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217. Structural Transformation, Amorphization, and Fracture in Nanowires: A Multi-million Atom Molecular Dynamics Study

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219. Scalable Atomistic Simulation Algorithms for Materials Research
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223. Hybrid Electronic-Density-Functional/Molecular-Dynamics Simulation on Parallel Computers: Oxidation of Si Surface
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225. Collaborative Simulation Grid: Multiscale Quantum-Mechanical/Classical Atomistic Simulations on Distributed PC Clusters in the US and Japan

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229. Multimillion Atom Simulations of Nanosystems on Parallel Computers
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230. Pressure induced Structural Transformation in Gallium Arsenide: A Molecular-Dynamics Study
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232. Atomistic Aspects of Crack Propagation in Brittle Materials: Multimillion Atom Molecular Dynamics Simulations
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233. Scalability of a Low-cost Multi-Teraflop Linux Cluster for High-end Classical Atomistic and Quantum Mechanical Simulations
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235. Hybrid Quantum Mechanical/Molecular Dynamics Simulation on Parallel Computers: Density Functional Theory on Real-space Multigrids
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R. K. Kalia, A. Nakano, P. Vashishta, C. L. Rountree, L. Van Brutzel, and S. Ogata, International Journal of Fracture **121**, 71-79 (2003).

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P. S. Branicio, R. K. Kalia, A. Nakano, J. P. Rino, F. Shimojo, and P. Vashishta, Applied Physics Letters **82**, 1057-1059 (2003).

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A. Sharma, R. K. Kalia, A. Nakano, and P. Vashishta
IEEE Computing in Science and Engineering **5** (2), 26-33 (2003).

240. Multimillion Atom Molecular Dynamics Simulations of Nanoparticles on Parallel Computers
P. Vashishta, R. K. Kalia, and A. Nakano, Journal of Nanoparticle Research **5**, 119-135 (2003).

241. Molecular Dynamics Study of Structural, Mechanical, and Vibrational Properties of Crystalline and Amorphous $Ga_{1-x}In_xAs$ alloy:

P. S. Branicio, J. P. Rino, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta, Journal of Applied Physics **94**, 3840-3848 (2003).

242. Immersive and Interactive Exploration of Billion-Atom Systems
A. Sharma, P. Miller, X. Liu, A. Nakano, R. K. Kalia, P. Vashishta, W. Zhao, T. J. Campbell, and A. Haas, Presence: Teleoperators and Virtual Environments **12**, 85-95 (2003).

243. Scalable and Portable Implementation of the Fast Multipole Method on Parallel Computers
S. Ogata, T. J. Campbell, R. K. Kalia, A. Nakano, P. Vashishta, and S. Vemparala, Computer Physics Communications **153**, 445-461 (2003).

244. New Mechanisms for Wurtzite-to-Rocksalt Structural Transformation in Cadmium Selenide Under Pressure
F. Shimojo, S. Kodiyalam, I. Ebbsjö, R. K. Kalia, A. Nakano, and P. Vashishta, Physical Review Letters, submitted.

245. A Scalable Parallel Molecular Dynamics Algorithm for Large-scale Macromolecular Simulations
S. Vemparala, R. K. Kalia, B. Karki, A. Nakano, and P. Vashishta, Parallel Computing, submitted.

246. Million Atom Walkthrough: Octree-based Fast Visibility Culling and Multiresolution Rendering for Scalable Atomistic Visualization

A. Sharma, P. Miller, X. Liu, A. Nakano, R. K. Kalia, P. Vashishta, T. J. Campbell, and A. Haas, Computing and Visualization in Science, submitted.

247. Multiple Grains in Nanocrystals: Effect of Initial Shape and Size on Transformed Structures Under Pressure
S. Kodiyalam, R. K. Kalia, A. Nakano, and P. Vashishta, Physical Review Letters, submitted.

248. Orientation-dependent Brittle Fracture Dynamics in Crystalline GaAs: A Molecular Dynamics Study
H. Kikuchi, S. Kodiyalam, A. Nakano, R. K. Kalia, and P. Vashishta, Applied Physics Letters, submitted.

249. Brittle Dynamic Fracture of Crystalline 3C-SiC via Molecular Dynamics Simulation
H. Kikuchi, S. Kodiyalam, A. Nakano, R. K. Kalia, and P. Vashishta, Journal of the American Ceramics Society, submitted.

250. Hypervelocity Impact on Diamond: Collision-to-Evaporation Crossover and Diamond-to-Graphite Transformation
A. Omeltchenko, R. K. Kalia, A. Nakano, and P. Vashishta, Physical Review Letters, submitted.

