

Douglas Edward Spearot

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EDUCATION

- Georgia Institute of Technology** **2005**
Doctor of Philosophy in Mechanical Engineering
Dissertation: Atomistic Calculations of Nanoscale Interface Behavior in FCC Metals
Advisors: Dr. David L. McDowell and Dr. Karl I. Jacob
Major: Mechanics of Materials
Minor: Computational Materials Science
- Georgia Institute of Technology** **2001**
Master of Science in Mechanical Engineering
- University of Michigan** **1999**
Bachelor of Science in Mechanical Engineering

PROFESSIONAL APPOINTMENTS

University of Arkansas – Fayetteville **August 2005 – Current**
Assistant Professor, Department of Mechanical Engineering

- Atomistic modeling (molecular dynamics and molecular mechanics) of nanoscale interface behavior in metallic and intermetallic materials.
- Identification of dislocation nucleation and propagation phenomena in metallic materials; relationship of specific interface features in nanoscale plasticity.
- Molecular dynamics simulation of metal catalyst assisted carbon nanotube nucleation and growth – role of catalyst structure and configuration on carbon nanotube chirality.
- Molecular dynamics simulation of metal-alkane interfaces – application to nanomachining processes.

Georgia Institute of Technology **1999-2005**
Graduate Research Assistant, Mechanics of Materials Research Group
G.W. Woodruff School of Mechanical Engineering

Sandia National Laboratories / Livermore, CA **Summer 2001**
Intern, Engineering Sciences Summer Institute
Mentor: Dr. Jonathan A. Zimmerman, Science-Based Mathematical Modeling Department

Visiting Researcher

Mentor: Dr. Steven J. Plimpton, Parallel Computational Sciences

TEACHING HISTORY

Semester	Number	Title	Level	Students
Fall 2005	MEEG 2023	Introductory Mechanics	Junior	51
Spring 2006	MEEG 591V	Multiscale Computational Modeling	Graduate	11
Fall 2006	MEEG 2023	Introductory Mechanics	Junior	40
Fall 2006	MEEG 2303	Introduction to Materials	Sophomore	63
Spring 2007	MEEG 491V	Mechanics of Composite Materials	Senior	9
Summer 2007	MEEG 2303	Introduction to Materials	Sophomore	14
Fall 2007	MEEG 2023	Introductory Mechanics	Junior	35
Fall 2007	MEEG 2303	Introduction to Materials	Sophomore	62
Spring 2008	MEEG 591V	Multiscale Computational Modeling	Graduate	5
Fall 2008	MEEG 2303	Introduction to Materials	Sophomore	
Fall 2008	MEEG 5013	Advanced Mechanics of Materials	Graduate	
Spring 2009	MEEG 491V	Mechanics of Composite Materials	Senior	

GRADUATE STUDENT ADVISING**Rahul Rajgarhia, Ph.D. Mechanical Engineering, Expected December 2008**

Dissertation: Grain boundary structure and mechanical properties in doped nanocrystalline Cu
 Co-advisor: Professor Ashok Saxena

Valliappa Kalyanasundaram, M.S. Mechanical Engineering, Expected May 2008

Thesis: Behavior of dielectric polymer chains with application to nano-machining processes
 Co-Advisor: Professor Ajay Malshe

Nikhil Joshi, M.S. Microelectronics and Photonics, Expected May 2008

Thesis: The study of the melting of nanosized metallic particles
 Co-Advisor: Professor Deepak Bhat

