Alejandro Strachan

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EDUCATION

Degree	Date	School
Ph.D., Physics	1999	University of Buenos Aires, Argentina
M.Sc., Physics	1995	University of Buenos Aires, Argentina
B.Sc., Physics	1995	University of Buenos Aires, Argentina

PROFESSIONAL EMPLOYMENT

Dates	Position
2011-present	Deputy Director, NNSA Center for Prediction of Reliability, Integrity and Survivability of Microsystems, Purdue University
2013-present	Professor, School of Materials Engineering, Purdue University
2010-2013	Associate Professor, School of Materials Engineering, Purdue University
2005-2010	Assistant Professor, School of Materials Engineering, Purdue University
2002-2005	Staff Member, Theoretical Division, Los Alamos National Laboratory
2001-2002	Scientist, Materials and Process Simulation Center, California Institute of Technology.
1999-2001	Postdoctoral Scholar, Materials and Process Simulation Center, California Institute of Technology
1995-1999	Graduate Teaching Assistant, Physics Department, University of Buenos Aires, Argentina

HONORS AND AWARDS

- Purdue Faculty Scholar (2012-2017)
- Purdue University College of Engineering Faculty Excellence Award. Team Award: PRISM, 2009.
- TMS Early Career Faculty Fellow Award, 2009.
- Purdue University *Teaching for Tomorrow* award, 2007.
- Purdue Seeds of Success Acorn Award given by Vice Provost for Research:
    - 2007 NSF *"Network for Computational Nanotechnology"*. PI: M. Lundstrom.
    - 2008 DoE-NNSA *"Center for the prediction of reliability and Survivability"*, PI: J. Murthy.
    - 2009 NSF *"Cyber-enabled Predictive Models for Polymer Nanocomposites: Multiresolution Simulations and Experiments"*, PI: A. Strachan.
    - 2009 The Boeing Company *"Atoms to aircraft program"*, PI: A. Strachan.
    - 2011 DTRA *"Multi-Resolution Modeling and Experiments of Nanostructured Reactive Materials"* PI: A. Strachan
- Schuhmann Best Undergraduate Teacher Award, School of Materials Engineering, Purdue University, 2007.

STUDENT AND POSTDOC MENTORING

NAME	DEGREE	GRADUATION DATE	NAME OF CO-CHAIR	TITLE
Arvind Arumbakam	MS	05/2007	-	Interface structure, coherency limits and mechanical properties of heteroepitaxial nanowires via molecular dynamics
Ya Zhou	PhD	06/2010	-	Thermal transport in nanoscale and nanostructured materials
Amrit Palaria	PhD	12/2010	Gerhard Klimeck (ECE)	First principles modeling of materials for electronic applications
Patrick Cantwell	PhD	06/2011	Eric Stach (MSE)	A quantitative study of microstructure and fiber texture in nickel electrodeposits for mems applications, including a new transmission electron microscopy (tem) technique for polycrystalline films
Yumi Park	PhD	12/2011	-	Molecular dynamics simulations of semiconductor heterostructures
Karthik Guda Vishnu	PhD	7/2012	-	Size effects in shape memory alloys
Nathan Anderson	PhD	7/2012	-	Point defects in dielectric interaces and free surfaces
Ravi Vedula	PhD	12/2013	M. Ashraf Alam (ECE)	First principles characterization of dielectric charging
Yae-ji Kim	PhD	12/2014		Thermo-mechanical properties of polymer nanocomposites
Keng-Hua Lin	PhD	12/2014		Thermal transport in nanoscale and nanostructured materials
Mathew Cherukara	PhD	12/2015	-	Thermal transport and energetic materials
Mitchel Wood	PhD	12/2016	-	Energy transfer mechanisms and chemistry initiation in high energy materials
Sean Sullivan	M.S	12/2014	-	Thermal transport at interfaces
Keith Morrison	M.S	12/2014	-	Nanoscale shape memory materials
David Guzman	PhD	8/2016		Electronic processes in dielectric materials
Kiettipong Banlusan	PhD	8/2016		Shock-energy absorption by endothermic chemistry

Postdoctoral scholars

- Shijin Zhao (at Los Alamos National Laboratory), Ph.D. Chinese Academy of Science, 2001. Research: *"Atomistic studies of fast chemical processes in nano-structured metastable composites"*. Co-advised with T. C. Germann, Los Alamos National Laboratory. 2004-2006.
- Gabriela Venturini, Ph.D. Caltech, 2010. Research: *"Predictive modeling and simulation of Microsystems and polymer slabs"*. 2010-2011.
- Hojin Kim. Ph.D. University of Utah, 2007. Research: *"Large-scale molecular dynamics simulations of microdevices"*. 2008-present.
- Chunyu Li. Ph.D. Harbin Institute of Technology, China, 1999. Research: *"Atomistic simulations of polymer and polymer composites"*. 2009-present.
- Benjamin Haley, Ph.D. UC Davis. Research: *"Developing and cyber-enabling simulation tools for polymer nanocomposites"*. 2010-present.
- Stanislav Advoshenko, Technical University of Dresden, Germany, 2009. Research: Ab initio modeling of optical properties of rare earth oxides. 2011-present.
- Nicolas Onofrio, Ph.D. University Joseph Fourier, Grenoble, France, 2011. Research: Molecular dynamic of tip-polymer interaction and uncertainties in atomistic simulations. 2011-present.
- Edwin Antillon, Ph.D. Purdue, 2012. Research: Shock-energy absorption via endothermic chemistry. 2012-present.

PROFESSIONAL ACTIVITIES

- Guest Editor with Profs. Gerhard Klimeck and Mark Lundstrom of Special Issue to appear in *Computing in Science and Engineering* on "Cyber-enabled simulations in nanoscale science and engineering" March/April 2010.
- Site Lead and Chair of the Steering Committee, NCN@Purdue Program, Network for Computational Nanotechnology, an NSF research and cyber-infrastructure center.
- Visiting Professor, Institute of High Performance Computing, Singapore, September 10-14, 2007.

Symposia and workshop organization

- MiniSymposium on *"Multiscale modeling of molecular solids"*, during the 9th World Congress on Computational Mechanics, Sydney, Australia July 19-23, 2010. Co-organized with: Stephen Christensen (Boeing), Alberto Cuitino (Rutgers University), Jonathan Gosse (Boeing), and Marisol Koslowski (Purdue University)
- Symposium on *"Thermo-Mechanical Response of Molecular Solids: Multi-Resolution Theory, Simulations, and Experiments"* during TMS 2010 Annual Meeting, Exhibition. February 14-18, 2010 in Seattle, WA. Co-organized with: Thomas Sewell (University of Missouri), Rodolfo Pinal (Industrial and Physical Pharmacy, Purdue), and Chunyu Li (MSE, Purdue).
- Purdue workshop on "*Predictive materials modeling and simulations: nano- and micro-mechanics*" planned for August 6 and 7, Purdue University, West Lafayette, IN. Co-organized with Marisol Koslowski (ME).
- Purdue School on High Performance and Parallel Scientific Computing, September 4 and 5, 2008. Purdue University, West Lafayette, IN. Co-organized with Faisal Saied (Rosen Center for Advanced Computing, Purdue).

- CECAM workshop on *"Materials under Extreme Conditions: Experimental Validation of Atomistic Modeling"*, May 26-28, 2004, Lyon, France.
- CECAM workshop on *"Reactive Classical Potentials versus Hybrid Methods: Towards Chemical Complexity"*, June 16-19, 2003, Lyon, France.
- CECAM workshop on *"Upscaling from ab initio to Molecular Dynamics: Interatomic Potentials and Hybrid Methods"*, July 8-12, 2002, Lyon, France.

NEW COURSES DEVELOPED

MSE270 *"Atomistic materials science"*, with Prof. Eric Stach. Strachan effort: 50%. First offered: Spring 2008.
MSE550 *"Properties of solids"*, first offered: Fall 2007.
MSE597G *"Materials modeling and simulation: methods and applications"*, with Prof. Edwin Garcia. Strachan effort 50%. First offered: Fall 2006.

PUBLICATIONS

BOOKS, MONOGRAPHS, AND BOOK CONTRIBUTIONS

1. *"Non-Equilibrium Molecular Dynamics Studies of Shock and Detonation Processes in Energetic Materials"*, Brad Lee Holian, Timothy C. Germann, Alejandro Strachan, and Jean-Bernard Maillet, in Chemistry at Extreme Conditions, Riad Manaa, (Ed.) Elsevier (2004).

