

# Yunfeng Shi

Assistant Professor of Materials Science and Engineering  
School of Engineering • Rensselaer Polytechnic Institute  
MRC RM311, 110 8th Street, Troy, NY 12180 • Email: shiy2@rpi.edu  
Office: (518) 276-6729 • Cell: (734) 355-6648 • Fax: (519) 276-8554

---

## Education

- 08/2002 - 02/2006    Ph.D., Materials Science  
Department of Materials Science and Engineering  
**University of Michigan**, Ann Arbor, MI  
Thesis title: “*Strain localization of non-crystalline solids*”
- 08/2000 - 08/2002    M.S., Materials Science  
Department of Materials Science and Engineering  
**University of Illinois**, Urbana-Champaign, IL  
Thesis title: “*First principle studies of metal-semiconductor interfaces: Ag on hydrogen-terminated silicon (111) surfaces*”
- 09/1996 - 07/2000    B.E., Materials Science  
Department of Materials Science and Engineering  
**Tsinghua University**, Beijing, China

## Professional Experience

- 08/2008 - present    Assistant Professor  
Department of Materials Science and Engineering, Rensselaer Polytechnic Institute
- 05/2006 - 08/2008    Postdoctoral Research Associate (Advisor: Dr. Donald W. Brenner)  
Department of Materials Science and Engineering, North Carolina State University
- 08/2002 - 05/2006    Research Assistant (Advisor: Dr. Michael L. Falk)  
Department of Materials Science and Engineering, University of Michigan
- 08/2000 - 08/2002    Research Assistant (Advisor: Dr. Jian-min Zuo)  
Department of Materials Science and Engineering, University of Illinois

## Research Interests

- Multiscale modeling
- Chemically powered biomolecular motors
- Nanoporous materials
- Shock-induced nanojetting applied in cell permeabilization
- Reactivity and sensitivity of energetic materials
- Plasticity of metallic glasses and nanocrystalline metals
- Metal-semiconductor interfaces

## Honors and Awards

- **Albert Yee Award** for Excellence in Graduate Student Research, University of Michigan, Ann Arbor, 2005
- **Young Researcher Fellowship Award**, the Third M.I.T. Conference on Computational Fluid and Solid Mechanics, Boston, 2005
- Rackham Conference Travel Grant, University of Michigan, Ann Arbor, 2005
- Rackham Conference Travel Grant, University of Michigan, Ann Arbor, 2004
- **MRS Best Poster Award**, MRS Fall Meeting, Boston, 2002
- Tsinghua Student Award for Social Work, Beijing, 1998
- Tsinghua Excellent Student Scholarship, Beijing, 1996

## Grants

- TeraGrid computing allocation grant TG-DMR070044N, "*Jetting and detonation initiation in shock induced collapse of nanometer scale voids*", Yunfeng Shi, (05/2007-05/2008).

## Professional Services

- Reviewer for Journal of Physics: Condensed Matter, IEEE Transactions on Nanotechnology, Journal of Physics: Applied Physics, Scripta Materialia.

## Selected Publications

5. Y. F. Shi, "A mimetic porous carbon model by quench molecular dynamics simulation", **Journal of Chemical Physics**, 128, 234707 (1-11) (2008).
4. Y. F. Shi, M. B. Katz, H. Li, M. L. Falk, "Evaluation of the 'disorder temperature' and free volume formalisms via simulations of shear banding in amorphous solids", **Physical Review Letters**, 98, 185505 (1-4) (2007).
3. Y. F. Shi, M. L. Falk, "Shear localization and percolation of stable structure in amorphous solids", **Physical Review Letters**, 95, 095502 (1-4) (2005).
2. Y. F. Shi, M. L. Falk, "Structural transformation and localization during simulated nanoindentation of a non-crystalline metal film", **Applied Physics Letters**, 86, 011914 (1-3) (2005).
1. J. Bording, B. Li, Y. F. Shi, J. M. Zuo, "Size- and shape-dependent energetics of nanocrystal interfaces: Experiment and simulation", **Physical Review Letters**, 90, 226104 (1-3) (2003).

## Complete Publication List (Peer Reviewed)

18. Y. F. Shi, "A mimetic porous carbon model by quench molecular dynamics simulation", **Journal of Chemical Physics**, 98, 185505 (1-4) (2008).