REFEREED PUBLICATIONS

1. Spearot, D.E. (2008) Evolution of the E structural unit during uniaxial and constrained tensile deformation, *Mechanics Research Communications*, 35, 81-88.
2. Spearot, D.E., Capolungo, L., Qu, J., Cherkaoui, M. (2008) On the elastic structural evolution of <100> bicrystal interfaces in copper, *Computational Materials Science*, 42, 57-67.
3. Kalyanasundaram, V., Virwani, K.R., Spearot, D.E., Malshe, A.P., Rajurkar, K.P. (2008) Understanding behavior of machining interface and dielectric molecular medium in nanoscale electro-machining, *CIRP Annals - Manufacturing Technology*, accepted.
4. Kalyanasundaram, V., Virwani, K.R., Spearot, D.E., Rajurkar, K.P., Malshe, A.P. (2008) In situ characterization and repeatability analysis of nano-EM tool machining performance, *Transactions of the NAMRI/SME*, vol. 36.
5. Spearot, D.E. (2008) Dislocation nucleation from ledges and disconnections in grain boundaries, *Plasticity 2008 Proceedings*, in press.
6. Rajgarhia, R., Spearot D.E., Saxena, A (2008) Plastic deformation behavior of single crystal copper-antimony alloy, *Plasticity 2008 Proceedings*, in press.
7. Rajgarhia, R.K., Koh, S.-W., Spearot, D., Saxena, A. (2008) Microstructure stability of nanocrystalline materials using dopants, *Molecular Simulation*, in press.
8. Tschopp, M.A., Spearot, D.E., McDowell, D.L. (2008), Influence of Grain Boundary Structure and Dislocation Nucleation in FCC Metals, in: *Dislocations in Solids, Volume 14 – A tribute to F.R.N. Nabarro*, Elsevier, in press.
9. Tschopp, M.A., Spearot, D.E., McDowell, D.L. (2007) Atomistic simulations of homogeneous dislocation nucleation in single crystal copper, *Modeling and Simulation in Materials Science and Engineering*, 15, 693-709.
10. Capolungo, L., Spearot, D.E., Cherkaoui, M., McDowell, D.L., Qu., J. and Jacob, K.I. (2007) Dislocation nucleation from bicrystal interfaces and grain boundary ledges: Relationship to nanocrystalline deformation, *Journal of the Mechanics and Physics of Solids*, 55, 2300-2327.
11. Spearot, D.E., Tschopp, M.A., Jacob, K.I. and McDowell, D.L. (2007) Tensile strength of <100> and <110> tilt interfaces in copper, *Acta Materialia*, 55, 705-714.
12. Spearot, D.E., Jacob, K.I. and McDowell, D.L. (2007) Dislocation nucleation from bicrystal interfaces with dissociated structure, *International Journal of Plasticity*, 23, 143-160.
13. Rajgarhia, R.K., Koh, S.-W., Spearot, D., Saxena, A., Selvam, P. and Tummala, R. (2007) Influence of stress and temperature on the microstructure stability of nanocrystalline materials, *Technical Proceedings of the 2007 Nanotechnology Conference and Trade Show (NSTI-Nanotech 2007) Volume 4*, 543-546.
14. Spearot, D.E., Jacob, K.I. and McDowell, D.L. (2005) Nucleation of dislocations from [001] bicrystal interfaces in aluminum, *Acta Materialia*, 53, 3579-3589.

15. Spearot, D.E., Jacob, K.I., McDowell, D.L. and Plimpton, S.J. (2005) Effect of deformation path sequence on the behavior of nanoscale copper bicrystal interfaces, *Journal of Engineering Materials and Technology*, 127, 374-382.
16. Spearot, D., Jacob, K. and McDowell, D. (2005) Molecular dynamics simulations of dislocation nucleation from bicrystal interface in FCC metals, *Proceedings of the ASME Materials Division 2005*, v 100 MD, 505-513.
17. Spearot, D.E., Jacob, K.I. and McDowell, D.L. (2004) Nonlocal separation constitutive laws for interfaces and their relation to nanoscale simulations, *Mechanics of Materials*, 36, 825-847.
18. Spearot, D., Jacob, K. and McDowell, D. (2004) Molecular Dynamics Simulations of Grain Boundary Decohesion in FCC Copper and Aluminum, *Collection of Technical Papers – 45th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference*, v 3, 2083-2093.
19. Spearot, D., Jacob, K. and McDowell, D. (2003) MD Simulation of Grain Boundary Fracture in Copper and Connections to Interface Separation Potentials, *Collection of Technical Papers - AIAA/ASME/ ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference*, v 3, 1902-1911.

CONFERENCE PRESENTATIONS

1. Spearot, D.E., Rajgarhia, R., Saxena, A., Atomistic simulation of dislocation nucleation from homogeneous and doped copper grain boundaries, presented at: TMS2008, 137th Annual Meeting and Exhibition, March 9-13, 2008, New Orleans, LA.
2. Spearot, D.E., Dislocation nucleation from ledges and disconnections in grain boundaries, presented at: Plasticity2008, January 3-8, 2008, Kona, HI.
3. Rajgarhia, R., Spearot, D.E., Saxena, A., Plastic deformation behavior of single crystal copper-antimony alloys, presented at: Plasticity2008, January 3-8, 2008, Kona, HI.
4. Spearot, D.E., Atomistic simulation of elastic and inelastic grain boundary evolution during tensile deformation, presented at: 9th U.S. National Congress on Computational Mechanics, July 23 – 26, 2007, San Francisco, CA.
5. Rajgarhia, R., Koh, S.W., Spearot, D., Saxena, A., Selvam, P., Tummala, R., Influence of stress and temperature on the microstructure stability of nanocrystalline materials, presented at: NSTI Nanotechnology Conference, May 20-24, 2007, Santa Clara, CA.
6. Joshi, N., Spearot, D.E., Bhat, D., Molecular dynamics simulation of nanocluster melting: application to carbon nanotube nucleation, presented at: Materials Research Society 2007 Spring Meeting, April 9-13, 2007, San Francisco, CA.
7. Spearot, D.E., McDowell, D.L., Jacob, K.I., Atomistic simulation of dislocation nucleation from grain boundaries in FCC metals, presented at: The 7th World Congress on Computational Mechanics, July 16-22, 2006, Los Angeles, CA.