JOURNAL PUBLICATIONS

1. *"Multiscale contact mechanics model for RF MEMS switches with quantified uncertainties"*, Hojin Kim, Nurul Huda Shaik, Xin Xu, Arvind Raman, Alejandro Strachan. Journal of the Mechanics and Physics of Solids (submitted).
2. *"Model form uncertainty versus intrinsic atomic variability in amorphous silicon oxides and nitrides"* Nathan L. Anderson,1 Ravi Pramod Vedula and Alejandro Strachan, Modelling and Simulation in Materials Science and Engineering (submitted).
3. *"Molecular dynamics simulation of PMMA slabs"*,Y-J Kim, K-H Lin and A. Strachan, Modelling and Simulation in Materials Science and Engineering (submitted).
4. *"Functional uncertainty quantification for error estimation and minimization via optimal high-fidelity simulations"*, A. Strachan, S. Mahadevan, V. Hombal, Modelling and Simulation in Materials Science and Engineering (submitted).
5. "*Role of atomic variability in dielectric charging: a first principles-based multiscale modeling study*", R. P. Vedula, S. Palit, M. A. Alam, and A. Strachan. Physical Review Letters (submitted).
6. *"Molecular dynamic simulation of tip-polymer interaction in tapping-mode AFM"* Nicolas Onofrio, Gabriela N. Venturini and Alejandro Strachan. Journal of Applied Physics (submitted).
7. *"Modeling Amorphous polymers at nanoHUB.org"*, Benjamin P. Haley, Chunyu Li, Nathaniel Wilson1, Eugenio Jaramillo, Alejandro Strachan, Computer Physics Communications (submitted).
8. *"Shape memory metamaterials with tunable thermo-mechanical response via hetero-epitaxial integration"*, K. Guda Vishnu and A. Strachan, Journal of Applied Physics (accepted with minor modifications).

9. *"Lectures and Simulation Laboratories to Improve Learners' Conceptual Understanding"*, Alejandra Magana, Sean Brophy and Alejandro Strachan, Advances in Engineering Education (in press).
10. *"Phonon thermal transport outside of local equilibrium in nanowires via molecular dynamics"* Ya Zhou and Alejandro Strachan, *Journal of Chemical Physics* (in press).
11. *"Thermal Transport in SiGe Superlattice Thin Films and Nanowires: Effects of Specimen and Periodic Lengths"*, K-H Lin* and A. Strachan, Physical Review B, **87**, 115302 (2013). DOI: 10.1103/PhysRevB.87.115302
12. *"Molecular dynamics simulations on cyclic deformation of an epoxy thermoset"*, C. Li,* E. Jaramillo, and A. Strachan, Polymer, **54**, 881-890 (2013). DOI: 10.1016/j.polymer.2012.12.007
13. *"Molecular dynamics study of dynamical contact between a nanoscale tip and substrate for AFM experiment"*, Hojin Kim,* Gabriella Venturini and Alejandro Strachan, Journal of Applied Physics, **112,** 094325 (2012). DOI: 10.1063/1.4762016
14. *"Atomistic Simulations on Multilayer Graphene Reinforced Epoxy Composites"*, Chunyu Li, Andrea Browning, Stephen Christensen and Alejandro Strachan, Composites Part A,**43**, 1293-1300 (2012). DOI: 10.1016/j.compositesa.2012.02.015
15. *"Defect level distributions and atomic relaxations induced by charge trapping in amorphous silica"*, Nathan L. Anderson, Ravi Pramod Vedula, Peter A. Schultz, R. M. Van Ginhoven, and Alejandro Strachan, Applied Physics Letters, **100,** 172908: 1-3 (2012). DOI: 10.1063/1.4707340
16. *Effect of topological disorder on structural, mechanical, and electronic properties of amorphous silicon nitride: An atomistic study*, Ravi Pramod Vedula, Nathan Anderson, and Alejandro Strachan, Physical Review B, **85,** 205209 (2012). DOI: 10.1103/PhysRevB.85.205209
17. *"High-energy amorphous intermolecular reactive composites"* Karthik Guda Vishnu, Mathew Cherukara, Hojin Kim and Alejandro Strachan, Physical Review B, **85,** 184206 (2012). DOI: 10.1103/PhysRevB.85.184206
18. *"Estimating in-plane Young's modulus of polycrystalline films in MEMS"*, Patrick R. Cantwell, Hojin Kim, Matthew M. Schneider, Hao-Han Hsu, Dmitrios Peroulis, Eric A. Stach, Alejandro Strachan, Journal of Microelectromechanical Systems, **21,** 840-849 (2012). DOI: 10.1109/JMEMS.2012.2191939
19. *"Molecular Dynamics Simulations and Experimental Studies of the Thermomechanical Response of an Epoxy Thermoset Polymer"*, Chunyu Li, Grigori Medvedev, Eun-Woong Lee, Jaewoo Kim, James Caruthers, Alejandro Strachan, Polymer, **53,** 4222-4230 (2012). DOI: 10.1016/j.polymer.2012.07.026
20. *"Tailored Reactivity of Ni+A1 Nanocomposites: Microstructural Correlations"*, Khachatur Manukyan, Aaron Mason, Lori Groven, Ya-Cheng Lin, Mathew Cherukara, Steven Son, Alejandro Strachan , Alexander Mukasyan, The Journal of Physical Chemistry C, **116,** 21027-21038 (2012). DOI: 10.1021/jp303407e
21. *"Role of nanostructure on reaction and transport in Ni/Al intermolecular reactive composites"*, Mathew Cherukara, Karthik Guda Vishnu, Alejandro Strachan, Physical Review B, **86,** 075470 (2012). DOI: 10.1103/PhysRevB.86.075470
22. *"Size effects in NiTi from density functional theory calculations"*, Karthik Guda Vishnu and Alejandro Strachan, Physical Review B **85,** 014114 (2012). DOI: 10.1103/PhysRevB.85.014114
23. *"Energy-based yield criterion for PMMA from large-scale MD simulations"*, Eugenio Jaramillo, Nathaniel Wilson, Stephen Christensen, Jonathan Gosse, and Alejandro Strachan, Physical Review B, **85**, 024114 (2012). DOI: 10.1103/PhysRevB.85.024114

24. *"Effect of thickness on the thermo-mechanical response of free-standing thermoset nanofilms from molecular dynamics"*, Chunyu Li and Strachan, Alejandro, Macromolecules, **44**, 9448–9454 (2011). DOI: 10.1021/ma201927n
25. *"Strain engineering via amorphization and recrystallization in Si/Ge heterostructures"*, Yumi Park and Alejandro Strachan, Physical Review B **84**, 125412 (2011). DOI: 10.1103/PhysRevB.84.125412
26. "*Uncertainty propagation in a multiscale model of single crystal plasticity*", M. Koslowski and A. Strachan, Reliability Engineering and System Safety **96**, 1161-1170, (2011). DOI: 10.1016/j.ress.2010.11.011
27. *"Role of surface orientation on ALD Al2O3/GaAs interface structure and Fermi level pinning: a DFT study"*, Ganesh Hegde, Gerhard Klimeck, and Alejandro Strachan, Applied Physics Letters, **99**, 093508 (2011). DOI: 10.1063/1.3624897
28. "*Molecular dynamics predictions of thermal and mechanical properties of thermoset polymer EPON862/DETDA"* Chunyu Li and Alejandro Strachan, Polymer **52**, 2920-2928 (2011). DOI: 10.1016/j.polymer.2011.04.041
29. "*First-Principles Investigation of Low Energy E' Center Precursors in Amorphous Silica"* Nathan L. Anderson, Ravi Pramod Vedula, Peter A. Schultz, R.M. Van Ginhoven, and Alejandro Strachan, Physical Review Letters, **106**, 206402 (2011). DOI: 10.1103/PhysRevLett.106.206402
30. *"Thermal decomposition of condensed-phase nitromethane from molecular dynamics using the reactive force field ReaxFF",* Si-ping Han, Adri C. T. van Duin, William A. Goddard, III, and Alejandro Strachan, Journal of Physical Chemistry B, **115**, 6534-6540 (2011). DOI: 10.1021/jp1104054
31. *"Effect of core energy on mobility in a continuum dislocation model"*, Dong Wook Lee, Hojin Kim, Alejandro Strachan, and Marisol Koslowski, Phys. Rev. B 83, 104101 (2011). DOI: 10.1103/PhysRevB.83.104101
32. *"Molecular dynamics characterization of the contact between clean metallic surfaces with nanoscale asperities"*, H. Kim and A. Strachan, Physical Review B 83, 024108 (2011). DOI: 10.1103/PhysRevB.83.024108
33. *"Molecular Simulations of Cross-linking Process of Thermosetting Polymers"*, C. Li and A. Strachan, Polymer **51**, 6058-6070 (2010). DOI: 10.1016/j.polymer.2010.10.033
34. "*Molecular Dynamics Simulations of Strain Engineering and Thermal Transport in Nanostructured Materials*", Y. Park, Y. Zhou, J. Jhaveri, and A. Strachan, Computing In Science & Engineering **12** 36-42 (2010). DOI: 10.1109/MCSE.2010.44
35. *"Cyber-Enabled Simulations in Nanoscale Science and Engineering INTRODUCTION"*, Strachan A, Klimeck G, Lundstrom M, Computing In Science & Engineering, **12** 12-17 (2010). DOI: 10.1109/MCSE.2010.38
36. "*Nanoscale metal-metal contact physics from molecular dynamics: the strongest contact size"*, H. Kim and A. Strachan, Physical Review Letters **104**, 215504 (2010). DOI: 10.1103/PhysRevLett.104.215504
37. *"Phase stability and transformations in NiTi from density functional theory calculations"*, K. Guda Vishnu and A. Strachan, Acta Materialia, **58,** 745–752 (2010). *1st Tier.* DOI: 10.1016/j.actamat.2009.09.019
38. *"Size effects on martensitic microstructure in Zr nanowires via molecular dynamics"*, A. Thompson and A. Strachan, Physical Review B, **81** 085429 (2010). DOI: 10.1103/PhysRevB.81.085429
39. *"Thermal conduction in molecular materials using coarse grain dynamics: role of mass diffusion and quantum corrections for MD simulations"*, Y. Zhou and A. Strachan, Journal of Chemical Physics **131** 234113 (2009). *1st Tier.* DOI: 10.1063/1.3272028