251. InAs/GaAs Square Nanomesas: Multimillion-atom Molecular Dynamics Simulations on Parallel Computers
X. Su, R. K. Kalia, A. Nakano, P. Vashishta, and A. Madhukar, Journal of Applied Physics, submitted

252. Electric Field Induced Switching of Poly (ethylene glycol) (PEG) Terminated Self-Assembled Monolayers: A Parallel Molecular Dynamics Simulation
S. Vemparala, R. K. Kalia, A. Nakano, and P. Vashishta, Journal of Chemical Physics, submitted.

253. Large-scale Molecular Dynamics Simulations of Alkanethiol Self-Assembled Monolayer
S. Vemparala, B. B. Karki, R. K. Kalia, A. Nakano, and P. Vashishta, Journal of Chemical Physics, submitted.

254. Oxidation Dynamics of Aluminum (111) Surface
G. Aral, S. Ogata, T. J. Campbell, R. K. Kalia, A. Nakano, and P. Vashishta, Journal of Chemical Physics, submitted

255. Reactive Wetting of Al/α-Al_2O_3 Systems: A Parallel Molecular Dynamics Simulation Study

G. Aral, R. K. Kalia, A. Nakano, and P. Vashishta, Journal of Applied Physics, submitted.

256. Environmental Effects of H_2O on Fracture Initiation in Silicon: A Hybrid Electronic-Density-Functional/Molecular-Dynamics Study
S. Ogata, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta, Journal of Applied Physics, submitted.

257. Nanoindentation-Induced Amorphization in Silicon Carbide
I. Szlufarska, R. Kalia, A. Nakano, and P. Vashishta, Physical Review Letters, submitted.

INVITED TALKS

- Melting of a Two-Dimensional Electron Solid
Annual Meeting of the American Physical Society, Phoenix, AZ, March 1981.
- Molecular Dynamics Study of 2D Melting: Long Range Potentials
NATO Advanced Study Institute on Nonlinear Phenomena at Phase Transitions and Instabilities, Geilo, Norway, March 29-April 9, 1981.
- Melting and Nucleation of a Two-Dimensional Coulomb Solid
International Conference on Physics of Intercalation Compounds, I.C.T.P. Trieste, Italy, July 6-10, 1981.
- Melting and Freezing in Two Dimensions: A Molecular Dynamics Study
9th Midwest Solid State Theory Symposium, Argonne National Laboratory, Argonne, IL. Nov. 2-3, 1981.
- Electrons on Smooth and Corrugated Surfaces
10th Midwest Solid State Theory Symposium, Michigan State University, East Lansing, MI, Oct. 8-9, 1982.
- Microscopic Structure of Electron Glass in Two Dimensions
12th Midwest Solid State Theory Symposium, University of Minnesota, October 1984.
- Fractal Dimensions of Brown Trails and Isosets in Superionic and Molten Ag_2I
Electrochemical Society Meeting, Las Vegas, NV, October 14-18, 1985.
- Monte Carlo and Molecular Dynamics Simulations of Condensed Matter Systems
Workshop on the Electronic Structure of Defects, Argonne National Laboratory, Argonne, IL, June 2-13, 1986.
- Random Resistance Fluctuations in 1D MOSFETs
Summer Institute in Theoretical Physics, Workshop on the Physics of Artificially Structured Materials, Queen's University, Canada, July 1986.
- Molecular Dynamics Simulations of Classical and Quantum Systems
Universidade de São Paulo, São Carlos, Brazil, September 1986.
- Computer Simulations in Condensed Matter Physics
Universidade Federal de Ceara, Forta Leza, Brazil, September 1986.
- Computer Experiments on Classical Systems
Fundacao Universidade de Amazonas, Manaus, Brazil, September 1986.
- Conductance Fluctuations in 1D MOSFETs
Universidade Federal de São Carlos, São Carlos, Brazil, October 1986.