17. Y. F. Shi, D. W. Brenner, "*Molecular Simulation of the Influence of Interface Faceting on the Shock Sensitivity of a Model Plastic Bonded Explosive*", **Journal of Physical Chemistry B**, in press (2008).
16. Y. F. Shi, D. W. Brenner, "*Jetting and detonation initiation in shock induced collapse of nanometer scale voids*", **Journal of Physical Chemistry C**, 112, 6263-6270 (2008).
15. Y. F. Shi, D. W. Brenner, "*Hotspot formation in shock induced void collapsing*", **Solid State Phenomena**, 139, 77-82 (2008).
14. Y. F. Shi, M. L. Falk, "*A computational analysis of the deformation mechanisms of a nanocrystallite-metallic glass composites*", **Acta Materialia**, 56, 995-1000 (2007).
13. Y. F. Shi, D. W. Brenner, "*Simulated thermal decomposition and detonation of nitrogen cubane by molecular dynamics*", **Journal of Chemical Physics**, 127, 134503 (1-7) (2007).
12. Y. F. Shi, M. B. Katz, H. Li, M. L. Falk, "*Evaluation of the 'disorder temperature' and free volume formalisms via simulations of shear banding in amorphous solids*", **Physical Review Letters**, 98, 185505 (1-4) (2007).
11. Y. F. Shi, M. L. Falk, "*Stress-induced structural transformation and shear banding during simulated nanoindentation of a metallic glass*", **Acta Materialia**, 55, 4317-4324 (2007).
10. Y. F. Shi, M. L. Falk, "*Simulations of nanoindentation in a thin amorphous metal film*", **Thin Solid Films**, 515, 3179-3182 (2007).
9. Y. F. Shi, M. L. Falk, "*Atomic-scale simulations of strain localization in three-dimensional model amorphous solids*", **Physical Review B**, 73, 214201 (1-10) (2006).
8. Y. F. Shi, M. L. Falk, "*Does metallic glass have a backbone? The role of percolating short range order in strength and failure*", **Scripta Materialia**, 54, 381-386 (2006).
7. Y. F. Shi, M. L. Falk, "*Shear localization and percolation of stable structure in amorphous solids*", **Physical Review Letters**, 95, 095502 (1-4) (2005).
6. Y. F. Shi, M. L. Falk, "*Atomic-scale simulations of strain localization in a single-component three-dimensional model amorphous solid*", **Mat. Res. Soc. Proc.**, 903E, Z16.05.1-6 (2005).
5. Y. F. Shi, M. L. Falk, "*Structural transformation and localization during simulated nanoindentation of a non-crystalline metal film*", **Applied Physics Letters**, 86, 011914 (1-3) (2005).
4. J. Bording, B. Li, Y. F. Shi, J. M. Zuo, "*Size- and shape-dependent energetics of nanocrystal interfaces: Experiment and simulation*", **Physical Review Letters**, 90, 226104 (1-4) (2003).
3. M. L. Falk, Y. Shi, "*Strain Localization in a Molecular-Dynamics Model of a Metallic Glass*", **Mat. Res. Soc. Proc.**, 754, CC6.20.1-6 (2003).
2. B. Q. Li, Y. F. Shi, J. Bording, J. M. Zuo, "*Nanocluster Epitaxy by Annealing: Ag on H-terminated Si(111) Surfaces*", **Mat. Res. Soc. Proc.**, 749, W2.10.1-6 (2003).

1. J. M. Zuo, Y. F. Shi, "Complementary Structural Information from Diffraction Patterns in STEM: Accurate Thickness Measurement with Pattern Matching", **Microscopy and Microanalysis**, 7, S224-225 (2001).

### Other Publications

2. Y. F. Shi, M. L. Falk, "Uniaxial tensile test on an amorphous solid with embedded quasi-crystallites: a molecular dynamics study", *Computational Fluid and Solid Mechanics*, ed. by K. J. Bathe, 485-487, Elsevier (2005).

1. Y. F. Shi, M. L. Falk, "Shear Banding and Short Range Order in Simulated nanoindentation of a Metallic Glass", *Proceedings of the Third International Conference on Multiscale Materials Modeling*, September 18-22, 2006, Freiburg, Germany, pp. 296-301.

### Invited Seminars

6. Y. F. Shi, "Simulating non-equilibrium phenomena at the atomic scale: from high explosives to molecular motors", College of Nanoscale Science and Engineering, University at Albany, Albany (2008).

5. Y. F. Shi, "Simulating non-equilibrium phenomena at the atomic scale: from high explosives to molecular motors", Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy (2008).

4. Y. F. Shi, "Strain Localization of Non-crystalline Solids", Nonlinear physics group, Department of Physics, North Carolina State University, Raleigh (2007).

3. Y. F. Shi, "Strain Localization of Non-crystalline Solids", T-12 group, Los Alamos National Laboratory, Los Alamos (2006).

