Dr. Donald W. Brenner
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Education

- Ph.D. in Chemistry, Pennsylvania State University, 1987
- B.S. in Chemistry, State University of New York, 1982

Professional Experience

- Associate Department Head, Dept. of Materials Science and Engineering, NC State University, 2009-present
- Kobe Steel Distinguished Professor, Dept. of Materials Science and Engineering, NC State University, 2008-present
- Professor, Dept. of Materials Science and Engineering, NC State University, 2003-present.
- Associate Faculty Member, Department of Chemistry, NC State University, 1996-present.
- Associate Professor, Department of Materials Science and Engineering, NC State University, 1994-2003.
- Research Chemist, Theoretical Chemistry Section, Naval Research Laboratory, Washington, DC, 1987-1994.

Honors and Awards

- Alexander Quarles Holladay Medal for Excellence, 2016. This is the highest honor given by NC State University to one of its faculty.
- Alcoa Foundation Distinguished Engineering Achievement Award, 2013.
- Best Poster, Fall 2011 MRS Meeting “First Principles Studies of Oxygen Transfer at Buried Metal/Metal-Oxide Interfaces: Implications for the Performance of Energetic Nanolaminates”, presented in the symposium *Advances in Energetic Materials Research.*
- Co-author, paper included in the “*Modelling and Simulation in Materials Science and Engineering* Highlights of 2010”.
- Reynolds Award for Excellence in Research, Teaching and Outreach, NC State College of Engineering, 2009.
- Best Poster, Fall MRS meeting, Symposium “Multi-Physics Modeling in Materials Design”, 2009
- NSMMS Outstanding Poster (1st Prize), Operating in Space Session, 2005.
- Feynman Award for Research in Nanotechnology (theory), 2002.
- Co-author, 1st Prize for Technical Publication from the Institute for Metals Superplasticity Problems, Russian Academy of Science, Ufa, Russia (paper co-authored with A. Nazarov) 2001.
- Alcoa Foundation Engineering Research Achievement Award, 2000.
- Co-author, Veridian Medal Paper, 1999.
- NC State College of Engineering Outstanding Teacher Award, 1999.
- Inducted into the North Carolina State University Academy of Outstanding Teachers, 1999.
- Co-author, 2nd Prize for Technical Publication from the Institute for Metals Superplasticity Problems, Russian Academy of Science, Ufa, Russian (paper co-authored with A. Nazarov) 1999.
- NSF Faculty Early Career Development Award, 1995.

- Naval Research Laboratory Chemistry Division Young Investigator, 1991.
- Naval Research Laboratory Chemistry Division Berman Award for Outstanding Technical Publication, 1990.
- Xerox Award in Materials Science (Best Thesis), Penn. State, 1987.
- American Vacuum Society Student Award, 1986.
- Sam Molnar Award, SUNY Athletic Conference Outstanding Senior Scholar Athlete, 1982.
- NCAA Div. III Cross Country All-American, 1980.

Consulting Activities

- Comalco Aluminum Limited, North Carolina. Industrial Al/Na processing (1995).
- Monterey Technologies, Cary, NC. Virtual reality for military training (1996).
- Nanotechnology Partners, L.P. Member Scientific Advisory Board (2001-2011).
- Apex Nanotechnologies, Member Scientific Advisory Board (2002-2008).
- Junius Tech. Consultant on molecular modeling in Nanotechnology (2002-2004).
- Member, Editorial Board, *Molecular Simulation* (2002-2008).
- Member, Editorial Board, *Journal of Computational and Theoretical Nanoscience*, (2003-present).
- Consultant, International Technology Research Institute (2003).
- Member, Panel of Technology Experts, Nalysts, LLC. (2004-2009).
- Consultant, Army Research Office (2007).
- Consultant, WTEC on Nano-Modular Systems (2014).

Research Program: Computational Materials Science and Engineering

- Atomistic simulation of reactive chemical dynamics in condensed phases.
- Development & application of multiscale modeling, many-body potentials & tight-binding models.
- Use of first principles total energy methods for materials design.