- Simulated Annealing Approach to Density Functional and Other Optimization Problems in Condensed Matter
  Canadian Association of Physicists Congress, June 15-17, 1987.
- Nature of Gigantic Resistance Fluctuations in 1D MOSFETs
  11th Int. Workshop on Condensed Matter Theory, Oulu, Finland, July 27-August 1, 1987.
- Computer Simulation of Classical and Quantum Systems
  Int. Adv. School on Statistical Physics, Chandigarh, India, Sept. 28-Oct. 9, 1987.
- Structural Correlations and Phonon Density of States in a-$GeSe_2$
  IFF in Kernforschungsanlage, Jülich, West Germany, Nov. 1987.
- Computer Simulation of Systems with Long-Range Interactions
  CECAM Workshop in Paris, France, January 11-22, 1988.
- Electron Bubbles in Helium Gas - A Quantum Molecular Dynamics Simulation
  XII Int. Workshop on Condensed Matter Theories, Taxco, Mexico, August 14-20, 1988.
- Quantum Molecular Dynamics Simulations
  CECAM Meeting on Computational Problems of Glasses and Networks, Amersfoort, The Netherlands, Sept. 10-14, 1988.
- Quantum Molecular Dynamics Simulation of Electron Self-Trapping in Helium
  "Many-Body Encounter in Minnesota," University of Minnesota, Minneapolis, May 12-13, 1989.
- Quantum Molecular Dynamics Simulation of Electron Mobility in a Dense Helium Gas
  International Workshop on Condensed Matter Theories," Campos dõ Jordão, Brazil, August 7-12, 1989.
- Simulation of Electron Transport in Disordered Systems Using Quantum Molecular Dynamics Technique
  XXIV Yamada Conference on "Strongly Coupled Plasma Physics," Lake Yamanaka, Japan, August 29-September 2, 1989.
- Behavior of Excess Electrons in Disordered Media Using Quantum Molecular Dynamics Simulation
  17th Midwest Solid State Theory Symposium, Indiana University, Bloomington, IN, October 9-10, 1989.
- Electron Transport in Disordered Systems - A Quantum Molecular Dynamics Simulation
  Annual Meeting of the American Physical Society, Anaheim, CA, March 12-16, 1990.
- Electron Transport in Amorphous Materials - A Quantum Molecular Dynamics Study
  Fortieth Annual American Crystallographic Association Meeting, New Orleans, LA, April 8-13, 1990.
- Materials Simulations using Quantum Molecular Dynamics Technique
  University of Tokyo, June 21, 1991.
- Simulation of Mixed Classical-Quantum Systems
  NEC Corporation, Tsukuba, Japan, July 19, 1991.

- Quantum Molecular Dynamics Simulation of Electron Transport in Devices
  Okayama University, Japan, July 30, 1991.
- Simulation of Classical and Quantum Systems
  Niigata University, Japan, August 1, 1991.
- Materials Simulations using Quantum Molecular Dynamics Technique
  Tohoku University, Japan, August 20, 1991.
- Multiple-time-step Molecular Dynamics Simulations on Distributed Memory MIMD Machines
  XIth Parallel Circus, Minnesota Supercomputer Institute, Minneapolis, MN, April 24-25,1992.
- Concurrent Classical and Quantum Simulations
  AFOSR Workshop on Parallel Computing in Chemistry, Washington, DC, October 25-29, 1992.
- Molecular Dynamics Simulations on Parallel Architectures
  XII SLAFES, Pichidangui, Chile, November 22-28, 1992.
- Atomistic Simulations on Parallel Architectures
  Sanibel Symposia, St. Augustine, FL, March 13-20, 1993.
- Atomistic Simulations of Condensed Phase Materials on Parallel Architectures
  High Energy Density Matter Conference, Woods Hole, MA. June 6-8, 1993.
- Structural Transformations in Glasses
  University of Amsterdam, The Netherlands, July 16, 1993.
- Large-Scale Materials Simulations on Parallel Architectures
  Symposium at Brown University, Providence, RI, September 3-4, 1993.
- Probing Amorphous Materials with Computer Experiments on Parallel Architectures
  Battelle Pacific Northwest Laboratory, Richmond, WA, November 9, 1993.
- Computer Simulation of Porous Glasses on Parallel Architectures
  1994 Simulation Multiconference, San Diego, CA, April 10-15, 1994.
- Morphology of Pores and Fracture Surfaces in Porous Silica - Multimillion Particle Molecular-Dynamics Simulations
  XVIII Int. Workshop on Condensed Matter Theories, Valencia, Spain, June 6-10, 1994.
- Massively Parallel Simulations of Nanostructured Materials
  Texas A&M University, College Station, TX.
- Multiresolution Molecular Dynamics Simulations of Real Materials Using Parallel Architectures
  Livermore National Laboratory, CA.
- Fracture and Sintering of Ceramic Materials by Parallel Molecular Dynamics
  High Performance Computational Chemistry Workshop, Pleasanton, CA.
- Large Scale Molecular Dynamics Simulation of High Temperature Ceramics
  XIX International Workshop on Condensed Matter Theories, Caracas, Venezuela.
- Studies of Nanoclusters and Amorphous Materials by Parallel Molecular Dynamics Simulations
  Annual Meeting of the American Ceramic Society, Cincinnati, OH.
- Multimillion Atom Molecular Dynamics Experiments on Parallel Architectures

