award (2006)
- Presidential Early Career Award for Scientists and Engineers (PECASE, 2005)