2. Y. F. Shi, "Visualization for Computer Simulations", Liquid Crystal Institute, Kent State University, Kent (2006).

1. Y. F. Shi, "Strain Localization of Non-crystalline Solids", special department seminar for the Albert Yee Award, Department of Materials Science and Engineering, University of Michigan, Ann Arbor (2005).

### Presentations in Conferences or Workshops

14. Y. F. Shi, D. W. Brenner, "A Molecular Dynamics Study of Model Energetic Crystals under Shock Loading", MRS Fall Meeting, Boston (2007)

13. M. L. Falk, Y. F. Shi, "Atomistic Simulations of Shear Banding in Metallic Glasses", MRS Fall Meeting, Boston (2007)

12. Y. F. Shi, B. Broom, Y. H. Hu, D. W. Brenner, "Atomic simulations of heterogeneous detonation dynamics", Multiscale Modeling to Predict Sensitivity of Energetic Materials-MURI Review Meeting, Aberdeen (2007)

11. Y. F. Shi, M. L. Falk, "Mechanical behaviors of nanocrystallites-amorphous matrix", MRS Fall Meeting, Boston (2006).

10. Y. F. Shi, M. L. Falk, "*Atomic-scale simulations of localization during nanoindentation of metallic glasses*", MRS Fall Meeting, Boston (2005).
9. Y. F. Shi, M. L. Falk, "*Localization and Percolation of Short Range Ordering in Bulk Metallic Glasses*", MRS Fall Meeting, Boston (2005).
8. Y. F. Shi, M. L. Falk, "*Uniaxial tensile test on an amorphous solid with embedded quasicrystallites*", Third M.I.T. Conference, Boston (2005).
7. Y. F. Shi, M. L. Falk, "*Shear Localization and Percolation in a Simulated Model Metallic Glass*", TMS Annual Meeting, San Francisco (2005).
6. Y. F. Shi, M. L. Falk, "*Simulations of Nanoindentation in Thin Amorphous Metal Films*", TMS Annual Meeting, San Francisco (2005).
5. J. M. Zuo, Y. F. Shi, J.K. Bording, B. Q. Li, "*Structure of supported Ag nanoclusters on silicon surfaces, theory and experiment*", APS March Meeting, Montreal, Canada (2004).
4. Y. F. Shi, M. L. Falk, "*Shear Localization and Defect Dynamics in a Model 2D Binary Glass*", APS March Meeting, Montreal, Canada (2004).
3. M. L. Falk, F. Albano, Y. F. Shi, "*Relating Structure to Mechanical Properties in Simulation Studies of Model Metallic Glasses*", Fluctuation Electron Microscopy and Nanoscale Ordering in Amorphous Materials, Urbana-Champaign (2003)
2. Y. F. Shi, M. L. Falk, "*A Technique for the Creation of Aperiodic Large-Scale Glass Systems*", APS March Meeting, Austin (2003).
1. Y. F. Shi, J. K. Bording, B. Q. Li, J. M. Zuo, "*A Molecular Dynamics Study of the alignment of silver nano-clusters on H-terminated Si(111)*", APS March Meeting, Indianapolis (2002).

### **Poster Presentations**

6. Y. F. Shi, D. W. Brenner, "*Detonation sensitivity of defected energetic crystals under shock loading*", Gordon Research Conferences (Energetic Materials), Tilton, NH (2008).
5. Y. F. Shi, M. L. Falk, "*Structural transformation and localization during simulated nanoindentation of a non-crystalline metal film*", Gordon Research Conferences (Physical Metallurgy), Plymouth (2004).
4. Y. F. Shi, M. L. Falk, "*Structural transformation and localization during simulated nanoindentation of a non-crystalline metal film*", ASM-Detroit Chapter University Night, Ann Arbor (2004).
3. M. L. Falk, Y. F. Shi, "*Strain Localization in a Molecular-Dynamics Model of a Metallic Glass*", **MRS Best Poster Award Winner**, MRS Fall Meeting, Boston (2002).
2. Y. F. Shi, J. K. Bording, B. Q. Li, J. M. Zuo, "*Molecular Dynamics Study of the Growth of Silver Clusters on H-Si(111) Surfaces*", MRS Fall Meeting, Boston (2002).
1. J. K. Bording, Y. F. Shi, B. Q. Li, J. M. Zuo, "*Finite Size Effects on Interface Energy*", MRS Fall Meeting, Boston (2002).

**Memberships**

American Physical Society (APS)

Materials Science Society (MRS)

Minerals, Metals & Materials Society (TMS)