Other Professional Activities

- Member review panel, Institute for NEXT Generation IT Systems, 2016.
- Member NSF International Study Group, Assessment of Nano-modular Systems, 2014-2015;
- Member Mid-Term Review Team, Energy Frontier Research Centers, 2012 (2 centers), 2016 (3 centers).
- Academic Lead Organizer, 2014 NSF Nanoscale Science and Engineering Grantees Conference, December 9 and 10, 2014, Washington, DC.
- Invited Tutorial, 'Atomic Modeling and the Computational Design of New Materials, Surface and Interfaces', AVS 61st International Symposium and Exhibition, Baltimore, MD, Nov. 14, 2014
- Co-Organizer, Symposium "Multi-scale Modeling of Materials Behavior in Extreme Environments", 12th U.S. National Congress on Computational Mechanics, Raleigh, NC July, 2013.
- Co-Organizer, Symposium "Multi-scale Thermo-Mechanical Response of Molecular Solids: Theory, Simulation, Modeling, and Experiments", 12th U.S. National Congress on Computational Mechanics, Raleigh, NC July, 2013.
- Invited Lecturer, CAMS NSF Summer School "Simulation of Complex Microstructure in Materials", May 19-24, 2013.
- Member local organizing committee for 12th U.S. National Congress on Computational Mechanics, Raleigh, NC July, 2013.

- Organizer, “Workshop on Meeting Grand Challenges in Computational Materials Design”, North Carolina State University, Raleigh, NC January 15 and 16, 2013.
- Member, Advisory Board for the “Cyberinfrastructure for Atomistic Materials Science”, 2012-present.
- Member International Scientific Committee, 12th U.S. National Congress on Computational Mechanics.
- Organizer, Symposium “Innovations in Molecular Modeling: New Tools and Applications”, Southeastern Regional Meeting of the American Chemical Society, Raleigh, NC, Nov. 14-17, 2012.
- Invited Tutorial, “Structure, Characterization and Modeling of Domain Interfaces and Grain Boundaries in Materials: Atomic Scale Computation and Theory”, Fall National Meeting of the Materials Research Society, Boston, MA November 25, 2012.
- Guest co-editor, Materials Research Society Bulletin “Three Decades of Many-Body Potentials”, May 2012.
- Co-organizer, Symposium “Theory and Modeling of the Individual and Collective Properties of Nanoparticles”, 241st American Chemical Society National Meeting, March 27-31, 2011.
- Section Editor for *Molecular Modeling and Its Role in Advancing Nanotechnology*, Springer Encyclopedia of Nanotechnology, 2011
- Panel Moderator, “Reaching Our Societal Goals with CI”, Cyber Infrastructure Days, NC State, Sept. 8, 2010
- Member Scientific Advisory Committee, Center for Nanoscale Materials, Argonne National Lab, 2010-present
- Member Proposal Review Panel, Center for Nanophase Materials Sciences, Oak Ridge National Lab, 2010-present.
- Plenary Lecturer, Computational Engineering and Science/HPC: Enabling New Discoveries, Lehigh University, Oct. 5,6, 2009
- Member NC State College of Engineering Research Committee, 2009-2014 (Chair 2010-2012).
- Member NC State University Research Committee, 2009-2014 (Chair 2011-2012).
- Member *Army Chemistry Coordinating Group on Energetic Materials*, Army Research Lab, March 26, 2008
- Co-organizer, Symposium “Modeling of Covalent Bonding Interactions”, Southeastern Regional Meeting of the American Chemical Society, Greenville, SC, Oct. 24 and 25, 2007.
- Member workshop program committee, IEEE/ACM HPCNano06, 2006.
- Member Argonne National Laboratory *Center for Nanoscale Materials* Proposal Evaluation Board, 2006-present.
- Co-organizer for the focus session “Theory of Nanotubes and Carbon Based Nanostructures”, March Meeting of the American Physical Society, 2004.
- Member, Nanoscale Technologies Focus Group of the *Research Triangle Regional Partnership for Economic Development*, 2003.
- Presenter for Tutorial “Nanotechnology and Multifunctional Materials: Bio/Nano Structures, Multiscale Designs and Multiphysics”, Annual Conference of Society for Experimental Mechanics, Charlotte, SC, May 31, 2003
- Keynote Speaker, Army Symposium on Solid Mechanics, Charleston, SC, May 6, 2003.
- Chair, 9th Foresight Conference on Molecular Nanotechnology, Santa Clara, CA, Nov. 10-12, 2001.
- Presented Layperson Overview “Nanotechnology: Fact and Fiction", Duke Institute for Learning in Retirement, Durham, NC, November 7, 2000.
- Invited Presenter, NSF Workshop on Materials Theory (WOMT2000), Washington, DC, Oct. 4-6, 2000