40. *"Strain relaxation in Si/Ge/Si nanoscale bars from molecular dynamics simulations"*, Y Park, M. Aktuga, A. Grama and A. Strachan, Journal of Applied Physics, **106**, 034304-1-6 (2009). DOI: 10.1063/1.3168424
41. *"Coarse grain modeling of spall failure in molecular crystals: role of intra-molecular degrees of freedom"* K. Lynch,* A. Thompson, and A. Strachan, Modeling and Simulation in Materials Science and Engineering, **17,** 015007-1-13 (2009). DOI: 10.1088/0965-0393/17/1/015007
42. *"Structures and energetics of silicon nanotubes from molecular dynamics and density functional theory"*, A. Palaria, G. Klimeck, and A. Strachan, Physical Review B, **78**, 205315-1-5 (2008). DOI: 10.1103/PhysRevB.78.205315
43. *"Phonon Thermal Conductivity in Nanolaminated Composite Metals via Molecular Dynamic"*, Y. Zhou, B. Anglin, and A. Strachan, Journal of Chemical Physics, **127**, 184702-1-11 (2007). DOI: 10.1063/1.2802366
44. *"Melting and alloying of Ni/Al nanolaminates induced by shock loading: A molecular dynamics simulation study"*, S. Zhao, T. C. Germann, and A. Strachan, Physical Review B, **76**, 104105-1-5 (2007). DOI: 10.1103/PhysRevB.76.104105
45. *"Molecular dynamics simulation of dynamical response of perfect and porous Ni/Al nanolaminates under shock loading"*, S. Zhao, T. C. Germann, and A. Strachan, Physical Review B, **76**, 014103-1-6 (2007). DOI: 10.1103/PhysRevB.76.014103
46. *"Atomic-Level View of Inelastic Deformation in a Molecular Crystal"*, E. Jaramillo, T. D. Sewell, and A. Strachan, Physical Review B, **76**, 064112-1-6 (2007). DOI: 10.1103/PhysRevB.76.064112
47. *"Heteroepitaxial integration of metallic nanowires: transition from coherent to defective interfaces via molecular dynamics"*, A. Arumbakkam, E. Davidson, and A. Strachan, Nanotechnology, **18**, 345705-1-7 (2007). DOI: 10.1088/0957-4484/18/34/345705
48. *"Molecular dynamics characterization of the response of Ni/Al nanolaminates under dynamical loading"*, S. Zhao, Timothy C. Germann, and Alejandro Strachan, Journal of Propulsion and Power, **23**, 693-697 (2007). DOI: 10.2514/1.25727
49. *"Reply to "Comment on 'Melting dynamics of superheated argon: Nucleation and growth"'"*, S-N. Luo, L. Zheng, A. Strachan, D. Swift, Journal of Chemical Physics, **126**, 187102 (2007). DOI: 10.1063/1.2732744
50. *"Melting dynamics of superheated argon: Nucleation and growth"*, S-N. Luo, L. Zheng, A. Strachan, D. Swift, Journal of Chemical Physics, **126**, 34505-1-7 (2007). DOI: 10.1063/1.2424715
51. *"Atomistic simulations of shock-induced alloying reactions in Ni/Al nanolaminates"*, S. Zhao, T. C. Germann, and A. Strachan, Journal of Chemical Physics, **125**, 164707-1-8 (2006). DOI: 10.1063/1.2359438
52. *"Vibrational density of states and Lindemann melting law"*, S-N. Luo, A. Strachan, D. Swift, Journal of Chemical Physics, **122**, 194709-1-5 (2005). DOI: 10.1063/1.1902948
53. *"Deducing Solid-liquid interfacial energy of H_2O at 0-0.3 GPa deduced from supercooling experiments"*, S-N. Luo, A. Strachan, D. Swift, Modelling and Simulation Materials Science and Engineering, **13**, 321-328 (2005). DOI: 10.1088/0965-0393/13/3/002
54. *"Large electrostrictive strain at Gigahertz frequencies in a PVDF nano-actuator: computational device design"*, A. Strachan and W. A. Goddard, Applied Physics Letters, **86**, 83103-1-3 (2005). DOI: 10.1063/1.1862343
55. *"Thermal decomposition of RDX from reactive molecular dynamics"*, A. Strachan, E. Kober, A. C. T. van Duin, J. Oxgaard, and W. A. Goddard, Journal of Chemical Physics, **122**, 54502-1-10 (2005). DOI: 10.1063/1.1831277
56. *"Energy exchange between mesoparticles and their internal degrees of freedom"*, A. Strachan and B. L. Holian, Physical Review Letters, **94**, 014301-1-4 (2005). DOI: 10.1103/PhysRevLett.94.014301

57. *"Density functional theory and molecular dynamics studies of the energetics and kinetics of Electroactive polymers: PVDF and P(VDF-TrFE)"*, H. Su, A. Strachan, and W. A. Goddard, III, Physical Review B, **70**, 064101-1-8 (2004). DOI: 10.1103/PhysRevB.70.064101
58. *"Properties of Asphaltenes Through Computer Assisted Structure Elucidation and Atomistic Simulations. 1. Bulk Arabian Light Asphaltenes"*, M. S. Diallo, A. Strachan, J. L. Faulon, and W. A. Goddard III , Petroleum Science and Technology, **22**, 877-899 (2004). DOI: 10.1081/LFT-120040254
59. *"Calculating the Peierls energy and Peierls stress from atomistic simulations of screw dislocation dynamics: application to bcc tantalum"*, G. Wang, A. Strachan,* T. Cagin and W. A. Goddard III, Modelling and Simulation in Materials Science and Engineering, **12**, S371-S389 (2004). DOI: 10.1088/0965-0393/12/4/S06
60. *"First principles force field for metallic tantalum"*, A. Strachan, T. Cagin, O. Gülseren, S. Mukherjee, R. E. Cohen and W. A. Goddard III, Modelling and Simulation in Materials Science Engineering, **12**, S445-S459 (2004). DOI: 10.1088/0965-0393/12/4/S10
61. *"Non-equilibrium melting and crystallization of a model Lennard-Jones System"*, S-N. Luo, A. Strachan, D. Swift, Journal of Chemical Physics, **120**, 11640-1-10 (2004). DOI: 10.1063/1.1755655
62. *"Normal modes and frequencies from covariances in molecular dynamics or Monte Carlo simulations"*, A. Strachan, Journal of Chemical Physics, **120**, 1-4 (2004). DOI: 10.1063/1.1635364
63. *"Atomistic simulations of kinks in 1/2a < 111 > screw dislocations in bcc tantalum"*, G. Wang, A. Strachan, T. Cagin, W. A. Goddard, Physical Review B, **68**, 224101-1-15 (2003). DOI: 10.1103/PhysRevB.68.224101
64. *"Maximum superheating and undercooling: Systematics, molecular dynamics simulations, and dynamic experiments"*, S-N. Luo, T. Ahrens, T. Cagin, A. Strachan, W. A. Goddard, D. Swift, Physical Review B, **68**, 134206-1-11 (2003). DOI: 10.1103/PhysRevB.68.134206
65. *"Shock waves in high-energy materials: The initial chemical events in nitramine RDX"*, A. Strachan, A. van Duin, D. Chakraborty, S. Dasgupta, and W. A. Goddard, Physical Review Letters, **91**, 098301-1-4 (2003). DOI: 10.1103/PhysRevLett.91.098301
66. *"Ab initio and finite-temperature molecular dynamics studies of lattice resistance in tantalum"*, D. Segall, A. Strachan, W.A. Goddard, III, S. Ismail-Beigi, T. A. Arias, Physical Review B, **68**, 014104-1-11 (2003). DOI: 10.1103/PhysRevB.68.014104
67. *"ReaxFF$_{SiO}$ reactive force field for silicon and silicon oxide systems"*, A. van Duin, A. Strachan, S. Stewman, Q. Zhang, X. Xu, and W. A. Goddard, III, Journal of Physical Chemistry A, **107**, 3803-1-9 (2003). DOI: 10.1021/jp0276303
68. *"Role of core polarization curvature of screw dislocations in determining the Peierls stress in bcc Ta: A criterion for designing high-performance materials"*, G. Wang, A. Strachan, T. Cagin, W. A. Goddard, Physical Review B**,** **67**, 140101-1-4 (2003). DIO: 10.1103/PhysRevB.67.140101
69. *"Molecular Dynamics Modeling of Stishovite"*, S-N. Luo, T. Cagin, A. Strachan, W. A. Goddard, III and T. J. Ahrens, Earth and Planetary Science Letters, **202**, 147-157 (2002). DOI: 10.1016/S0012-821X(02)00749-5
70. *"Kinks in a/2<111> screw Dislocation in Ta"*, Guofeng Wang, A. Strachan, T. Cagin and W. A. Goddard III, Journal of Computer Aided Materials Design, **8**, 117-125 (2002). DOI: 10.1103/PhysRevB.68.224101
71. *"A Multiscale Approach for Modeling Crystalline Solids"* A. Cuitino, L. Stainier, G. Wang, A. Strachan, T. Cagin, W. A. Goddard, III and M. Ortiz, Journal of Computer Aided Materials Design, **8,** 127-149 (2002). DOI: 10.1023/A:1020012431230

