Jeffrey M. Rickman
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Department of Materials Science and Engineering and Department of Physics
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A. Education

Ph.D. in Physics, August 1989. Carnegie Mellon University Pittsburgh, Pa.
Thesis: "Some Effects of Strain on Diffusion in Crystalline Solids" (Advisor: R. F. Sekerka)
M.S. in Physics, August 1984. Carnegie Mellon University Pittsburgh, Pa.
B.S. in Physics, December 1982. Miami University Oxford, Ohio.
B.A. in Mathematics, December 1982. Miami University Oxford, Ohio.

Professional Experience

Senior Technical Expert – GrainBound, Inc. – we identify the key grain boundaries that govern material performance to provide a processing-design solution with better control for product reliability

Professor, Department of Materials Science and Engineering and Department of Physics, Lehigh University (2005)

Associate Professor, Department of Materials Science and Engineering, Lehigh University, 1999-2005.

Assistant Professor, Department of Materials Science and Engineering, Lehigh University, 1993 - 1999.

Summer Visitor, Los Alamos National Laboratory, 1995 - .

Consultant, Biosym Technologies, Inc., 1992 - 1993 .

Postdoctoral Associate, Department of Materials Science and Engineering, University
of Michigan, 1991 - 1993.

Postdoctoral Associate, Materials Science Division, Argonne Nat. Lab., 1989 - 1991.

Research Interests

Some of my research interests include:

1.) Materials informatics

We are applying the methodologies of data science to analyze big data in materials science, including the characterization of abnormal grain growth in ceramic oxides and the prediction of the plastic response of high-entropy alloys.

2.) Modeling of dynamics of line defects (dislocations) leading to plastic behavior.

Monte Carlo and Langevin dynamics are employed to describe the mutual interactions and kinetics associated with interacting dislocations.

3.) Simulation of kinetics and pattern formation associated with phase transitions.

We have assessed the role of defects on nucleation and growth phenomena that attend first-order phase transitions, enabling generalizations of kinetic models that describe the temporal evolution of these transitions.

4.) Grain-boundary chemistry and mechanical properties of ceramic oxides.

We employed atomic-level simulation (energy minimization and molecular dynamics) to describe segregation to interfaces in aluminum oxide using empirical potentials with long-ranged Coulombic interactions. We have also examined diffusive transport at internal interfaces via experiment and simulation.

5.) Analysis of atomic-level simulation data using cumulant (histogram) techniques and free-energy calculations.

These methods permit the extraction of thermodynamic information over a wide range of parameter space from simulations at one point in that space, thereby enabling highly-efficient simulations. This effort has also shed new light on modern methods of Monte Carlo data analysis (e.g., histogram techniques) by employing cumulant expansions to examine these methods from a complementary perspective.

6.) Defect elasticity.

Areas of interest include the energetics (electrostatic and elastostatic) of twin domain formation in ferroelectrics and the energetics governing eutectic morphologies.

My many other research interests include: mesoscale simulations of grain growth, sintering and creep, analysis of transmission electron microscope (TEM) images, colloidal self-assembly and the implementation of parallel computing strategies. Both analytical and simulational tools (e.g., field theories, Monte Carlo methods, etc.) are employed in various efforts to obtain a quantitative description of material behavior.

B. Publications

Book Chapters

"Grain Boundary Chemistry and Creep Resistance of Alumina," Y. Z. Li, M. P. Harmer, H. M. Chan and J. M. Rickman in *Ceramic Microstructures '96: Control at the Atomic Level* , ed. by A. P. Tomsia and A. Glaeser (Plenum Press).

"Grain Boundary Chemistry and Creep Resistance of Alumina," M. P. Harmer, H. M. Chan, J. M. Rickman, J. Cho and Y.-Z. Li in *Computer-Aided Design of High-Temperature Materials* , ed. by A. Pechenik *et al*. (Oxford University Press, Oxford, 1999), p. 18.

"Free Energy Calculations in Materials Research", J. M. Rickman and R. LeSar, Ann. Rev. Mater. Res. **32**, 195 (2002). (review)

"Coarse-Graining of Dislocation Structure and Dynamics", R. LeSar and J. M. Rickman, for *Continuum Scale Simulation of Engineering Materials*, ed. by D. Raabe, to be published in 2004. (invited)

"Coarse-Graining Methodologies for Dislocation Energetics and Dynamics," J. M. Rickman and R. LeSar, *Handbook for Materials Modeling*, ed. S. Yip, 2325-2335 (2005) (invited).

"Microstructural Characterization Associated With Solid-Solid Transformations", J. M. Rickman and K. Barmak, *Handbook for Materials Modeling*, ed. S. Yip, 2397-2408 (2005) (invited).

"Multiscale Modeling of Deformation and Fracture in Metallic Materials", D. Farkas and J. M. Rickman, to be published in *Applied Computational Materials*

Modeling: Theory, Experiment, and Simulations, ed. by G. Bozzolo, R. Noebe, and P. Abel, Springer (2007) (invited).

"Janus Ellipsoids: Self-Assembly and Applications," Wei Li, Jeffrey M. Rickman, Ya Liu and James D. Gunton, *Soft, Hard and Hybrid Janus Structures: Synthesis, Self-Assembly and Application*s, ed. by B. Li and Z. Lin, Ch. 7, 277-314 Imperial College Press (2017) (invited).

Journal Articles (refereed)

"Temperature Dependence of Thermodynamic Quantities From Simulations at a Single Temperature", J. M. Rickman and S. R. Phillpot, Phys. Rev. Lett. **66**, 349 (1991).