1995 Simulation Multiconference, The Society of Computer Simulation, Phoenix, AZ.

- Parallel Molecular-Dynamics Simulation of Amorphous Materials
  8th Annual Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, Univ. of Georgia, Athens, GA.
- Multimillion Particle Molecular-Dynamics Simulations for Amorphous Materials on Parallel Architectures
  Los Alamos National Laboratory, Los Alamos, NM.
- Structure, Fracture and Sintering of Silicon Nitride by Parallel Molecular Dynamics
  AFOSR Contractors' Conference, Washington, DC.
- Dynamics of Fracture in Nanophase Silicon Nitride: Million Atom Molecular-Dynamics Simulations on Parallel Machines
  AFOSR Meeting in Boulder, CO.
- Structure, Mechanical Properties, and Fracture in Nanophase Silicon Nitride: Million Atom Molecular Dynamics Simulations on Parallel Computers
  TMS Meeting, Orlando, FL.
- Morphology of Pores and Interfaces and Dynamic Fracture in Nanophase Silicon Nitride
  IMRC Meeting in Cancun, Mexico.
- Molecular-Dynamics Simulations of Nanostructured Materials
  Inelastic Nuclear Resonant Scattering Workshop, Argonne, IL.
- Massively Parallel Atomistic Simulations of Dynamic Fracture in Nanophase Materials
  Niigata Univ., Japan.
- Multimillion Atom Molecular Dynamics Simulations of Nanophase Materials on Massively Parallel Computers
  Niigata Univ., Japan.
- Multimillion Atom Molecular Dynamics Simulations of Nanophase Materials on Massively Parallel Computers
  Institute for Solid State Physics, Univ. of Tokyo.
- MD Simulation of Fracture
  Gordon Research Conference, La Barga, Italy.
- Dynamic Fracture in Nanophase Ceramics: Multimillion Atom Molecular Dynamics Simulations on Parallel Computers
  Saclay, France.
- Large Scale Simulations of High Temperature Structural Materials on Massively Parallel Computers
  DoD Challenge Meeting, Houston, TX.
- Crack Propagation and Fracture in Nanostructured Ceramics: Multimillion Atom Parallel Molecular Dynamics Simulations
  WCTCC 98, Pacific National Northwest Laboratory, Richmond, WA, June 21-23, 1998.
- Multimillion Atom Molecular Dynamics Simulations of High Temperature Ceramics

International Conference on "New Developments in High Temperature Ceramics," Istanbul, Turkey.

- Structure and Dynamic Fracture in Nanophase Silicon Nitride and Silicon Carbide: Multimillion Atom Molecular Dynamics Simulations on Massively Parallel ComputersWorkshop on "*Advanced Materials for Extreme Environments: New Experimental Opportunities in Neutron Scattering*," Argonne National Laboratory, Illinois, September 11-12, 1998.
- Grand Challenge Materials Simulations: Multimillion Atom Molecular Dynamics Simulations on Parallel Computers, SSI Collaboration Meeting, Jefferson Laboratory, Newport News, Virginia, January 20-22, 1999.
- Massively Parallel Atomistic Simulations of Nanostructured Materials, Physics Department Colloquium, Auburn University, Auburn, Alabama, February 24-25, 1999.
- Designing Novel Materials on Parallel Computers, Links for Success, The 1999 Annual Board of Regents Louisiana NSF EPSCoR Conference, Pennington Biomedical Research Conference Center, Baton Rouge, Louisiana, April 13-14, 1999.
- Computational Assisted Development of High Temperature Structural Materials, Ninth Annual DoD High Performance Computing Modernization Program Users Group Conference, Monterey, California, June 7-10, 1999.
- Multimillion Atom Molecular Dynamics Simulations of Nanostructured Materials on Parallel Machines, ACS Annual Meeting in New Orleans, August 22-26, 1999.
- Multimillion Atom Molecular Dynamics Simulations of Nanostructured Materials on Parallel Machines, International Materials Research Congress, Symposium: Theory and Computer Simulation of Materials, Cancun, Mexico, August 29 - September 2, 1999.
- Massively Parallel Materials Simulations, Colloquium in the Department of Chemical Engineering, Univ. of Cincinnati, October 21, 1999.
- Multiscale Simulations of Nanostructred Materials on Massively Parallel Compters
  CERCA, Montreal, Canada, December 8, 1999.
- Multiscale Simulations of Nanostructred Materials on Massively Parallel Compters
  Steacie Institure for Molecular Sciences, National Research, Council of Canada, Ottowa, Canada, December 10, 1999.
- Parallel Multiscale Simulations of Nanostructured Materials
  CSW 2000 EPOCHAL TSUKUBA International Congress Center, March 13-15, 2000.
- Information Technology and the Dual-Degree Program
  Amercian Physical Society, Minneapolis, Minnesota, March 20, 2000.
- Parallel Multiscale Simulations of Nanostructured Materials
  Iowa State University and Ames Research Laboratory, Ames, Iowa, April 3, 2000.
- Multiscale Simulations of Oxidation and Fracture in Nanostructured Solids
  HPaC Seminar, TU Delft, The Netherlands, April 14, 2000.
- Parallel Multiscale Simulations of Nanostructured Materials