72. *"Crack propagation in a Tantalum nano-slab"*, A. Strachan, T. Cagin and W. A. Goddard III, Journal of Computer Aided Materials Design, **8**, 151-159 (2002). DOI: 10.1023/A:1020046914392
73. *"Accurate Calculations of the Peierls Stress in Small Periodic Cells"*, D. E. Segall, T. A. Arias, A. Strachan, and W. A. Goddard, III, Journal of Computer Aided Materials Design, **8**, 161-172(2002).
    DOI: 10.1023/A:1020001527113
74. *"Ab-initio Studies of Pressure Induced Phase Transitions in BaO"*, M. Uludogan, T. Cagin, A. Strachan, and W. A. Goddard, III, Journal of Computer Aided Materials Design, **8**, 193-202 (2002).
    DOI: 10.1023/A:1020085006640
75. *"Large scale atomistic simulations of screw dislocation structure, annihilation and cross-slip in FCC Ni"*, Y. Qi, A. Strachan, T Cagin, and W. A. Goddard, III, Materials Science and Engineering A **309**, Sp. Iss. SI, 156-159 (2001). DOI: 10.1016/S0921-5093(00)01716-0
76. *"Molecular dynamics simulations of 1/2 a<111> screw dislocation in Ta"*, G. Wang, A. Strachan, T Cagin, and W. A. Goddard, III, Materials Science and Engineering A, **309**, Sp. Iss. SI, 133-137 (2001). DOI: 10.1016/S0921-5093(00)01739-1
77. *Reply to "Comment on 'Phase diagram of MgO from density-functional theory and molecular-dynamics simulations' "*, A. Strachan, T. Cagin, and W. A. Goddard, Physical Review B **63,** 096102 (2001). DOI: 10.1103/PhysRevB.63.096102
78. *"Critical behavior in spallation failure of metals"*, A. Strachan, T. Cagin, and W. A. Goddard, III, Physical Review B, **63**, 060103-1-4 (2001). DIO: 10.1103/PhysRevB.63.060103
79. *"Phase diagram of MgO from density-functional theory and MD simulations"*, A. Strachan, T. Cagin, and W. A. Goddard, Physical Review B, **60**, 15084-15093 (1999). DOI: 10.1103/PhysRevB.60.15084
80. *"Fragmentation of hot drops"*, C. O. Dorso and A. Strachan, Computer Physics Communications **121**, Sp. Iss. SI, 240-243 (1999). DOI: 10.1016/S0010-4655(99)00321-5
81. *"Temperature and energy partition in fragmentation"*, A. Strachan and C. O. Dorso, Physical Review C, **59**, 285-294 (1999). DOI: 10.1103/PhysRevC.59.285
82. *"Caloric curve in fragmentation"*, A. Strachan and C. O. Dorso, Physical Review C, **58**, R632-R636 (1998). DOI: 10.1103/PhysRevC.58.R632
83. *"Statistical thermodynamics of cluster phase transitions"* A. Strachan and C. O. Dorso, Physica A, **257**, 526-529 (1998). DOI: 10.1016/S0378-4371(98)00187-3
84. *"Time scales in fragmentation"*, A. Strachan and C. O. Dorso, Physical Review C, **55**, 775-787 (1997). DOI: 10.1103/PhysRevC.55.775
85. *"Fragment recognition in molecular dynamics"*, A. Strachan and C. O. Dorso, Physical Review C, **56**, 995-1001 (1997). DOI: 10.1103/PhysRevC.56.995
86. *"Onset of fragment formation in periodic expanding Systems"*, C. O. Dorso, A. Strachan, Physical Review B, **54**, 236-243 (1996). DOI: 10.1103/PhysRevB.54.236

REFEREED CONFERENCE PROCEEDINGS

(* indicates postdoc author, + graduate student author, # undergraduate student author)

1. *"Molecular dynamics simulations of shock-induced chemical mechanical, and thermal processes in Ni/Al nanolaminates"* S. Zhao, *T.C. Germann, A. Strachan, A. AIP Conference Proceedings, 845, 593-596 (2006). Conference of the American Physical Society Topical Group on Shock Compression of Condensed Matter, Jul. 31 – Aug. 05, 2005 Baltimore, MD
2. *"Reactive force fields based on quantum mechanics for applications to materials at extreme conditions"*, A.C.T. van Duin,* S. V. Zybin, K. Chenoweth, L. Zhang, S-P. Han, A. Strachan,

and W. A. Goddard, AIP Conference Proceedings, **845**, 581-1-4 (2006). Conference of the American-Physical-Society-Topical-Group-on-Shock-Compression-of-Condensed-Matter, JUL 31-AUG 05, 2005 Baltimore, MD.

3. *"Initial chemical events in the energetic material RDX under shock loading: role of defects"*, A. Strachan,* A. C. T. van Duin, and W. A. Goddard, III, Shock Compression of Condensed Matter-2003, Proceedings of the APS Topical Group on Shock Compression of Condensed Matter, **706**, 895-1-4.
4. *"The ReaxFF polarizable reactive force fields for molecular dynamics simulation of ferroelectrics"*, W. A. Goddard, III, Qingsong Zhang;* M. Uludogan, A. Strachan, T. Cagin, AIP Conference Proceedings, **626**, 45-1-11 (2002). Conference: Fundamental Physics of Ferroelectrics 2002, 3-6 Feb. 2002, Washington, DC, USA.
5. *"Fragment formation in finite and infinite expanding systems"*, C. O. Dorso* and A. Strachan, Revista Mexicana de Fisica. **41**, 96 (1995). XVIII Symposium on Nuclear Physics, JAN 04-07, 1995 Oaxtepec, Mexico.

PRESENTATIONS

INVITED AND KEYNOTE CONFERENCE PRESENTATIONS

1. KEYNOTE: *"Cyber-enabled predictive simulations of materials and devices via nanoHUB.org"*, Nanotech conference & Expo 2013, Washington, D.C. (scheduled May 2013).
2. KEYNOTE: *"Predictive materials modeling with quantified uncertainties and cyber-enable via nanohub-org."*, Alejandro Strachan, Colombia-US Workshop on Nanotechnology in Energy and Medical Applications, Medellin, Colombia, March 11 – 13, 2013.
3. *"Multi-resolution modeling & experiments of energetic materials"*, Alejandro Strachan, Materials Research Society Fall Meeting and Exhibit, Boston, Massachusetts, November 25-30, 2012.
4. *"Role of size and nanostructure on the thermo-mechanical response of shape memory alloys"*, Alejandro Strachan, 6th International Conference on Multiscale Materials Modeling, Biopolis, Singapore, October 15-19, 2012.
5. *"Multi-resolution modeling & experiments of nanostructured intermolecular reactive composites"*, Alejandro Strachan, Chemistry in Dynamic Extremes Workshop, Buffalo Thunder Resort, Santa Fe, NM, January 18-20, 2012.
6. KEYNOTE: *"Role of size and nanostructure on the thermo-mechanical response of shape memory alloys"*, Karthik Guda and Alejandro Strachan, International Conference on Plasticity, San Juan, Puerto Rico, January 3-8, 2012.
7. *"Challenges in multiscale, multiphysics modeling for Materials Genome: -Quantifying uncertainties & variability -Verification & validation -Cyber-enabling tools for research & edu"* Alejandro Strachan, Materials Genome Initiative Workshop, University of Michigan, Ann Arbor, MI December 12, 2011.
8. *"Quantifying variability and uncertainties in multiscale, multiphysics modeling"*, Alejandro Strachan, Nanotechnology for Defense Applications, Bellevue, WA October 26, 2011.
9. *"Online materials simulations @ nanoHUB.org, and more…"*, Ravi Vedula, Ben Haley and Ale Strachan, TMS Annual Meeting Lunch and Learn Series, San Diego Convention Center, San Diego, California, February 27 - March 3, 2011.
10. *"Session on Molecular Modeling"*, Alejandro Strachan (Discussion Leader), Gordon Research Conference on Energetic Materials, Tilton NH, (2010).