"Calculation of the Free Energy of Solids from the Energy Distribution Function", S. R. Phillpot and J. M. Rickman, J. Chem. Phys. **93**, 1454 (1991).

"Molecular Dynamics Study of the Effects of Strain on Interstitial Diffusion in a Hard-Sphere Model of a Binary Crystalline Solid", J. M. Rickman, Jorge Viñals, and R. F. Sekerka, Phys. Rev. B **43**, 8251 (1991).

"Calculation of Elastic Constants From a Replica Monte Carlo Simulation", J. M. Rickman and J. A. Jaszczak, Phys. Rev. B **43**, 13285 (1991).

"On the Mechanism for Grain-Boundary Migration in Metals: A Molecular-Dynamics Study", J. M. Rickman, S. R. Phillpot, D. Wolf, D. L. Woodraska, and S. Yip, J. Mat. Res. **6**, 2291 (1991).

"Calculation of the 'Absolute' Free Energy and the Entropy of Classical Solids From the Motion of Particles", J. M. Rickman and S. R. Phillpot, J. Chem. Phys. **95**, 7562 (1991).

"Temperature Dependence of the Thermodynamic Properties of a Liquid From Simulations at a Single Temperature", S. R. Phillpot and J. M. Rickman, Mol. Phys. **75**, 189 (1992).

"Effects of Long-range Crystalline Order on Collective Diffusion in Binary Solids", J. M. Rickman, Jorge Viñals, R. F. Sekerka, and W. W. Mullins, Phys. Rev. B **45**, 7750 (1992).

"Finite-Temperature Properties of Perfect Crystals and Defects From Zero-Temperature Energy Minimization", J. M. Rickman, R. Najafabadi, L. Zhao, and D. J. Srolovitz, J. Phys.: Condens. Matter **4**, 4923 (1992).

“Simulated Quenching to the Zero-Temperature Limit of the Grand-Canonical Ensemble”, S. R. Phillpot and J. M. Rickman, J. Chem. Phys. **97**, 2651 (1992).

"Defect Interactions on Solid Surfaces," J. M. Rickman and D. J. Srolovitz, Surf. Sci. **284**, 211 (1993).

"A Modified Local Harmonic Model for Solids," J. M. Rickman and D. J. Srolovitz, Phil. Mag. A **67**, 1081 (1993).

"Efficient Determination of Thermodynamic Properties From a Single Simulation," J. M. Rickman and D. J. Srolovitz, J. Chem. Phys. **99**, 7993 (1993).

"Thermoelastic Analysis of Matrix Crack Growth in Particulate Composites, " N. Sridhar, J. M. Rickman and D. J. Srolovitz, Acta metall. mater. **43**, 1669 (1995).

"Effect of Reinforcement Morphology on Matrix Microcracking," N. Sridhar, J. M. Rickman and D. J. Srolovitz, Acta metall. mater. **44**, 915 (1996).

"A Simulation Study of Grain Boundary Diffusion Kinetics," Y. Wang, J. M. Rickman and Y. T. Chou, Acta metall. mater. **44**, 2505 (1996).

"Finite-Temperature Properties of Materials From Analytical Statistical Mechanics," R. LeSar and J. M. Rickman, Phil. Mag. B **73**, 627 (1996).

“The Effects of Particle Size Distribution and Induced Unpinning During Grain Growth," G. S. Thompson, J. M. Rickman, M. P. Harmer and E. A. Holm, J. Mat. Res. **11**, 1520 (1996).

"Twinning in Thin Films: I. Elastic Analysis," N. Sridhar, J. M. Rickman and D. J. Srolovitz, Acta mater. **44** , 4085 (1996).

"Twinning in Thin Films: II. Equilibrium Microstructures," N. Sridhar, J. M. Rickman and D. J. Srolovitz, Acta mater. **44** , 4097 (1996).

"Modeling of Dislocation Structures in Materials," J. M. Rickman and Jorge Viñals, Phil. Mag. A **75**, 1251 (1997).

"Impact of Heterogeneous Boundary Nucleation on Transformation Kinetics and Microstructure," J. M. Rickman, W. S. Tong and K. Barmak, Acta mater. **45**, 1153 (1997).

"Microstructural Stability of Stressed Eutectic Composites" N. Sridhar, J. M. Rickman and D. J. Srolovitz, Acta mater. **45**, 2715 (1997).

"Impact of Heterogeneous Boundary Nucleation on Product Grain Size Distribution," W. S. Tong, J. M. Rickman and K. Barmak, J. Mater. Res. **12**, 1501 (1997).

"Effect of Y and La on the Tensile Creep Behavior of Aluminum Oxide," J. Cho, M. P. Harmer, H. M. Chan, J. M. Rickman and A. M. Thompson, J. Am. Ceram. Soc. **80**, 1013 (1997).

"Evolution of Grain Structure in Thin Film Reactions," K. Barmak, J. M. Rickman and C. Michaelsen, J. Elec. Mat. **26**, 1009 (1997). (invited)

"Multilayer Film Stability," N. Sridhar, J. M. Rickman and D. J. Srolovitz, J. Appl. Phys. **82**, 4852 (1997).

"A Simulation Study of Nucleation in a Phase-Field Model," A. Roy, J. M. Rickman, J. D. Gunton and K. R. Elder, Phys. Rev. E. **57**, 2610 (1998).

"Grain Boundary Chemistry and Creep Resistance of Oxide Ceramics," M. P. Harmer, H. M. Chan, J. M. Rickman, J. Cho, and C. M. Wang, in *The Science of Engineering Ceramics II*, eds. K. Nihara, T. Sekino, E. Yasuda and T. Sasa (Trans. Tech. Publ. Ltd., Switzerland, 1998), pp. 139-144.