- Co-chair, 8th Foresight Conference on Molecular Nanotechnology, Bethesda, MD, Nov. 5-8, 2000
- Presented invited tutorial `Analytic Potentials and Molecular Dynamics Simulation' as part of the 'Tutorial on Critical Enabling Technologies for Nanotechnology', 5th (1997), 6th (1998) and 7th (1999) Foresight Conferences on Molecular Nanotechnology.
- Chair of 'Tutorial on Foundations of Nanotechnology', 7th Foresight Conference on Molecular Nanotechnology, October 14, 1999.
- Member program committee for `5th Foresight Conference on Molecular Nanotechnology', Nov. 5-8, 1997.
- Member organizing committee for 9th International Congress of Quantum Theory Satellite Symposium `Quantum Theory and Simulation of Bulk, Surface, and Interface Phenomena', NC State University, Raleigh, NC, June 9-14, 1997.
- Convener for session 'Surface Science' at the `First Electronic Molecular Graphics and Modeling Society Conference'. Held on the internet Oct. 7-18, 1996
- Member expert panel on future of nanotechnology for *Wired Magazine, Reality Check Feature,* August, 1995.
- Organizer and chair for session `Properties and Engineering of Novel Interfaces: Theory and Simulation', 1995 March Meeting of the American Physical Society.
- Developed web-base tutorial entitled "Molecular Dynamics and Nanotechnology", 1995.
- Reviewer for Nature, Science, Computer Simulations in Engineering and Science, Computational Materials Science, Applied Mechanics Reviews, J. Am. Chem. Soc., Phys. Rev. Lett., Phys. Rev. B, Nanotechnology, Diamond and Related Materials, J. Phys. Chem., Surface Science, Journal of Nanoscience and Nanotechnology, Langmuir.
- Proposal reviewer for The National Science Foundation, Army Research Office, Air Force Office of Scientific Research, Research Corporation, Department of Energy, Livermore National Laboratory, Arkansas Science and Technology Authority, American Chemical Society Petroleum Research Fund, Science Foundation of Ireland.

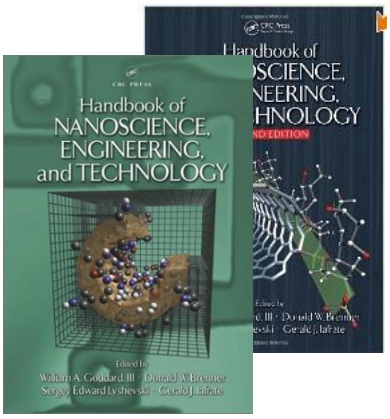
Courses Taught

- Computer Applications in Materials Science and Engineering
- Mathematical Methods for Materials Engineers.
- Introduction to Engineering Materials
- Structure of Materials at the Nanoscale
- Materials Engineering Special Projects
- Computer Simulations in Materials Science (Graduate Course)
- Modeling from the Nanoscale to the Macroscale (Team-Taught Graduate Course)
- Nanoscale Simulation and Modeling (Team-Taught Graduate Course)

Summary of Publication Record

- Total Refereed Publications: 251
- Invited Review Articles and Book Chapters: 32; Books Edited: 1 (3 editions)
- No. Citations/h-index(through 12/28/16): 11,842/41 (web of science), 19,052/49 (Google scholar)

Complete List of Professor Brenner's Publications by Topic Area



Books Edited

"Handbook of Nanoscience, Engineering and Technology", W. Goddard, D. Brenner, S. Lyshevski and G. Iafrate, Eds., CRC Press, October 2002.