11. *"First Principles-Based Modeling Of Nanostructured Materials"*, Ya Zhou, Jane Lin, and Alejandro Strachan, XIX International Materials Research Congress, Cancun, Mexico, August 15–19, 2010.
12. Young Leader Tutorial Luncheon Lecture: *"Atomistic and Mesoscale Modeling of Materials: Towards Predictive Tools for Materials Design"*, A. Strachan.* TMS 2009 Annual Meeting, San Francisco, California, February 16, 2009. E.5.34.
13. *"Shape memory in nanoscale metallic alloys"*, A. Strachan.* MS&T, Pittsburgh, Pennsylvania, October 7, 2008. E.5.33.
14. "*Dynamics with implicit degrees of freedom in materials simulations: coarse grain polymer and electrons in metals"*, A. Strachan.* Gordon Research Conference on Energetic Materials, June 18, 2008, Tilton, New Hampshire. E.5.31.
15. *"Atomistic and mesoscale modeling of chemical and thermo-mechanical processes in molecular crystals"*, A. Strachan.* 234th American Chemical Society National Meeting & Exposition. August 23, 2007, Boston, Massachusetts. E.5.28.
16. *"Atomistic and mesoscale modeling of the response of molecular crystals to dynamical loading"*, Alejandro Strachan.* E. Jaramillo, and T. Sewell, The Sixth Biennial Conference, New Models and Hydrocodes for shockwave processes in Condensed Matter, April 11, 2006, Dijon, France. E.5.22.
17. *"Atomistic and mesoscale modeling of mechanical and chemical processes in energetic materials"*, Alejandro Strachan,* T. D. Sewell, E. Jaramillo, A.C.T. van Duin, W.A. Goddard. 14th APS Topical Conference on Shock Compression of Condensed Matter, July 31st-August 5th, Baltimore, MD. E.5.20.
18. *"Reactive molecular dynamics and mesoscopic modeling of the mechanical and chemical response of materials under dynamical loading"*, A. Strachan,* B.L. Holian, E.M.Kober, A.C.T. van Duin, S-P. Han, W.A. Goddard, III. Special Focus Session on Simulations of Matter at Extreme Conditions of the American Physical Society meeting, March 21-25, 2005, Los Angeles, California. E.5.18.
19. *"First principles-based atomistic modeling of materials: ferroelectric polymers and chemistry at extreme conditions"*, A. Strachan,* H. Su, W.A. Goddard, III. 3rd International Conference on Computational Modeling of Materials, May 30-June 4, 2004, Acireale, Sicily, Italy. E.5.15.
20. *"Plastic deformation and failure from First Principles"*, A. Strachan,* T. Cagin, W.A. Goddard, Centre Européen de Calcul Atomique et Moléculaire (CECAM) International Workshop on Stress driven solid-solid phase transformations, July 23-25, 2001, Lyon France. E.5.10.

INVITED COLLOQUIUM/SEMIAR SERIES PRESENTATIONS

1. *"First Principles, Multiscale Modeling of Materials with Quantified Uncertainties: Towards Computational Materials Design"*, Alejandro Strachan,* Mechanical Engineering Seminar Series, Mechanical and Nuclear Engineering, Pennsylvania State University, University Park, Pennsylvania, January 15, 2013.
2. "Modelado de MEMS desde primeros principios con cuantificación de incerteza", Alejandro Strachan,* Physics Department, University of Buenos Aires, Argentina. December 20, 2012.
3. *"First Principles, Multiscale Modeling of Materials with Quantified Uncertainties: Towards Computational Materials Design"*, Alejandro Strachan,* DMSE Colloquia, Materials Science and Engineering, Case Western, Cleveland, Ohio, April 17, 2012.
4. "Predictive materials modeling and simulations", Alejandro Strachan* and Chunyu Li, Rolls Royce Materials Forum, Indianapolis, Indiana, September 20, 2011.

5. "Multiscale Modeling - Certification by Analysis", A. Strachan* and R. B. Pipes, April 15, 2011, Air Force Research Laboratory, Dayton, Ohio.
6. *"Size effects in materials response from atomistic simulations: contact physics and shape memory alloys"*, Condensed Matter Seminar, Physics Department, Purdue University, West Lafayette, Indiana, December 10, 2010.
7. *"Cyber-enabled first principles-based materials modeling: uncovering new behavior at the nanoscale using a web-browser"*, Physics Seminar, Ball State University, Muncie, Indiana, October 7, 2010.
8. *"First principles-based atomistic simulations of molecular solids"*, A. Strachan. Mechanical Engineering, McGill University, Montreal, Quebec Canada, April 27, 2009.
9. *"Atomistic and mesoscale modeling of materials at extreme conditions"*, Alejandro Strachan.* NASA Ames Research Laboratories, Moffett Field, CA April 16, 2009.
10. *"Predictive materials modeling and simulation"*, Alejandro Strachan. Purdue University Department of Industrial and Physical Pharmacy Seminar, West Lafayette, Indiana, December 5, 2008.
11. *"Dinámica con grados de libertad implícitos en simulaciones de materiales: electrones en metales y dinámica de meso-partículas"*, Alejandro Strachan,* Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Buenos Aires, Argentina, December 20, 2007.
12. *"Modelado atomístico y molecular de nano-materiales"*, Alejandro Strachan.* Facultad de Ingeniería, Universidad de Buenos Aires, Buenos Aires, Argentina, December 21, 2007.
13. *"Dynamics with implicit degrees of freedom in materials simulations: coarse grain polymer and electrons in metals"*, Alejandro Strachan. Sandia National Laboratories, Albuquerque, New Mexico December 10, 2007.
14. *"Atomistic and mesoscale predictive modeling of materials: from nanoelectronics and ferroelectrics to structural materials"*, Alejandro Strachan. Institute of High Performance Computing, A*STAR (Agency for Science, Technology and Research), Singapore, September 12, 2007.
15. *"Atomic structure, hetero-integration and thermo-mechanical response of semiconductor and metallic one dimensional nanostructures"*, Alejandro Strachan.* Institute of High Performance Computing, A*STAR (Agency for Science, Technology and Research), Singapore, September 10, 2007.
16. *"Size and geometrical effects on ferroelectricity and martensitic microstructure: towards computational materials design and optimization"*, Alejandro Strachan.* Institute of High Performance Computing, A*STAR (Agency for Science, Technology and Research), Singapore, September 11, 2007.
17. *"Multiscale modeling of mechanical response of materials"*, Alejandro Strachan.* Institute of High Performance Computing, A*STAR (Agency for Science, Technology and Research), Singapore, September 13, 2007.
18. *"Atomistic and mesoscale modeling of materials: thermal, mechanical and chemical phenomena"*, A. Strachan. Physical Chemistry Seminars, Department of Chemistry, Purdue University, November 8, 2006, West Lafayette, Indiana.
19. *"Atomistic and mesoscale modeling of mechanical and chemical processes in materials"*, A. Strachan. February 15, 2006, Computer Research Institute Nano-Computational Seminar, Purdue University, West Lafayette, Indiana.
20. *"Atomistic and Mesoscale Modeling of the Mechanical and Chemical Behavior of Materials"*, A. Strachan. Mechanical Engineering Graduate Seminars, Purdue University, West Lafayette, Indiana.