MD Meeting, University of Illinois at Urbana, April 16-17, 2000.

- Massively Parallel Multiscale Simulations of Nanostructured Materials
  Intel Corporation, May 1, 2000.
- Massively Parallel Multiscale Simulations of Nanostructured Ceramics
  American Ceramic Society Symposium on Advances in Theory, Modeling, and Simulations of Materials, St. Louis, Missouri, May 3, 2000.
- Computer Simulations of Ceramic Interfaces
  AFOSR Contractors' Meeting in Ceramic Materials and Composites, St. Louis, Missouri, May 5, 2000.
- Computational Assisted Development of High Temperature Structural Materials
  DoD Challenge User's Group Meeting, Albuquerque, New Mexico, June 8, 2000.
- Parallel Molecular Dynamics Simulations of Nanostructured Materials
  Corsica Meeting on Fracture, June 6-17, 2000.
- Parallel Molecular Dynamics Simulations of Nanostructured Materials
  Canadian Computational Chemistry Meeting, Bishop University, Lennoxville, Quebec, Canada, July 31 - August 3, 2000.
- Simulations of Nanostructured Materials
  TU Delft, The Netherlands, September 25, 2000.
- Multiscale Materials Simulations: Importance of Neutron Scattering
  Argonne National Laboratory, November 20, 2000.
- Multiscale Materials Simulations
  National Research Council, Ottawa, Canada, November 23, 2000.
- Multiscale Simulations of Nanostructured Solids on Massively Parallel Computers
  International Conference on Science & Technology of Nanostructured Materials, Puri, India, January 4-8, 2001.
- Massively Parallel, Multiscale Simulations of Interfacial Materials
  Saclay, France, March 29, 2001.
- Massively Parallel Multiscale Simulations
  DoD Computational Materials Science Workshop, St. Louis, MO, April 24-25, 2001.
- Hybrid Atomistic-Continuum Simulations of Nanopixels
  DoD Users Group Conference, Biloxi, MI, June 18-22, 2001.
- Intercontinental Computational Physics Course
  Niigata University, Japan, June 25, 2001.
- Massively Parallel Simulations of Nanosystems Under Extreme Conditions
  Mission Computing Conference, Washington DC, February 4, 2002.

- Multiscale Simulations of Nanosystems
  IPNS Nanocomposite Workshop, Argonne National Lab, Chicago, IL, March 28, 2002.
- Mulstiscale Simulations of Nanosystems
  Oak Ridge National Lab, TN, April 18, 2002.
- Multiscale Fracture and Nanoindentation Simulations and Visualization

DoD High-Performance Computing Users Group Conference, Austin, TX, June 12, 2002.

- Mulstiscale Simulation of Atomistic Processes in Nanostructured Materials
  NSF Workshop, University of Illinois at Urbana-Champaign ,June 10, 2002.
- Massively Parallel, Multiscale Simulations of Nanostructured Materials
  CIMTEC 2002, Florence, Italy, July 11, 2002.
- Multiscale Algorithms and Simulations of Nanoceramics and Nanocomposites
  Multi-algorithm Methods for Multiscale Simulations Conference, January 14-16, 2004, Livermore, CA.
- Multiscale Algorithms and Simulations of Nanosystems
  Joint Physics and Computer Science Colloquium, Florida State University, November 10, 2003.
- Multimillion Atom Simulations of Nanoscale Dynamics and Fracture
  CECAM workshop, Lyon, France, October 13-15, 2003.
- Multiscale Material Simulation Challenges on a Grid
  APS March Meeting, Montreal, Canada, March 2005.