"Analysis of Dislocation Microstructures: Impact of Force Truncation and Slip Systems," H. Y. Wang, R. LeSar and J. M. Rickman, Phil. Mag. A **78**, 1195 (1998).

"Influence of Yttrium Doping on Grain Misorientation in Aluminum Oxide," J. Cho, H. M. Chan, M. P. Harmer and J. M. Rickman, J. Am. Ceram. Soc. **81**, 3001 (1998).

"A Methodology for Automated Quantitative Microstructural Analysis of Transmission Electron Micrographs," D. T. Carpenter, J. M. Rickman and K. Barmak, J. Appl. Phys. **84**, 5843 (1998).

"Quantitative Analysis of Spatial Distribution of Nucleation Sites: Microstructural Implications," W. S. Tong, J. M. Rickman and K. Barmak, Acta Mater. **47**, 435 (1999).

"Modeling of Grain-Boundary Segregation Behavior in Aluminum Oxide", J. Cho, J. M. Rickman, H. M. Chan and M. P. Harmer, J. Am. Ceram. Soc. **83**, 344 (2000).

"Defect Model of Twinning in Ferroelectric Thin Films," J. M. Rickman, N. Sridhar and D. J. Srolovitz, Acta Mater. **47**, 1325 (1999).

"Codoping of Alumina to Enhance Creep Resistance," Yan Z. Li, C. Wang, H. M. Chan, Jeffrey M. Rickman and Martin P. Harmer, J. Am. Ceram. Soc. **82**, 1497 (1999).

"Ex-Situ Characterization of Phase Transformations and Associated Microstructures in Polycrystalline Thin Films" K. Barmak, J. M. Rickman, C. Michaelsen, R. A. Ristau, J. Kim, G. A. Lucadamo, D. T. Carpenter and W. S. Tong, J. Vac. Sci. and Technol. **17**, 1950 (1999).

"Evolution of Perimeter Fraction During a Phase Transformation", W. S. Tong, J. M. Rickman and K. Barmak, Acta mater. **48**, 1181 (2000).

"Issues Associated with the Analysis of Thin-Film Grain Size Data", D. T. Carpenter, J. R. Codner, K. Barmak and J. M. Rickman, Mater. Lett. **41**, 296 (1999).

"Nucleation and Growth in Thin Film Transformations: Theory, Simulation and Experimental Perspectives", K. Barmak and J. M. Rickman, Metals, Materials and Processes **11**, 177 (1999).

"Dislocation Motion in the Presence of Diffusing Solutes: A Computer Simulation Study", Y. Wang, D. J. Srolovitz, J. M. Rickman and R. LeSar, Acta Mater. **48**, 2163 (2000).

"Scanning Transmission Electron Microscopy Analysis of Grain Boundaries in Creep-Resistant Yttrium- and Lanthanum-Doped Alumina Structures", J. Bruley, J. Cho, H. M. Chan, M. P. Harmer and J. M. Rickman, J. Am. Ceram. Soc. **82**, 2865 (1999).

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"Stress Calculation in Atomistic Simulation of Perfect and Defected Solids", J. Cormier, J. M. Rickman and T. J. Delph, J. Appl. Phys. **89**, 99 (2001).

Reply to "Comment on 'Influence of Yttrium Doping on Grain Misorientation in Aluminum Oxide", H. M. Chan, M. P. Harmer and J. M. Rickman, J. Am. Ceram. Soc. **83**, 1324 (2000).

"Impact of Local Interactions on the Evolution of a Phase Transformation", W. S. Tong, J. M. Rickman and K. Barmak, J. Chem. Phys. **114**, 915 (2001).

"Microstructure Evolution during Solid State Reactions of Nb/Al Multilayers", G. Lucadamo, K. Barmak, D.T.Carpenter and J.M. Rickman, Acta mater. **49**, 2813 (2001).

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"Improved tensile creep properties of yttrium- and lanthanum-doped alumina: a solid solution effect", J. Cho, C. M. Wang, H. M. Chan, J. M. Rickman, and M P. Harmer. J. Mater. Res. **16**, 425-29 (2001).

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"Coble-Creep Response and the Variability of Grain-Boundary Properties", W. S. Tong, J. M. Rickman, H. M. Chan and M. P. Harmer, J. Mat. Res. **17**, 348 (2002).

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"A Computational Materials Science Course for Undergraduate Majors", J. M. Rickman and R. Vinci, Dec. 2003, JOM-e <www.tms.org/pubs/journals/JOM/0312/ Rickman/Rickman-0312.html>.

"Incorporation of Local Structure in Continuous Dislocation Theory", R. LeSar and J. M. Rickman, Phys. Rev. B **69**, 172105 (2004).

"Efficient Algorithms for Parallelizing Monte Carlo Simulations for 2D Ising Spin Models", E. E. Santos, J. M. Rickman, G. Muthukrishnan, and S. Feng, J. Supercomput. **44**, 274-290 (2008).

"Unified Framework for Dislocation-Based Defect Energetics", J. M. Rickman, J. Vinals, and R. LeSar, Phil. Mag. **85**, 917-929 (2005).

"The Calculation of Elastic Constants from Displacement Fluctuations", M . T. Meyers, J. M. Rickman, and T. J. Delph, J. Appl. Physics **98**, 066106 (2005).