8. Capolungo, L., Spearot, D.E., Cherkaoui, M., Qu, J. Dislocation nucleation from bicrystal interface and grain boundary ledges: Relationship to nanocrystalline deformation, presented at: The 7th World Congress on Computational Mechanics, July 16-22, 2006, Los Angeles, CA.
9. Spearot, D.E., Tschopp, M.A., McDowell, D.L., Grain Boundary Structure and Dislocation / Dislocation Mechanics in Plasticity of FCC Metals, keynote lecture: Plasticity 2006, July 17-22, 2006, Halifax, Nova Scotia.
10. Capolungo, L., Spearot, D.E., Cherkaoui, M., Qu, J. Dislocation nucleation from bicrystal interface and grain boundary ledges: Relationship to nanocrystalline deformation, presented at: Plasticity 2006, July 16-22, 2006, Halifax, Nova Scotia.
11. McDowell, D., Spearot, D.E., Tschopp, M.A., Atomistic Simulations of Grain Boundary Dislocation Structure and Evolution in FCC Metals, presented at: The 2005 Fall Meeting of the Materials Research Society, November 27-December 1, 2005, Boston, MA.
12. Spearot, D., Jacob, K. and McDowell, D., Molecular dynamics simulations of dislocation nucleation from bicrystal interface in FCC metals, presented at: 2005 ASME International Mechanical Engineering Congress and Exposition, November 5-11, 2005, Orlando, FL.
13. Spearot, D.E., Jacob, K.I., McDowell, D.L., Atomistic calculations of interface structure and dislocation nucleation during tensile deformation of Cu and Al, presented at: The 2005 Joint ASME/ASCE/SES Conference on Mechanics of Materials, June 1-3, 2005, Baton Rouge, LA.
14. Spearot, D.E., Jacob, K.I., McDowell, D.L., Fracture of CSL boundaries in Cu and Al, presented at: 11th International Conference on Fracture, March 20-25, 2005, Turin, Italy.
15. Spearot, D.E., Jacob, K.I., McDowell, D.L., Molecular dynamics simulations of grain boundary decohesion in FCC copper and aluminum, presented at: 45th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, April 19-22, 2004, Palm Springs, CA.
16. Spearot, D.E., Jacob, K.I., McDowell, D.L., Molecular dynamics calculations of interface behavior copper and aluminum, presented at: 5th Georgia Tech Conference on Nanoscience and Nanotechnology, November 10-11, 2004, Atlanta, GA.
17. Spearot, D.E., Jacob, K.I., McDowell, D.L., MD simulation of grain boundary fracture in copper and connections to interface separation potentials, presented at: 44th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, April 7-10, 2003, Norfolk, VA.
18. Spearot, D.E., Jacob, K.I., McDowell, D.L., Constitutive laws for metallic interface separation motivated by nanoscale simulations, presented at: U.S. National Congress on Computational Mechanics VII, July 27 – August 1, 2003, Albuquerque, NM.
19. Spearot, D.E., Jacob, K.I., McDowell, D.L., Separation constitutive laws for interfaces informed by nanoscale simulations, presented at: 5th European Solid Mechanics Conference, August 17-22, 2003, Thessaloniki, Greece.
20. Spearot, D.E., Jacob, K.I., McDowell, D.L., Nonlocal separation constitutive laws for interfaces informed by nano-scale simulations, presented at: 39th Annual Technical Meeting of the Society of Engineering Science, October 13-16, 2002, State College, PA.

21. Spearot, D.E., Zimmerman, J.A., Jacob, K.I., McDowell, D.L., Identification of dislocation structure during separation of Cu-Cu and Cu-Al interfaces using MD simulations, presented at: U.S. National Congress on Computational Mechanics VI, August 1-3, 2001, Dearborn, MI.
22. Spearot, D.E., Jacob, K., Zhou, M., McDowell, D.L., Nonlocal separation constitutive laws for interfaces and their relation to nano-scale simulations, presented at: 1st Georgia Tech Conference on Nanoscience and Nanotechnology, October 16-18, 2000, Atlanta, GA.

HONORS AND AWARDS

- Ralph E. Powe Junior Faculty Enhancement Award, Oak Ridge Associated Universities, Engineering or Applied Science Division, 2007.
- Most Outstanding Teacher Award, Department of Mechanical Engineering, University of Arkansas, 2007.
- Recipient of Georgia Institute of Technology Presidential Fellowship, Fall 2001.
- Recipient of AESF Graduate Scholarship, Fall 2001.
- Recipient of G.W. Woodruff Fellowship, Spring 2001.
- University of Michigan Engineering Dean's List, Spring 1996 - Spring 1999.
- Inducted into Tau Beta Pi, Engineering Honor Society, Fall 1997.
- Inducted into Pi Tau Sigma, Mechanical Engineering Honor Society, Fall 1996.
- Eagle Scout, May 1990.

PROFESSIONAL SOCIETY MEMBERSHIPS

- Materials Research Society (MRS)
- American Society of Mechanical Engineering (ASME)
- American Society of Engineering Education (ASEE)
- International Association for Computational Mechanics (IACM)