21. *"Atomistic and mesoscale modeling of advanced materials: from nanotechnology to single crystal plasticity"*, A. Strachan. April 6, 2005, College of Engineering, Purdue University, West Lafayette, Indiana.
22. *"Multiscale modeling of mechanical and chemical properties of materials"*, A. Strachan. April 4, 2005, Department Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania.
23. *"Atomistic and mesoscale modeling of mechanical and chemical properties of materials"*, A. Strachan. March 22, 2005, Department of Materials Science, Caltech, Pasadena, California.
24. *"Atomistic and mesoscale modeling of mechanical and chemical properties of materials"*, A. Strachan. Feb. 27, 2005, Department of Engineering Science and Mechanical Engineering, Virginia Tech, Blacksburg, VA.
25. *"First principles-based multiscale modeling of materials"*, A. Strachan, G Wang, T. Cagin, W.A. Goddard, III, M. Ortiz, L. Stainer, A. Cuitino. March 26, 2003, Materials Lectures Series, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM.
26. *"Full-physics, full-chemistry multiscale modeling of materials"*, A. Strachan. May 2002, Los Alamos National Laboratory, Los Alamos, NM.
27. *"Full-physics, full-chemistry multiscale modeling of materials"*, Alejandro Strachan. April 2002, Sandia National Laboratories, Albuquerque, NM.
28. *"Multiscale modeling: from nanotechnology to materials science"*, Alejandro Strachan. Colloquium series of the Mechanical and Aerospace Engineering, November 2001, Rutgers University, Piscataway, NJ.
29. *"Spall failure in Ta from First Principles"*, Alejandro Strachan, T. Cagin, W.A. Goddard. February 2001, T-12 Group, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM.

CONFERENCE AND OTHER PRESENTATIONS

1. Poster: *"Size effects and nanoengineering in shape memory materials"*, Keith Morrison, Karthik Guda, Mathew Cherukara, and Alejandro Strachan, Mechanical Behavior and Radiation Effects of Materials Principal Investigators' Meeting, Potomac, Maryland, March 25 – 27, 2013.
2. "*Shape Memory Metamaterials with Tunable Thermo-Mechanical Response Via Hetero-Epitaxial Integration"*, Alejandro Strachan, Karthik Guda Vishnu and Keith Morrison, TMS Annual Meeting & Exhibition, San Antonio, Texas, March 3 – 7, 2013.
3. *"Prediction of Contact Mechanics for Microsystems by a Multiscale Model with Uncertainties Quantification"* , Hojin Kim and Alejandro Strachan, TMS Annual Meeting & Exhibition, San Antonio, Texas, March 3 – 7, 2013.
4. *"Adaptive Atomistic-Phase-Field Dislocation Dynamics Model"*, Lei Cao, Hojin Kim, Alejandro Strachan, Marisol Koslowski, TMS Annual Meeting & Exhibition, San Antonio, Texas, March 3 – 7, 2013.
5. *"Ab-initio characterization of high-emissivity oxide coatings"*, Alejandro Strachan, Aerospace Materials for Extreme Environments Program Review, Arlington, Virginia, February 11-15, 2013.
6. *"Ab- initio modeling in RRAM switching"*, Alejandro Strachan, FCRP Function Accelerated nanoMaterials Engineering Center Kickoff Meeting, Los Angeles, California, February 5 – 6, 2013
7. Poster: *"Ab Initio of RRAM Switching"*, Alejandro Strachan, Gerhard Klimeck and Nicolas Onofrio, FCRP Function Accelerated nanoMaterials Engineering Center Kickoff Meeting, Los Angeles, California, February 5 – 6, 2013.
8. Poster: *"Theoretical Prediction of Performance Enhancements in Asymmetric Strain Relaxed Ge-PMOS Nanowires"*, Ravi Pramod Vedula * and Alejandro Strachan, Materials Research Society Fall Meeting and Exhibit, Boston, Massachusetts, November 25 – 30, 2012.

9. *"Electron Trapping Dynamics in a-Si3N4: Application to multi-scale dielectric charging mode"*, Ravi Pramod Vedula* and Alejandro Strachan, Materials Research Society Fall Meeting and Exhibit, Boston, Massachusetts, November 25 – 30, 2012.
10. "*Electrical and Phonon Thermal Conductivity of A1 from Molecular Dynamics Simulation"*, Keng-Hua Lin* and Alejandro Strachan, Materials Research Society Fall Meeting and Exhibit, Boston, Massachusetts, November 25 – 30, 2012.
11. *"Effect of Nanostructure on Transport and Sensitivity of Ni/Ai Intermolecular Reactive Composite"*, Mathew Cherukara* and Alejandro Strachan, Materials Research Society Fall Meeting and Exhibit, Boston, Massachusetts, November 25 – 30, 2012.
12. *Electromagnetic and Thermal Induced Chemical Decomposition in the Molecular Explosive HMX via Reactive Molecular Dynamics Simulation"*, Mitchell Wood* and Alejandro Strachan, Materials Research Society Fall Meeting and Exhibit, Boston, Massachusetts, November 25 – 30, 2012.
13. "*Shape Memory Metamaterials with Tunable Thermo-mechanical Response via Hetero-epitaxial Integration"*, Karthik Guda, Keith Morrison and Ale Strachan, Materials Research Society Fall Meeting and Exhibit, Boston, Massachusetts, November 25 – 30, 2012.
14. *"Role of Atomic and Nano-scale Structure on the Thermo-Mechanical Response of Ni/Al Intermolecular Reactive Composites"*, Alejandro Strachan,* Mathew Cherukara and Karthik Guda Vishnu, 6th International Conference on Multiscale Materials Modeling, October 15-19, 2012 Biopolis, Singapore.
15. Poster: *"Cyber-Enabled Predictive Models for Polymer Nanocomposites: Multiresolution Simulations and Experiments"* Alejandro Strachan,* Marisol Koslowski, R. Byron Pipes, Arvind Raman, Benjamin Haley, A. Mendoza, J.L. Martin, Yae-Ji Kim, Hank Thompson, Rocio Misiego, 2012 NSF CMMI Engineering Research and Innovation Conference, July 9 – 12, 2012, Boston, Massachusetts.
16. "*Prediction of failure onset in multilayer graphene reinforced epoxy composites using Molecular Dynamics simulations "*, Chunyu Li* and Alejandro Strachan, International Conference on Mechanics of Nano, Micro and Macro Composite Structures, Turin, Italy, June 18-20, 2012.
17. "*Multi-resolution modeling & experiments of nanostructured intermolecular reactive composites"*, Alejandro Strachan,* Mathew Cherukara, and Karthik Guda Vishnu, 5th Annual Symposium of the International Center for Applied Computational Mechanics, June 13, 2012, New York, New York.
18. "*Predictive science with quantified uncertainties for decision-making"*, Alejandro Strachan,* MGI Workshop on Building the Materials Innovation Infrastructure: Data and Standards, Washington DC, May 14-15, 2012.
19. "*The Kinetics of reactive intermetallic composites",* Mathew Cherukara* and Alejandro Strachan, TMS Annual Meeting and Exhibition, Orlando, Florida, March 11-15, 2012.
20. "*First principles, predictive simulations of AFM tip-polymer interactions"*, Gabriela Venturini, Hojin Kim,* A. Strachan TMS Annual Meeting and Exhibition, Orlando, Florida, March 11-15, 2012.
21. Poster: *"Size and asperity height effect on the contact hardness in nanoscale metallic asperities contact: molecular dynamics simulation"*, Hojin Kim* and Alejandro Strachan, TMS Annual Meeting and Exhibition, Orlando, Florida, March 11-15, 2012.
22. Poster: *"Cyber-Enabled Ab Initio Simulations in nanoHUB.org: Simulation Tools and Learning Modules"*, Ravi Vedula,* Ben Haley, and Alejandro Strachan, TMS Annual Meeting and Exhibition, Orlando, Florida, March 11-15, 2012.
23. "*Predictive Simulations of AFM tip-polymer interactions"*, Hojin Kim*, Gabriela Venturini, Alejandro Strachan, TMS Annual Meeting and Exhibition, Orlando, Florida, March 11-15, 2012.
24. "*Mechanical Response of the PMMA-CNT Nanocomposite via Molecular Dynamics"*, Yae-ji Kim*, Eugenio Jaramillo, Benjamin Haley, Alejandro Strachan, TMS Annual Meeting and Exhibition, Orlando, Florida, March 11-15, 2012.
25. "*Multi-resolution modeling & experiments of nanostructured intermolecular reactive composites"*, Alejandro Strachan,* Mathew Cheruraka, and Karthik Guda Vishnu, Chemistry in Dynamic Extremes Workshop, Buffalo Thunder Resort, Santa Fe, NM, January 18-20, 2012.
26. *"Challenges in multiscale, multiphysics modeling for Materials Genome: -Quantifying uncertainties & variability -Verification & validation -Cyber-enabling tools for research &*

edu", A. Strachan,* Materials Genome Initiative Workshop, Ann Arbor, MI December 12, 2011