"Densification and Grain Growth of Fe-Doped and Fe/Y Codoped Alumina: Effect of Fe Valency", J. Am. Ceram. Soc. **88**, 3369-3373 (2005).

"Impact of Microstructure on Grain-Boundary Diffusion in Polycrystals", K. Bedu-Amissah, J. M. Rickman, H. M. Chan, and M. P. Harmer, J. Appl. Phys. **98**, 063511 (2005).

"Issues in the Coarse Graining of Dislocation Energetics and Dynamics", J. M. Rickman and R. LeSar, Scripta Mater. **54**, 735-739 (2006).

"Three-Dimensional Simulation of Isotropic Coarsening in Liquid Phase Sintering-I. Model", S.-B. Lee, J. M. Rickman, and A. D. Rollett, Acta Mater. **55**, 615-626 (2007).

"Biased Diffusive Transport and Solute Trapping Near a Crack", P. Kansuwan, J. M. Rickman, and T. J. Delph, Phys. Rev. B **75**, 024106 (2007).

"Grain-Boundary Diffusion of Cr in Pure and Y-doped Alumina", K. Bedu-Amissah, J. M. Rickman, H. M. Chan, and M. P. Harmer, J. Am. Ceram. Soc. **90**, 1551-1555 (2007).

"The Role of Segregating Impurities in Grain-Boundary Diffusion", P. Kansuwan and J. M. Rickman, J. Chem. Phys. **126**, 094707 (2007).

"The Impact of Obstacles on Dislocation Patterning", J. M. Rickman, M. Haataja, and R. LeSar, Phys. Rev. B **77**, 174105 (2008).

"The Effect of Yttrium on Oxygen Grain Boundary Transport in Polycrystalline Alumina Measured Using Ni Marker Particles", H. Cheng, S. J. Dillon, H. S. Caram, J. M. Rickman, H. M. Chan, and M. P. Harmer, J. Amer. Ceram. Soc. **91**, 2002-2008 (2008).

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"Elastic Response of Binary Hard-Sphere Fluids", J. M. Rickman and H. D. Ou-Yang, Phys. Rev. E **84**, 012401 (2011).

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"A Numerical Coarse-Grained Description of a Binary Alloy", J. M. Rickman, T. J. Delph, E. B. Webb III and R. Fagan, J. Chem. Phys. **137**, 054108 (2012).

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"Grain-Boundary Layering Transitions in a Model Bicrystal," J. M. Rickman, H. M. Chan, M. P. Harmer and J. Luo, Surf. Sci. **618**, 88-93 (2013).

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"Hybrid Atomistic Simulation of Fluid Uptake in a Deformable Solid," Mahyar M. Moghadam and J. M. Rickman, Phys. Rev. E **89**, 012305 (2014).

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"Orientational Anisotropy and Interfacial Transport in Polycrystals," M. M. Moghadam, J. M. Rickman, M. P. Harmer, and H. M. Chan, Surf. Sci. **646**, 204-209 (2016).

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J. M. Rickman, H. M. Chan, M. P. Harmer, J. A. Smeltzer, C. J. Marvel, A. Roy and G. Balasubramanian, "Materials Informatics for the Screening of Multi-Principal Elements and High-Entropy Alloys," accepted for publication in Nature Communications, https://doi.org/10.1038/s41467-019-10533-1.

J.A. Smeltzer, C.J. Marvel, B.C. Hornbuckle, A.J. Roberts, J.M. Marsico, A.K. Giri, K.A. Darling, J.M. Rickman, H.M. Chan and M.P. Harmer, "Achieving Ultra Hard Refractory Multi-Principal Element Alloy Via Mechanical Alloying," submitted for publication to Materials Science and Engineering A.

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"Calculation of Free Energy From the Internal Energy Distribution Function", S. R. Phillpot and J. M. Rickman, Mat. Res. Soc. Symp. **193**, 211 (1990).

"Molecular Dynamics Study of Grain-Boundary Migration in Metals", J. M. Rickman, S. R. Phillpot, and D. Wolf, Mat. Res. Soc. Symp. **193**, 325 (1990).

"Reconstruction of a High-Angle Twist Grain Boundary by Grand-Canonical Simulated Quenching", S. R. Phillpot and J. M. Rickman, Mat. Res. Soc. Symp. **238**, 183 (1992).

"Finite-Temperature Properties from a Single Zero-Temperature Energy Minimization", J. M. Rickman, R. Najafabadi, and D. J. Srolovitz, published in the Proceedings of the MRS Spring Symposium, San Francisco, CA, 27 April - 1 May 1992.

"Thermal Misfit and Thermal Fatigue Induced Damage in Brittle Composites," N. Sridhar, J. M. Rickman and D. J. Srolovitz, Mat. Res. Soc. Symp. Proc **350**, 267 (1994).

"Elastic Analysis of Twinning in Misfitting Thin Films," N. Sridhar, J. M. Rickman and D. J. Srolovitz, Mat. Res. Soc. Symp. **389**, 149 (1995).

"Reactive Phase Formation in Thin Films: Evolution of Grain Structure," K. Barmak, C. Michaelsen, J. Rickman and M. Dahms, Mat. Res. Soc. Symp. Proc. **403**, 51 (1996). (Invited)

"Microstructural Stability of Stressed Lamellar Eutectics," N. Sridhar, J. M. Rickman and D. J. Srolovitz, Mat. Res. Soc. Symp. Proc. **398**, 445 (1996).

"A Microstructural Model of the Electrical Failure of an Interconnect Resulting From Flux Divergences," J. M. Rickman, D. A. Smith and C. S. Nichols, Mat. Res. Soc. Symp. Proc. **403**, 627 (1996).