"Handbook of Nanoscience, Engineering and Technology, 2nd edition", W. Goddard, D. Brenner, S. Lyshevski and G. Iafrate, Eds., CRC Press, May 2007.

"Handbook of Nanoscience, Engineering and Technology, 3rd edition", W. Goddard, D. Brenner, S. Lyshevski and G. Iafrate, Eds., CRC Press, 2012.

Invited Book Chapters and Review Articles

1. D.W. Brenner and B.J. Garrison, `Mechanisms of Organic Molecule Ejection in SIMS and FABMS', *Springer Series in Chemical Physics* (Springer-Verlag, Berlin) **44**, 462 (1986).

2. D.W. Brenner and B.J. Garrison, `Gas-Surface Reactions: Molecular Dynamics Simulations of Real Systems', *Adv. Chem. Phys*, (Wiley, New York) **76**, 281 (1989).

3. D.W. Brenner, `Molecular Potentials for Simulating Shock-Induced Chemistry', in *Shock Compression of Condensed Matter*, S.C. Schmidt, R.D. Dick, J.W. Forbes and D.G. Tasker, Eds. (North-Holland, Amsterdam), pg. 115 (1992).

4. D.W. Brenner and J.A. Harrison, `Atomistic Simulations of Diamond Films', *Ceramic Bulletin* **71**, 1821 (1992).

5. J.A. Harrison, C.T. White, R.J. Colton and D.W. Brenner, `Atomistic Simulations of Friction at Sliding Diamond Interfaces', *Materials Research Society Bulletin* **18**, 50 (1993).

6. C.T. White, J.W. Mintmire, R.C. Mowrey, D.W. Brenner, D.H. Robertson, J.A. Harrison and B.I. Dunlap, `Predicting Properties of Fullerenes and their Derivatives', in *Buckminsterfullerene*, W.E. Billups and M. Ciufolini, Eds. (VCH Publishers, 1993) pg. 125.

7. J.A. Harrison and D.W. Brenner, `Atomic-Scale Simulation of Tribological and Related Phenomena', Chapter 10 in the *CRC Handbook of Micro/Nanotribology*, Bushan, ed. (CRC Publishers, 1995).

8. D.H. Robertson, D.W. Brenner and C.T. White, `Molecular Dynamics Analysis of Shock Phenomena', in *High-Pressure Shock Compression of Solids-III*, Davison & M. Shahinpoor, Eds. (Springer-Verlag, 1998).

9. D.W. Brenner, `Chemical Dynamics and Bond-Order Potentials', *Materials Research Society Bulletin* **21**, 36 (1996).

10. D.W. Brenner, O.A. Shenderova and D.A. Areshkin, `Quantum-Based Analytic Interatomic Forces and Materials Simulation', *Reviews in Computational Chemistry*, K.B. Lipkowitz and D.B. Boyd, Eds., (VCH Publishers, New York, 1998), pp 213-245.

11. J.A. Harrison, S.J. Stuart and D.W. Brenner, `Atomic-Scale Simulation of Tribological and Related Phenomena', Chapter 10 in the *CRC Handbook of Micro/Nanotribology, Second Edition*, Bushan, ed. (CRC Publishers, 1998), pp. 525-596.

12. S.B.Sinnott, L.Qi, O.A.Shenderova and D.W. Brenner, 'Modeling Condensed-Phase Chemistry with Analytic Potentials: Application to Hydrocarbon Cluster Dynamics', Chapter 1 in *Molecular Dynamics of Clusters, Surfaces, Liquids and Interfaces*, Volume IV of *Advances in Classical Trajectory Methods',* W.L. Hase, ed. (JAI Press, Inc, Stamford Ct, 1999), pp.1-26.