27. "*Molecular Dynamics Simulations Of Thermosetting Polymer And Their Properties*", Chunyu Li* and Alejandro Strachan, High Performance Resins, Cincinnati, Ohio, Sep 28, 2011.
28. *"Quantifying variability and uncertainties in multiscale modeling of MEMS"*, Alejandro Strachan,* PSAAP V&V/UQ workshop, Stanford University, Stanford, California, August 16-18, 2011.
29. Poster: *"Cyber-Enabled Ab Initio Simulations in nanoHUB.org: Simulation Tools and Learning Modules"*, Ravi Vedula, Ben Haley,* and Alejandro Strachan, 1st World Congress on Integrated Computational Materials Engineering, July 10-14, 2011, Seven Springs Mountain Resort, Seven Springs, Pennsylvania.
30. Poster: *"PolymerModeler at nanoHUB.org"*, Benjamin P. Haley,* Nate Wilson, Chunyu Li, Andrea Arguelles, Eugenio Jaramillo, Alejandro Strachan, 1st World Congress on Integrated Computational Materials Engineering, July 10-14, 2011, Seven Springs Mountain Resort, Seven Springs, Pennsylvania.
31. "*Cyber-enabled Materials Simulations @ nanoHUB.org: towards cloud ICME*", Alejandro Strachan,* 1st World Congress on Integrated Computational Materials Engineering, July 10-14, 2011, Seven Springs Mountain Resort, Seven Springs, Pennsylvania.
32. *"Uncertainty quantification in atomistic-based multiscale materials models"*, Alejandro Strachan,* PSAAP V&V/UQ workshop, July 7, 2010, University of Texas at Austin, Austin, Texas.
33. "*Quantifying variability and uncertainties in multiscale modeling of MEMS"* Uncertainty Quantification and Multiscale Materials Modeling Workshop, Santa Fe, New Mexico, June 13-15, 2011.
34. *"NSF's nanoHUB.org: Impact on Research and Education"*, Alejandro Strachan and Gerhard Klimeck, The Seventh International Nanotechnology Conference on Communication and Cooperation, College of Nanoscale Science and Engineering (CNSE), Albany, New York, May 16, 2011.
35. *"Molecular Dynamics Simulations on Thermal Transport in Hetero-epitaxial Si/Ge Nanolaminates and Nanowires"*, Keng-Hua Lin* and Alejandro Strachan, MRS Spring Meeting and Exhibit, San Francisco, CA, May 2011.
36. "*Strain Relaxation on Si-core/Ge-shell Heterostructure Nanowires via Molecular Dynamics*", Yumi Park* and Alejandro Strachan, MRS Spring Meeting and Exhibit, San Francisco, CA, May 2011.
37. "*First Principles Investigation of Structure and Electronic Properties of amorphous Si3N4"*, Ravi Vedula, Nathan L. Anderson, and Alejandro Strachan, American Physical Society March Meeting, Dallas, Texas, March 2011.
38. *"First-principles investigation of low energy E' center precursors in amorphous silica"*, Nathan L. Anderson, Ravi Pramod Vedula, Peter A. Schultz, R.M. Van Ginhoven, and Alejandro Strachan, American Physical Society March Meeting, Dallas, Texas, March 2011.
39. *"Molecular Dynamics Study of the Contact Strengths between Clean Metallic Surfaces with nanoscale asperities"*, Hojin Kim and Alejandro Strachan, American Physical Society March Meeting, Dallas, Texas, March 2011.
40. *"Online materials simulations @ nanoHUB.org, and more…"*, Ravi Vedula, Ben Haley and Ale Strachan,* TMS Annual Meeting Lunch and Learn Series, San Diego Convention Center, San Diego, California, February 27 - March 3, 2011.
41. *"First principles study of the energetics of ideal GaAs surfaces and adsorption of Al and O as a function of surface orientation"* Ganesh Hegde, Gerhard Klimeck and Alejandro Strachan,41st IEEE Semiconductor Interface Specialists Conference, San Diego, California, December 2-4, 2010.

42. "*Role of size and nanostructure on the thermo-mechanical response of shape memory alloys"*, Karthik Guda Vishnu, Alejandro Strachan, IX Argentinean Congress of Computational Mechanics, Buenos Aires, Argentina, November 15-19, 2010.
43. *"Molecular Simulations of Thermosetting Polymer EPON862/DETDA and Its Properties"*, C. Li and A. Strachan, 25th Annual Conf of American Society for Composites, Sep 20-22, 2010, Dayton, Ohio.
44. *"Ultimate Mechanical Response of PMMA from Large- scale MD Simulations"* A. Strachan, 25th Annual Conf of American Society for Composites, Sep 20-22, 2010, Dayton, Ohio.
45. *"Thermo-mechanical response of amorphous polymers from MD"*, Chunyu Li,* Nate Wilson, Eugenio Jaramillo, and Alejandro Strachan, World Congress on Computational Mechanics, July 19-23, 2010, Sydney, Australia.
46. The Strongest Contact and Size Effect in Nanoscale Metal-Metal Contact: Molecular Dynamics Simulation Study: Hojin Kim;* Alejandro Strachan, TMS Annual Meeting and Exhibition, February 14-18, 2010, Seattle, Washington.
47. Strain Engineering on Si/Ge Nanoscale Heterostructures: Yumi Park,* Winnie Tan; Alejandro Strachan, TMS Annual Meeting and Exhibition, February 14-18, 2010, Seattle, Washington.
48. Molecular Dynamics Simulations of Crosslinked EPON862/DETDA Polymers: Chunyu Li,* Alejandro Strachan, TMS Annual Meeting and Exhibition, February 14-18, 2010, Seattle, Washington.
49. Role Loading Conditions on the Mechanical Response of PMMA from Molecular Dynamics: Eugenio Jaramillo,* Alejandro Strachan, TMS Annual Meeting and Exhibition, February 14-18, 2010, Seattle, Washington.
50. *"Phase stability and transformation paths in NiTi from DFT calculations"*, Karthik Guda Vishnu* and Alejandro Strachan, TMS Annual Meeting and Exhibition, February 14-18, 2010, Seattle, Washington.
51. *"Large-scale molecular dynamics simulations of the mechanical response of amorphous polymers"*, ICCM-17 17th International Conference on Composite Materials, July 27, 2009, Edinburgh, Scotland, UK.
52. *"Poster: Cyber-Enabled Predictive Models for Polymer Nanocomposites: Multiresolution Simulations and Experiments"* Alejandro Strachan*, Marisol Koslowski, R. Byron Pipes, Arvind Raman, Eugenio Jaramillo, 2009 NSF CMMI Engineering Research and Innovation Conference, June 22-25, 2009. Honolulu, Hawaii.
53. "*Thermal Transport in Atomistic and Mesoscale Simulations with Implicit Degrees of Freedom*", Y. Zhou* and A. Strachan. MRS Spring Meeting, San Francisco, California, April 16, 2009.
54. "*Mechanical Analysis of Macromodels of Biomimetic Composite Materials using Rapid Prototyping Techniques*", M. Cooper, K. Frank, P. Russel, M. Waters, A. Strachan, and P. D. Zavattieri.* MRS Spring Meeting, San Francisco, California, April 16, 2009.
55. "*Large-scale MD Simulations of Metal-metal Contacts: Size Dependent Interactions and Sub-surface Defect Generation*", Alejandro Strachan and Hojin Kim.* MRS Spring Meeting, San Francisco, California, April 15, 2009.
56. *"Atomistic simulations of interfacial structure and thermal properties"*, A. Strachan,* A. Arumbakkam, Y. Park , Y. Zhou. Frontiers in Scalable Nanostructured Materials and Interfaces, March 10-12, 2009. Purdue University, West Lafayette, Indiana.
57. Young Leader Tutorial Luncheon Lecture: *"Atomistic and Mesoscale Modeling of Materials: Towards Predictive Tools for Materials Design"*, A. Strachan.* TMS 2009 Annual Meeting, San Francisco, California, February 16, 2009.
58. *"Shape memory in nanoscale metallic alloys"*, A. Strachan,* A. Thompson and K. Guda Vishnu. MS&T, Pittsbugrh, Pennsylvania, October 7, 2008.