"Creep Behavior of Doped Aluminum Oxide: Experimental Results and Computer Simulation," J. Cho, J. M. Rickman, M. P. Harmer, H. M. Chan, J. Bruley, World Federation Meeting of Korean Scientists and Engineers (6/24/96 - 7/6/96), Seoul, Korea.

"Microstructure Evolution During Solid-State Reactions in Polycrystalline Nb/Al and Ti/Al Multilayer Thin Films", G. Lucadamo, K. Barmak, D. T. Carpenter, C. Lavoie, C. Cabral, Jr., C. Michaelsen and J. M. Rickman, Mat. Res. Soc. Symp.

Proc. **562**, 159 (1999).

“Coarse-Grained Free Energy Functional for Lennard-Jones Systems”, M. Gracheva, J. M. Rickman, J. D. Gunton and D. Coffey, Mat. Res. Soc. Symp. Proc. **580**, 363 (2000).

"Effects of Y and Zr Dopants on Grain Boundary Structure in Creep Resistant Polycrystalline Alumina", G. S. Cargill, C. M. Wang, J. M. Rickman, H. M. Chan and M. P. Harmer, Mat. Res. Soc. Symp. Proc. **654**, AA1.1.1 (2001).

"Scaling Relations for Dislocation Structure and Response", R. LeSar, M. Koslowski, R. Thomson, and J. M. Rickman, *Proceedings of Science*, International Conference on Statistical Mechanics of Plasticity and Related Instabilities, Bangalore, India (2006).

“Physics Based Modeling for the Development of Soft Segmentation and Reconstruction”, Amirkoushyar Ziabari, Jeffrey Rickman, Jeffrey Simmons and Charles A. Bouman, Proceedings of the Fifty-First Asilomar Conference on Systems, Signals and Computers, 2017.

Technical Reports

"Efficient Parallel Algorithms for 2-D Ising Spin Models, Technical Report LCID-01-110, Laboratory for Computation, Information and Distributed Computing, Virginia Polytechnic Institute and State University, 2001.

C. Honors and Awards

- National Young Investigator Award - National Science Foundation
- Fellow – ASM International
- Class of ’61 Professorship - Lehigh University
- Chambers Junior Professorship - Lehigh University
- Visiting Fellow – Princeton University (Spring 2002)
- Visitor – Los Alamos National Laboratory (Summer 2002)
- Member of Sigma Xi
- Member of Phi Beta Kappa
- Member of Phi Kappa Phi
- Summa Cum Laude graduate of Miami University
- Honors in physics at Miami University
- Culler prize and physics scholarship at Miami University

D. Funded Research (selected)

"Polycrystalline Multi-Principal-Element Alloys: Exploiting the Role of Grain Boundaries," with M. P. Harmer and H. M. Chan, Office of Naval Research (2018-2020).

"Data Curation in Materials Science Workshop", National Science Foundation, (Spring 2019).

"Workshop on the Convergence of Materials Research and Multi-Sensory Data Science" National Science Foundation (June 2018)

"Physics-Based Image Processing" (AFRL) Co-Pi with J. Simmons, 2016-2018.

"Tailoring of Atomic-Scale Interphase Complexions For Mechanism-Informed Material Design," (MURI) Co-Pi with M. Harmer, H. Chan , *et al*., $4,500,000

"Development of Attribute Maps for Grain-Boundary Transport in Doped Alumina," Co-Pi with M. Harmer and H. Chan, (ONR) $360,000

"Modeling the Coupling of Elastic Anisotropy and Network Topology in Poroelastic Transport", The Petroleum Research Fund, (2009-2011) $100,000

"Multiscale Modeling of Metallic Microstructures", Co-Pi with D. J. Srolovitz and R. LeSar, AFOSR, FA9550-05-1-0082 (2005-2009). $532,987

"Multiscale Modeling of Metallic Microstructures", Co-Pi with D. J. Srolovitz and R. LeSar, AFOSR, FA9550-05-1-0082 (2005) - supplement $30,000

"Effect of Impurities on O and Al Boundary Diffusion in Alumina: Application to Alumina Scale Growth in Alloys," with M. Harmer and H. Chan, ONR, (2005-).
$309, 881

"Acquisition of a High Performance Beowulf Cluster Computer for Materials Modeling", with T. J. Delph and J. D. Gunton, $100,445
National Science Foundation, DMR- 0420428 (2004-2005)

"Defect Interactions in Solids: Impact on Microstructure and $177,000
Materials Properties" (1999-2004), NSF Grant, DMR-9975384
Single Investigator

"Tailoring of Grain Boundary Chemistry for the Development of Super Creep-Resistant Ceramic Oxides," AFOSR Grant F49620-94-1-0284 (renewal, through 8/04) Co-Pi's: Professors M. Harmer and H. Chan	$785,000
Computational Materials Summer School Lawrence Livermore National Laboratory (graduate student support) Past	$8750
"NSF Young Investigator" NSF Grant, DMR-9458023, 1994-1999 Single Investigator	$125,000
"Evolution of Grain Structure in Thin Film Reactions," NSF Grant, 1997-2000 Co-Pi: Professor K. Barmak	$369,706
"Tailoring of Grain Boundary Chemistry for the Development of Super Creep-Resistant Ceramic Oxides AFOSR Grant F49620-94-1-0284, 1997-2001 (renewal) Co-Pi's: Professors M. Harmer and H. Chan	$655,000
"Tailoring of Grain Boundary Chemistry for the Development of Super Creep-Resistant Ceramic Oxides AFOSR Grant F49620-94-1-0284, 1994-1997 Co-Pi's: Professors M. Harmer and H. Chan	$600,000
"Low Cost Creep Resistant Alumina Fibers for High Temperature CMC Applications," STTR Program, AFOSR Grant F49620-97-C-0004, 1997 Co-Pi's: Professors M. Harmer and H. Chan	$100,000
LDRD Program with Sandia National Laboratory Co-Pi: Prof. K. Barmak, Spring 1998	$25,000
"Workshop on Current Issues on Nonequilibrium Statistical Mechanics and Materials", NSF, October 1997 Co-Pi's: Dr. A. Saxena and Prof. M. Grant	$4,000