13. D.W. Brenner, 'The Art and Science of an Analytic Potential', *Physica Status Solidi* B **217**, 23 (2000).

14. J. Bernholc, D. Brenner, M. Buongiorno Nardelli, V. Meunier and C. Roland, 'Mechanical and Electrical Properties of Nanotubes', *Annual Review of Materials Research* **32**, 347 (2002).

15. D.W. Brenner, 'Mysteries of Friction and Wear Unfolding: Computational Materials Science Advances the Field of Tribology', *Advanced Materials and Processes Technology Information Analysis Center Newsletter (Feature Article)* **5** (3), 1 (2001).

16. D.W. Brenner, O.A. Shenderova, D.A. Areshkin, J.D. Schall, 'Atomic Modeling of Carbon-Based Nanostructures as a Tool for Developing New Materials and Technologies', *Computer Modeling in Engineering and Sciences* **3**, 643 (2002).

17. D.W. Brenner, O.A. Shenderova, J. D. Schall, D.A. Areshkin, S. Adiga, J.A. Harrison and S.J. Stuart, 'Contributions of Molecular Modeling to Nanometer-Scale Science and Technology', Chapter 24 in the *Nanoscience, Engineering and Technology Handbook (*W. Goddard, D. Brenner, S. Lyshevski and G. Iafrate, Eds., CRC Press, Boca Raton, FL, 2002)

18. O.A. Shenderova, V. Zhirnov, and D.W. Brenner 'Carbon Materials and Nanostructures', *Critical Reviews in Solid State and Materials Sciences* **32**, 347 (2002).

19. B. Rice, T. Sewell, D. Brenner and B. Holian, 'Overview of Atomistic Molecular Simulation Methods', Chapter 2 in *ITRI Study of Molecular Dynamics Simulations of Detonation Phenomena*, (International Technology Research Institute, Inc, Laurel, MD, 2003).

20. D. Brenner, A. Redondo, B. Rice, T. Sewell, 'Interatomic Forces and Potential Energy Expressions, Chapter 3 in *ITRI Study of Molecular Dynamics Simulations of Detonation Phenomena*, (International Technology Research Institute, Inc, Laurel, MD, 2003).

21. T. Sewell, B. Rice and D. Brenner, 'Atomistic Molecular Simulation Results', Chapter 4 in *ITRI Study of Molecular Dynamics Simulations of Detonation Phenomena*, (International Technology Research Institute, Inc, Laurel, MD, 2003).

22. J.D. Schall, D.W. Brenner, A.D. Kelkar and R. Gupta, "Continuum and Atomistic Modeling of Thin Films Subjected to Nanoindentation" in Chapter 19 in the *Nanoengineering of Structural, Functional and Smart Materials* (CRC Press, Boca Raton, FL, 2005).

23. S.-J. Heo, S.B. Sinnott, D.W. Brenner and J.A. Harrison, "Computational Modeling of Nanometer-Scale Tribology", in *Introduction to Nanotribology and Nanomechanics,* Ed. B. Bhushan (Springer-Verlag, Heidelberg, Germany, 2005), p 623.

24. S.B. Sinnott, S.-J. Heo, D.W. Brenner and J.A. Harrison, "Computer Simulations of Nanometer-Scale Indentation and Friction" in *Springer Handbook of Nanotechnology, 2nd edition* (Springer-Verlag, Heidelberg, 2006), 1051.

25. D.W. Brenner, "Computer Modeling of Nanostructured Materials", Chapter 7 in *Nanostructured Materials*, 2nd Edition, Carl Koch, Ed., (Noyes Publications, Norwich, NY, 2006).

26. Y. Hu, O.A. Shenderova, Z. Hu, C.W. Padgett and D.W. Brenner, 'Carbon Nanostructures for Advanced Composites', *Reports on Progress In Physics* **69,** 1847-1895 (2006)

27. Y. Hu, O.A. Shenderova and D.W. Brenner, "Carbon Nanostructures: Morphologies and Properties", *J. Theoretical Comp. Nanoscience* **4**, 199 (2007).