59. "*Poster: Electronic structure and transport in devices with non-ideal bonding environments"*, A. Palaria,* G. Klimeck and A. Strachan. Techcon Conference, Austin Texas, 2008.
60. *"Dynamics with implicit degrees of freedom in materials simulations: coarse grain polymer and electrons in metals"*, A. Strachan.* Gordon Research Conference on Energetic Materials, Tilton, New Hampshire, June 18, 2008.
61. *"Dynamic friction in multi-walled carbon nanotubes: a molecular dynamics study"*, A. Strachan,* Luis Zalamea, R. Byron Pipes, E. Jaramillo, and T. D. Sewell. "US-Japan Conference on Composite Materials, Nihon University, Tokyo, Japan, June 6, 2008.
62. *"Shape memory in nanoscale metallic alloys"*, A. Strachan,* A. Thompson and K. Guda Vishnu. DoE BES Contractors Meeting, "Behavior of Defects in Materials", Warrenton, Virginia, April 15, 2008.
63. *"Atomistic and mesoscale modeling of chemical and thermo-mechanical processes in molecular crystals"*, A. Strachan.* 234th American Chemical Society National Meeting & Exposition. August 23, 2007, Boston, Massachusetts.
64. *"Phonon Thermal Conductivity in Nanolaminated Composite Metals via Molecular Dynamics"*, Y. Zhou,* B. Anglin, and A. Strachan, Materials Research Society Spring Meeting, San Francisco, CA, April 9-13, 2007.
65. *"One dimensional silicon nanostructures: atomic level structures and properties from MD and DFT"*, A. Palaria* and A. Strachan, Materials Research Society Spring Meeting, San Francisco, CA, April 9-13, 2007.
66. "Interfaces and limit of coherency in core-shell and axially heterogeneous metallic and semiconductor nanowires via molecular dynamics", A. Arumbakkam, Y. Park, and A. Strachan.* Materials Research Society Spring Meeting, San Francisco, CA, April 9-13, 2007.
67. *"Atomistic and mesoscale modeling of the response of molecular crystals to dynamical loading"*, A. Strachan,* E. Jaramillo, and T. Sewell. Materials Research Society Fall Meeting, Boston, MA, November 27 - December 1, 2006.
68. *"Poster: Heteroepitaxial integration of metallic nanowires: transition from coherent to defective interfaces via molecular dynamics"*, A. Arumbakkam,* E. Davidson and A. Strachan. Materials Research Society Fall Meeting, Boston, MA, November 27 - December 1, 2006.
69. *"Atomistic and mesoscale modeling of the response of molecular crystals to dynamical loading"*, A. Strachan,* E. Jaramillo and T. Sewell. The Sixth Biennial Conference, New Models and Hydrocodes for shockwave processes in Condensed Matter, April 11, 2006, Dijon, France.
70. *"Atomistic and mesoscale modeling of mechanical and chemical processes in energetic materials"*, A. Strachan,* B. L. Holian, E. M. Kober, A. van Duin and W. A Goddard, III. Materials Research Society Fall Meeting, Boston, MA, November 30, 2005.
71. *"Atomistic and mesoscale modeling of mechanical and chemical processes in energetic materials"*, A. Strachan,* T. D. Sewell, E. Jaramillo, A.C.T. van Duin, W.A. Goddard, III. APS Topical Conference on Shock Compression of Condensed Matter, July 31st-August 5th, 2005; 14th, Baltimore, MD.
72. *"Atomistic and mesoscale modeling of deformation in metallic alloys and molecular crystals"*, Alejandro Strachan.* Third MIT Conference on Computational Fluid and Solid Mechanics, Cambridge, Massachusetts, June 14-17, 2005.
73. *"Reactive molecular dynamics and mesoscopic modeling of the mechanical and chemical response of materials under dynamical loading"*, A. Strachan,* B. L. Holian, E.M.Kober, A.C.T. van Duin, S-P. Han, W.A. Goddard, III. Special Focus Session on Simulations of Matter at Extreme Conditions of the American Physical Society meeting, March 21-25, 2005, Los Angeles, California.

74. *"Atomistic and mesoscale modeling of shock loading in molecular crystals"*, Alejandro Strachan,* S-N. Luo, B.L. Holian. International Symposium on Plasticity, January 4-8, 2005, Kauai, HI.
75. *"Atomistic and Mesoscale Modeling of Mechanical and Chemical Processes in Molecular Crystals"*, Alejandro Strachan.* 2nd International Conference on Multiscale Materials Modeling, University of California Los Angeles, Los Angeles, California, October 11-15, 2004.
76. *"First principles-based atomistic modeling of materials: ferroelectric polymers and chemistry at extreme conditions"*, A. Strachan,* H. Su, W.A. Goddard. 3rd International Conference on Computational Modeling of Materials, May 30-June 4, 2004, Acireale, Sicily, Italy.
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78. *"Molecular Dynamics Simulations of Reactive Processes I: shock loading"*, A. Strachan.* 13th Biennial International Conference of the APS Topical Group on Shock Compression of Condensed Matter, Portland, Oregon, July 20 - 25, 2003.
79. *"Multiscale modeling of nano-structured complexity in ferroelectric polymers"*, A. Strachan* and W.A. Goddard. 225th American Chemical Society National Meeting", March 23-27, 2003, New Orleans, LA.
80. *"Polarizable reactive force field for molecular dynamics of ferroelectrics"*, Q. Zhang, A. Strachan, M. Uludogan, T. Cagin, W.A. Goddard*, Fundamental Physics of Ferroelectrics 2002. Washington DC, Feb. 3-6, 2002.
81. *"Plastic deformation and failure from First Principles"*, A. Strachan,* T. Cagin, W.A. Goddard, Centre Européen de Calcul Atomique et Moléculaire (CECAM) International Workshop on Stress driven solid-solid phase transformations, July 23-25, 2001, Lyon France.
82. *"Poster: Large scale atomistic simulations of dislocations Ni"*, Y. Qi, A. Strachan,* T Cagin, and W. A. Goddard, III, Dislocations 2000: An International Conference on the Fundamentals of Plastic Deformation, 19-22 June 2000, Gaithersburg, MD, USA.
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84. *"Statistical thermodynamics of cluster phase transitions"*, A. Strachan* and C. O. Dorso, V Latin American Workshop on Nonlinear Phenomena, Canela, Brazil, 28 Sept - 3 Oct, 1997.
85. *"Poster: Termodinamica estadistica de sistemas pequenos altamente excitados"*, A. Strachan* y C. O. Dorso. 82 Reunion Nacional de Fisica, San Luis, Argentina, Septiembre 1997.
86. *"Poster: On the time scales in fragmentation"*, A. Strachan* and C. O. Dorso, X National Meeting on Nonequilibrium Statistical Mechanics and Nonlinear Physics MEDYFINOL'96. Universidad de Tucuman, Tucuman, Argentina.
87. *"Poster: Fluctuations in nuclear multifragmentation"*, A. Strachan,* C. O. Dorso, and J. A. Lopez, Nuclear dynamics at long and short distances, Angra dos Reis, RJ, Brazil, 8-12 April, 1996.
88. *"Fragmentacion en el big-bang microscopico"*, C. O. Dorso, A. Strachan.* 80a. Reunion Nacional de Fisica, Bariloche, Rio Negro, Argentina, 2-6 de Octubre, 1995.
89. *"Poster: Early fragment formation in 2-D expanding infinite systems"*, A. Strachan,* C. O. Dorso. 79a. Reunion Nacional de Fisica, 1994, Villa Giardino, Cordoba, Argentina.
90. *"The onset of fragment formation"*, C.O.Dorso,* A. Strachan, 79a. Reunion Nacional de Fisica, 1994, Villa Giardino, Cordoba, Argentina.

SPECIAL PROJECTS AND SHORT COURSES

Web-enabled simulations tools available via NSF's nanoHUB.org:

1. Polymer Modeler, https://nanohub.org/resources/9230. Impact: 120 users and 2,111 simulations.
2. DFT calculations with Quantum ESPRESSO: https://nanohub.org/resources/9269. Impact: 228 users and 1,691 simulations.
3. nanoMATERIALS SeqQuest DFT: https://nanohub.org/resources/3982. Impact: 218 users and 4,060 simulations.
4. nano-Materials Simulation Toolkit: https://nanohub.org/resources/1692. Impact: 1,678 users and 13,675 simulations.

Online seminars and short courses:

1. *"MSE 597G An Introduction to Molecular Dynamics"*, A. Strachan, Posted 13 Nov 2008. Impact: 2,756 users. https://nanohub.org/resources/5838
2. *"Lectures on Molecular Dynamics Modeling of Materials"*, A. Strachan, Posted 09 Jan 2008. Impact: 1.919 users (July 15, 2009). https://nanohub.org/resources/3675
3. *"Materials strength: does size matter? nanoMATERIALS simulation toolkit tutorial"*, A. Strachan, Posted 01 Feb 2007. Impact: 1,921 users (July 15, 2009). https://nanohub.org/resources/2322
4. *"First Principles-Based Modeling of materials: Towards Computational Materials Design"*, A. Strachan, Posted 20 Apr 2006. Impact: 427 users (July 15, 2009). https://nanohub.org/resources/1239
5. *"First Principles-based Atomistic and Mesoscale Modeling of Materials"*, A. Strachan, Posted 01 Dec 2005. Impact: 2,048 users (July 15, 2009). https://nanohub.org/resources/434