E. Editorial Boards

- Guest Editor (with R. LeSar) for *Annual Reviews of Materials Science* (vol. 32)
- Editorial Board, *Computational Materials Science* (journal)
- Editor, *Acta Materialia* (journal)

F. Professional Memberships and Presentations

Memberships

-ASM International
- TMS
- American Ceramic Society (ACerS)
- American Physical Society (APS)

Selected Invited Presentations

“Some Effects of Strain on Diffusion in Crystalline Solids”, Argonne National Laboratory, May 1989.

" Histogram Methods and Cumulant Expansions to Calculate Materials Properties"

Argonne National Laboratory - November 1990
University of Michigan – May 1991
University of Michigan - February 1993

"Efficient Determination of Material Properties Using Computer Simulation"

Sandia National Laboratory - November 1993
Los Alamos National Laboratory - November 1993
Florida State University - May 1994

"Impact of Heterogeneous Boundary Nucleation on Product Grain Distributions," Penn State University, Oct. 1996.

"Kinetics of Phase Formation and Growth in Thin Films," Spring TMS Meeting, Feb. 1997, Orlando, FL.

"Heterogeneous Nucleation: Kinetics and Microstructure," University of Colorado, July 1997, Boulder, CO.

"Extended Defects in Materials: Microstructure and Kinetics," Fall MRS, Boston, 1997.

"Extended Defects in Materials: Microstructure and Kinetics," Fall TMS, Indianapolis, 1997.

"Doping to Enhance Creep Resistance in Alumina", Schloss Ringberg, 1999.

"Free Energy Calculations with Computer Simulation", Daresbury Laboratory, England 1999.

"Models of Idealized Defects", Congress on Computational Mechanics, Boulder, CO 1999.

Gordon Research Conference on Innovations in College Teaching of Materials Science and Engineering

"Computer Simulation as a Tool to Address Interesting Problems in Materials Science, Fall 1999. Materials Science Department - Carnegie Mellon University.

"Computer Simulation as a Tool to Address Interesting Problems in Materials Science, Fall 1999. Mechanical Engineering Department - Lehigh University.

"Heterogeneous Nucleation: Kinetics and Microstructure"
Spring 2000 TMS Meeting, Nashville
Spring 2000 APS Meeting, Minneapolis
Florida State University, September 2000
Los Alamos National Laboratory, November 2000

"Nucleation Kinetics and Microstructure"

Virginia Tech (Spring, 2001)
University of California Santa Barbara (Spring, 2001)
University of Wisconsin (Spring, 2001)
Princeton University (Spring 2002)
Lawrence Berkeley National Laboratory (Spring 2001)
Rockwell Science Center (Spring 2001)
Spring MRS Meeting (2001
Spring TMS Meeting (2002)

"Dislocation Energetics and Dynamics"

Lawrence Livermore National Laboratory (Spring 2002)
Los Alamos National Laboratory (Spring 2002)
Los Alamos National Laboratory - T-Division (Spring 2003)
University of Florida (Spring 2003)

Lawrence Livermore National Laboratory (Spring 2003)

Computational Materials Science - Education, TMS Meeting (Spring 2003)

"Materials Modeling at Different Length Scales" - Lehigh Physics Dept. (Fall 2003)
"Materials Modeling at Different Length Scales" – SUNY-Binghamton (Fall 2003)

"Materials Modeling at Different Length Scales" – Wright-Patterson AFB (Fall 2003)

"Dislocation Energetics and Dynamics" – 2nd International Workshop Multiscale Modeling of Strength and Fracture, Berkeley, CA (Spring 2004)

"Multiscale Modeling of Materials" – California State University-Northridge (Spring 2004)

"Multiscale Modeling of Materials" – Washington University (Spring 2004)

"Multiscale Modeling of Materials" – Virginia Tech (Spring 2004)

"Some Mathematical Methods in Materials Science" – Lehigh Mathematics Dept. (Spring 2004)

"Dislocation Energetics and Dynamics" – Gordon Research Conference, Physical Metallurgy (Summer 2004)

Air Force Program Review – Ceramics (Summer 2004)

Third Multiscale Modeling Workshop – DOE (Portland, Oregon – Fall 2004)

"Simulation of Nucleation and Growth Processes" – Fall TMS meeting

"Multiscale Modeling of Materials" – Carnegie Mellon – CEE Dept. (Spring 2005)

"Coarse-Grained Dislocation Dynamics" – AFOSR Deer Creek workshop (Spring 2005)

"Grain-Boundary Kinetics in Oxides" – ONR program review (Spring 2005)

"Modeling of Dislocation Energetics and Dynamics" – Plasticity 2006, Halifax, NS (Summer 2006).

"Modeling of Dislocation Dynamics" , SES meeting, Texas A&M, Fall 2007.

"Modeling of Dislocation Dynamics", Dept. of Physics, McGill University, Spring 2008.