28. Y. Hu, Z. Hu, C.W. Padgett, D.W. Brenner and O.A. Shenderova, "Carbon Nanostructures and Nanocomposites", *Nanoscience, Engineering and Technology Handbook, 2nd edition (*W. Goddard, D. Brenner, S. Lyshevski and G. Iafrate, Eds., CRC Press, Boca Raton, FL, 2007)

29. C.C. Koch and D.W. Brenner, "Bulk Nanostructured Materials", Chapter 22 in the *Nanoscience, Engineering and Technology Handbook, 3rd edition (*W. Goddard, D. Brenner, S. Lyshevski and G. Iafrate, Eds., CRC Press, Boca Raton, FL, 2012)

30. S.B. Sinnott and D.W. Brenner, "Three Decades of Many-Body Potentials in Materials Research", *MRS Bulletin* **37**, 469 (2012)

31. D.W. Brennner, "Challenges to Marrying Atomic and Continuum Modeling of Materials", Current Opinion in Solid State and Materials Science 17, 257-262. (2013)

32. S. Lu, D. Li and D.W. Brenner, "Molecular Dynamics Simulations of Plastic Damage in Metals", *Handbook of Damage Mechanics: Nano- to Macro- Scale for Materials and Structures*, Springer-Verlag, New York, pp. 453-486. (2015)

Other Refereed Publications (by subject area)

Diamond Deposition and Surface Structure

33. M. Page and D.W. Brenner, `Hydrogen Abstraction from a Diamond Surface. *ab initio* Quantum Chemical Study using Constrained Isobutane as a Model' *J. Am. Chem. Soc.*, **113** , 3270 (1991).

34. M. Page and D.W. Brenner, ` *ab initio* Quantum Chemical Study of Hydrogen Abstraction from Isobutane Constrained to Model a Diamond Surface', *New Diamond Science and Technology (Proceedings of the Second*

International Conference on New Diamond Science and Technology), R. Messier and J.T. Glass, Eds., MRS International Conference Proceedings Series (Materials Research Society, Pittsburgh) pg. 45 (1991).

35. J.W. Mintmire, D.W. Brenner, B.I. Dunlap, R.C. Mowrey and C.T. White, `First-Principles Simulations of Diamond Surface Formation via Radical Addition', *New Diamond Science and Technology (Proceedings of the Second International Conference on New Diamond Science and Technology)*, R. Messier and J.T. Glass, Eds., MRS International Conference Proceedings Series (Materials Research Society, Pittsburgh) pg. 57 (1991).

36. D.W. Brenner, B.I. Dunlap, J.W. Mintmire, R.C. Mowrey and C.T. White, `Molecular-Dynamics Simulations of the Reaction of Atomic Hydrogen with Diamond Surfaces', *New Diamond Science and Technology (Proceedings of the Second International Conference on New Diamond Science and Technology)*, R. Messier and J.T. Glass, Eds., MRS International Conference Proceedings Series (Materials Research Society, Pittsburgh) pg. 39 (1991).

37. B.J. Garrison, E.J. Dawnkaski, D. Srivastava and D.W. Brenner, `Molecular-Dynamics Simulations of Dimer Opening on a Diamond [001](2x1) Surface', *Science* **255** , 835 (1992).

38. D.W. Brenner, D.H. Robertson, R.J. Carty, D. Srivastava and B.J. Garrison, `Combining Molecular Dynamics and Monte Carlo Simulations to Model Chemical Vapor Deposition: Application to Diamond', *Mat. Res. Soc. Symp. Proc.* **278**, 255 (1992)

39. D.R. Alfonso, S.E. Ulloa, and D.W. Brenner, `Hydrocarbon Adsorption on a Diamond (100) Stepped Surface', *Phys. Rev B* **49** , 4948 (1994).

40. Y. Li, D. W. Brenner, X. Dong and C. Sun, 'First Principles Prediction of Gas-Phase Composition and Substrate Temperature for Diamond Film Growth', *Molecular Simulation* **25**, 41 (2000).