"Local Stress and Elastic Constants", SIAM, Philadelphia, Spring 2008.

"Modeling of Dislocation Energetics and Dynamics: Obstacles and Coarse Graining", SIAM, Philadelphia, Spring 2008.

"Effect of Impurities on O and Al Boundary Diffusion in Alumina: Application to Alumina Scale Growth in Alloys", ONR program review (Spring 2008).

"Effect of Impurities on O and Al Boundary Diffusion in Alumina: Application to Alumina Scale Growth in Alloys", ONR program review (Spring 2009).

"Kinetics of Nucleation and Growth Processes," Fall 2009 TMS Meeting, Pittsburgh, PA.

"Kinetics of Nucleation and Growth Processes," AFRL Nucleation Workshop, Maui, HI (Spring 2010).

"Effect of Impurities on O and Al Boundary Diffusion in Alumina: Application to Alumina Scale Growth in Alloys", ONR program review (Spring 2010).

"The Role of Obstacles in Determining Material Properties," Penn State Univ., department seminar (Fall 2010).

"Kinetics of Nucleation and Growth Processes," Spring 2011 TMS Meeting, San Diego.

"Some Applications of Computer Simulation in Engineering and Physics," University of Texas at El Paso, department seminar (Spring 2011).

"The Role of Obstacles in Determining Material Properties," Columbia Univ., department seminar (Spring 2012).

"Dislocation Dynamics Simulations and Coarse Graining", International Workshop on Computational Mechanics of Materials, Baltimore, MD (Fall 2012)

"Simulational Studies of Complexions in Ni-Bi System," International Conference on Materials Interfaces, Bear Creek, PA (Fall 2012)

"Linking Atomistic and Phase-Field Simulations using Numerically Coarse-Grained Free Energy Functionals ", Spring TMS Meeting, 2014.

"Length and Time Scale Issues in Simulation", a tutorial at Spring MRS Meeting, 2014.

"Complexion Diagrams in Bicrystals," MS&T 2015, Columbus, OH, Oct. 2015.

"Parsing Abnormal Grain Growth," Bear Creek Workshop on Interfaces, Macungie, PA, Sept. 2015.

"Parsing Abnormal Grain Growth," TMS Grain Growth and Recrystallization Meeting, Pittsburgh, July 2016.

"Layering Transitions at Interfaces and Phonon Engineering," MS&T 2016, Salt Lake City, UT, Oct. 2016.

"Physics-Based Image Processing of Materials," Electronic Imaging 2017, Burlingame, CA, Jan. 2017.

"Controlling the Microstructure and Properties of Polycrystalline Ceramic Oxides," Corning, Inc., Oct. 2017.

"Data Analytics and Ceramic Processing," MS&T 2017, Pittsburgh, PA, Oct. 2017.

"Computer Simulation of Interfacial Transitions at Surfaces and Grain Boundaries," Los Alamos Center for Non-linear Studies Conference, Santa Fe, NM, 2017.

"Microstructure and Kinetics Associated with a First-Order Phase Transformation," EMA 2018, Orlando, Florida, 2018.

"Data Analytics using Canonical Correlation Analysis and Monte Carlo Simulation," EMA 2018, Orlando, Florida, 2018.

"Materials informatics to study abnormal grain growth," Ceramic Expo, Cleveland, May 2018.

"Materials informatics to study abnormal grain growth," WCCM, New York, July 2018.

"Layering Transitions at Internal Interfaces," Columbia U., Oct. 2018.

"Layering Transitions at Internal Interfaces," Fall MS&T Meeting Oct. 2018.

Session Chairs (selected)

- Solidification Conference, Los Alamos, New Mexico, July 1996
- Spring ACerS Meeting, Cincinnati, OH, April 1997
- "Computer-Aided Design of Materials," Santa Fe, New Mexico, July-Aug. 1997
- Spring 1999 MRS Meeting
- Spring 2002 TMS Meeting
- Plasticity 2006 (Halifax, NS)
- Gordon Conference, Ceramics, 2008 (Andover, NH)

Conferences and Symposia Organized

- Conference Organizer, EMA 2019 (Orlando, Florida)
- Statistical Mechanics and Materials Science - Lehigh (1997)
- Current Issues in Pattern Formation in Materials Science- Carnegie Mellon University (Spring 2003)
- Symposium Organizer, MRS 1999 Spring Meeting
- Symposium Organizer, TMS 2000 Spring Meeting
- Symposium Organizer, High-Performance Computing Conference (Lehigh, 2009)
-Workshop on the Convergence of Materials Research and Multi-Sensory Data Science (June 2018)

G. Teaching and Advising

Courses Taught - Undergraduate

ENGR 1 - Engineering Computations (Spring 1994 and 1996) (2 credits)

Recitation Approximate enrollment: 30

MAT 317 - Imperfections in Crystals (Fall 1994, Spring 1996, Spring 1997, Fall 1998)
(3 credits)

Lecture Approximate enrollment: 9

MAT 33 - Engineering Materials and Processes (many times) (3 credits)

Large lecture Approximate enrollment: 210
Recitation Approximate enrollment: 40

MAT 20 - Computational Methods in Materials Science (many times) (2 credits)

Lecture/lab (2-3 sessions/week) Approximate enrollment: 10 per class

PHY 273 – Undergraduate Research (Summer 2004) (3 credits)

Daily meetings 1 student

PHY 21 – Introductory Physics: Electricity & Magnetism (Summer 2009, 2010) (4 credits)

Daily meetings 19 students

Courses Taught – Graduate

MAT 401 - Thermodynamics and Kinetics I (several times) (3 credits)