41. Y. Li, D.W. Brenner, X. Dong, and C. Sun, '*Ab Initio* Study of the Role of Entropy in the Kinetics of Acetylene Production in Filament-Assisted Diamond Growth Environments', J. Phys. Chem. **110**, 132 (2006).

Diamond Materials Properties and Multiscale Modeling

42. J. Yu, A. Omeltchenko, R.K. Kalia, P. Vashishta, and D.W. Brenner, `Large-Scale Molecular Dynamics Study of Amorphous Carbon and Graphite on Parallel Machines', *Mat. Res. Symp. Proc.* **408**, 113 (1996).

43. O. Shenderova and D.W. Brenner, `Coexistence of Two Carbon Phases at Grain Boundaries in Polycrystalline Diamond', *Mat. Res. Symp. Proc.* **442,** 693 (1997).

44. O. Shenderova, D.W. Brenner, A. Nazarov, A. Romanov, L. Yang, `Multiscale Modeling Approach for Calculating Grain Boundary Energies from First Principles', *Phys. Rev. B.* **57**, R3181(1998).

45. O. Shenderova, D.W. Brenner, L.H.Yang, A.Omeltchenko, A. Nazarov, `Atomistic Modeling of Polycrystalline Diamond', in Diamond Materials V, J.L. Davidson*, et al.,* editors, *Proceedings of the 192nd Meeting of the Electrochemical Society* **243** (1998).

46. O.A.Shenderova, D.W. Brenner, A. Omeltchenko, X. Su, L.H. Yang and A. Nazarov, `Multiscale Modeling of Polycrystalline Diamond', in *Proceedings of the Second International Conference on the Modeling and Simulation of Microsystems*, p. 61 (1999).

47. O.A. Shenderova, D.W. Brenner, A. Omeltchenko, X. Su and L.H. Yang, 'Atomistic Modeling of Grain Boundary Fracture in Diamond', *Mat. Res. Symp. Proc.* **539**, 319 (1998).

48. O.A. Shenderova, D.W. Brenner and L.H. Yang, 'Atomistic Simulations of Structures and Mechanical Properties of Polycrystalline Diamond: Symmetrical <001> Tilt Grain Boundaries'. *Phys. Rev. B* **62**, 3565(2000).

49. O.A. Shenderova and D.W. Brenner, 'Atomistic Simulations of Structures and Mechanical Properties of <011> Tilt Grain Boundaries and Their Triple Junctions in Diamond', *Phys. Rev. B* **60**, 7053(1999)

50. D.W. Brenner, Olga A. Shenderova, L.H. Lin, A.A. Nazarov, A.E.Romanov 'Multiscale Modeling Method for Predicting Mechanical Properties of Polycrystalline Covalent Ceramics from First Principles', in *Computer Aided Design of High Temperature Materials*, A.Pechenik, R.Kalia, P.Vashishta,ed. (Oxford University Press, New York, 1999) 461.

51. A. Omeltchenko, K. Tsuruta, A. Nakano, R. Kalia, P. Vashishta, O. A. Shenderova and D.W. Brenner, 'Dynamics Fracture in Nanophase Ceramics and Diamond Films: Multimillion Atom Parallel Molecular Dynamics Simulations', in *Computer Aided Design of High Temperature Materials*, A.Pechenik, R.Kalia, P.Vashishta,ed. (Oxford University Press, New York, 1999) 81.

52. O.A.Shenderova, D.W.Brenner, 'Predicted Electronic and Cleavage Properties of Diamond', in *Diamond Materials VI: Proceedings of the Sixth International Symposium*, J. C. Angus, W. D. Brown, and A. Gicquel, Ed. (1999).

53. O.A. Shenderova, D.W.Brenner, A.Omeltchenko, X.Su and L.H.Yang, 'Atomistic Modeling of Grain Boundary Fracture in Diamond', *Phys. Rev. B* **61**, 3877 (2000).

54. A Nazarov, O.A. Shenderova and D.W.Brenner, 'Elastic Models of <001> and <011> Tilt Grain Boundaries in Polycrystalline Diamond', *Phys. Rev. B*, **61**, 928 (2000).

55. A Nazarov, O.A. Shenderova, D.W.Brenner, 'On the Disclination-Structural Unit Model of Grain Boundaries', *Mat. Sci. Eng. A* **281***,* 148 (2000).

56. O.A.Shenderova, D.W.Brenner, A.Omeltchenko, X.Su, Lin H.Yang and A.Nazarov, 'Properties of Polycrystalline Diamond: Multiscale Modeling Approach', *Molecular Simulation* **24**, 197 (2000).

57. O.A.Shenderova and D.W.Brenner, 'Atomistic Simulation of Grain Boundaries, Triple Junctions and Related Disclinations', in *Local Lattice Rotations and Disclinations in Microstructures of Distorted Crystalline Materials*, edited by P. Klimanek, A.E. Romanov, B.M. Seefeldt, Solid State Phenom., Trans.Tech. Publ., Switzerland, 87, 318 (2002).

58. S.-H. Lee, T.-Y. Lee, S.-C. Lee, Y.-C. Chung, D.W. Brenner and K.-R. Lee, 'The Structure and Properties of ta-C Film with Dispersion of Incident Beam Energy', in Technical Proceedings of the 2005 NSTI Nanotechnology Conference, Vol. 2, Chapter 3, 218-221 (2005).

59. D.L. Irving, C. Padgett, Y. Guo, J. Mintmire and D. Brenner, "Multiscale Modeling of Metal-Metal Contact Dynamics under High Electromagnetic Stress: Timescales and Mechanisms for Joule Melting of Al-Cu Asperities". *IEEE Trans. Magnetics* **45**, 331 (2009).

60. S.P. Adiga, V.P. Adiga, R.W. Carpick and D.W. Brenner, "Vibrational Properties and Specific Heat of Ultracrystalline Diamond: Molecular Dynamics Simulations", *J. Phys. Chem*. C **115**, 21691 (2011).

61. S.P. Adiga, V.P. Adiga, R.W. Carpick and D.W. Brenner, "The Vibrational Properties of Ultracrystalline Diamond based on Molecular Dynamics Simulations", MRS Symposium Proceedings (2012).

62. Brenner, D.W. and Shenderova, O.A., "Theory and modelling of diamond fracture from an atomic perspective", *Phil. Trans. Royal Soc. A – Mathematical Phys. and Eng. Sci*. **373**, 20140139 (2015).

Education and Technology

63. C.M. Balik, R.J. Spontak, D.W. Brenner, R.O. Scattergood, Z. Sitar, J.L. Reed, J.L. Prebola and J. Weitzel, `Evolution of VIMS at North Carolina State University', *J. Mater. Educ* , **19**, 59 (1997).

64. A. Tragler, L. Srinivasan, M. McClauren and D.W. Brenner, 'Development of Cost-Effective Virtual Reality Tools for Materials Engineering Education' *J. Mater. Educ.* **21**, 119 (1999).

65. A. Tragler, L. Srinivasan, O.A. Shenderova, M. McClauren and D. W. Brenner, 'Novel Simulation Tools for Materials Engineering Education ', *Molecular Simulation* **25**, 121 (2000).

Energetic Materials and High Strain Rate/Shock Dynamics

66. M.L. Elert, D.M. Deaven, D.W. Brenner and C.T.White, `One-Dimensional Molecular-Dynamics Simulation of the Detonation of Nitric Oxide', *Phys. Rev. B.* **39** 1453 (1989).

67. D.W. Brenner, C.T. White, M.L. Elert and F.E. Walker, `Chemical Model for Intrinsic Detonation Velocities', *Int. J. Quantum Chem.:Quantum Chemistry Symposium* **23**, 333 (1989).

68. D.W. Brenner, M.L. Elert and C.T. White, `Incorporation of Reactive Dynamics in Simulations of Chemically-Sustained Shock Waves', in *Shock Compression of Condensed Matter* , S.C. Schmidt, J.N. Johnson and L.W. Davison, Ed. (North-Holland, Amsterdam), **263** (1990).

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