Lecture Approximate enrollment: 12

MAT 402 - Thermodynamics and Kinetics II (several times) (3 credits)

Lecture Approximate enrollment: 10

MAT 403 - Structure and Properties I (Fall 1995, Fall 1998) (3 credits)

Lecture Approximate enrollment: 12

MAT 404 - Structure and Properties II (Spring 1996) (3 credits)

Lecture Approximate enrollment: 10

MAT 405 - Mathematical Methods in Materials Science (several times) (3 credits)

Lecture Approximate enrollment: 10

MAT 495 – Crystalline Imperfections (Spring 2001) (3 credits)

Lecture/ Web course (Lehigh & Carnegie Mellon students) Approximate enrollment: 8

MAT 496- Independent Study (Spring 2004, Fall 2004) (3 credits)

Weekly meetings 2 students

PHY 431 – Theory of Solids

Weekly meetings 5 students

MAT 495 – Modeling and Simulation in Engineering

Weekly meetings 5 students

Undergraduate Advising

I typically advise about 6 undergraduate materials science majors per year. This work involves course scheduling and, for example, making arrangements for study abroad and national laboratory internships. In addition, I participate in various recruiting activities including Candidates' Day and departmental open houses for prospective students.

Advising – Research Direction

Current Ph.D. students:

Songul Kutlu, Thienbao Nguyen (jointly with Jim Gunton)
Nipun Goel (jointly with E. B. Webb and A. Oztekin)

Past Ph.D. students

Abigail Lawrence (jointly with Martin Harmer)

Qian Wu, Mahyar Mohebi Moghadam, 2014

Huikai Cheng, 2009

Kwame Bedu-Amissah, 2006

Thirumalesh Bannuru, 2007

Panya Kansuwan, 2007

Junghyun Cho ('95-'99) "Role of Rare-Earty Dopants on the Improved Creep Properties of Aluminum Oxide" (1999), postdoctoral appointment at U. C.- Santa Barbara, currently Assistant Professor in Dept. of Mech. Eng. at SUNY-Binghamton.

W. Scott Tong ('96-'99) "The Effect of Heterogeneous Nucleation on Two-Dimensional Phase Transformation Kinetics and Resultant Microstructure" (1999), postdoctoral appointment at Carnegie Mellon, currently research scientist at University of Wisconsin

Derrick Carpenter ('97-'98) "Improvements in the Characterization of Polycrystalline Thin Films: Microchemistry, Microtexture and Microstructure" (1998), National Research Council postdoctoral appointment at NIST

Gary Thompson ('95-'01) "Kinetic Model of Particle-Inhibited Grain Growth" (1999)

Past Master's students

Josh Cormier (Fall '99 - Spring '00 - along with T. Delph), "Stress Tensors and Measures in Atomistic Simulations" (1998), U. S. Marine Corps

W. Scott Tong ('96-'99) "The Effect of Heterogeneous Nucleation on Two-Dimensional Phase Transformation Kinetics " (1996), University of Wisconsin

Undergraduates

Matt Meyers (2004) – summer REU program
Michael Carone (1998) – undergraduate working on image processing software

M.S. & Ph.D. – Co-supervision of Students at Other Institutions

Sridhar Narayanaswamy (University of Michigan, 1993-1994), Y. Wang (Princeton, 1999-2000), S.-B. Lee (Carnegie Mellon, 2002-2003)

Postdoctoral and Visiting Scientists

Dr. Yufeng Wang (1996), Dr. M. Gracheva (1999-2000)

Summer Research

Joseph Stempo (2010), Emeka Ihuralem (2008)

Ph.D. Committees (selected)

Bruce Lindsley (1996), Daniel Lewis (2001), Alex Bandar (2005-expected), A. Shiryayev (Physics, 2005-expected), Vicki Keast (1998), Jason Goodelle (1999), C. Palanduz (1998), Gene Lucadamo (1999), Roger Ristau (1998), N. Wentzel (2007-expected), Steve Sweeney (2008), Hongqing Zhang (2008), Steven Lettieri (2008), Jeff Stephens (2010).

H. Service

University

- Selection committee for Phi Beta Kappa (1995-1997)
- Direct and establish the departmental computing facilities (1993-present)
- Departmental seminar coordinator (1994-1995, present)
- Graduate course committee (present)
- Search committees – chair of Mathematics Department, mechanical properties faculty (department), technical and support positions (department) (2000)
- Member of Cosmos Club (1994-1996, 2000)
- Campus workstation advisory committee (2000)
- Beowulf cluster advisory committee (present)
- Recruitment – Candidates' Day, MAT 240 (Research Option), Open Houses (present)

Professional

- Secretary, Vice President of Computer Simulation Committee (TMS)
- Secretary, President of Computer Simulation Committee (TMS)
- NASA Microgravity Panel Reviewer (1999, 2002)
- Reviewer for National Science Foundation, Department of Energy, Physical Review, Physical Review Letters, Journal of Applied Physics, Journal of the American Ceramic Society, the Journal of Materials Research, Acta Materialia, Scripta Materialia, Modeling and Simulation in Materials Science and Engineering, Computational Materials Science, Materials Science and Engineering, Nature, etc.
- Member - Computational Materials Science Network (present)
- Member - Chemistry and Physics of Materials Committee (TMS) (present)
- Society memberships
  – American Physical Society, TMS, Materials Research Society

References

Professor David J. Srolovitz
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Professor Richard LeSar
Chair, Dept. of Materials Science andEngineering
Iowa State University
2220C Hoover Hall
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Professor Jorge Viñals
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