DIMITRIOS MAROUDAS
Curriculum Vitae

Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003

Education and Training

National Technical University, Athens, Greece	Chemical Engineering	Diploma, 1987
Massachusetts Institute of Technology, Cambridge, MA, USA	Chemical Engineering Minor: Physics	Ph.D., 1992
IBM T. J. Watson Research Center Yorktown Heights, NY, USA	Computational Materials Physics	Postdoctoral Research, 8/1992–6/1994

Professional Experience

9/2023–present	Department Head, Department of Chemical Engineering, University of Massachusetts (UMass) Amherst
9/2022–present	Affiliated Faculty, Interdisciplinary Graduate Program in Materials Science and Engineering, UMass Amherst
10/2020–present	Adjunct Professor, Department of Chemistry, UMass Amherst
9/2008–8/2023	Founding Director, Materials Engineering Certificate Program, College of Engineering, UMass Amherst
7/2002–present	Professor, Department of Chemical Engineering, UMass Amherst
7/2001–6/2002	Professor, Department of Chemical Engineering, University of California Santa Barbara (UCSB)
9/2000–8/2001	Visiting Associate Professor, Department of Chemical Engineering, Massachusetts Institute of Technology
7/1999–6/2001	Associate Professor, Department of Chemical Engineering, UCSB
7/1994–6/1999	Assistant Professor, Department of Chemical Engineering, UCSB

Professional Honors and Awards

- Fellow, American Institute of Chemical Engineers (AIChE), 2020.
- Fellow, American Association for the Advancement of Science (AAAS), 2018.
- UMass Amherst Faculty Exceptional Merit Award, 2012.
- College of Engineering Outstanding Senior Faculty Award, UMass Amherst, 2009.
- Co-Organizer, Multiscale Modeling and Simulation, National Academy of Engineering's Tenth Annual Symposium on *Frontiers of Engineering*, September 2004, Irvine, California.
- Invited Participant, National Academy of Engineering's Ninth Annual Symposium on *Frontiers of Engineering*, September 2003, Irvine, California.

- Invited plenary speaker, National Research Council (NRC) workshop on *Challenges for the Chemical Sciences in the 21st Century*: *Information & Communications*, National Academies of Sciences, October/November 2002, Washington, D.C.
- Camille Dreyfus Teacher-Scholar Award, The Camille & Henry Dreyfus Foundation, Inc., 1999.
- Robert G. Rinker American Institute of Chemical Engineers (AIChE) Outstanding Teaching Award, Department of Chemical Engineering, UCSB, 1996.
- Faculty Research Fellowship Award, Oak Ridge Associated Universities, Oak Ridge Institute for Science and Education, 1996.
- Faculty Early Career Development (CAREER) Award, National Science Foundation (NSF), 1995.

Selected Professional Activities

Service in Professional Societies

- Director, Materials Engineering and Sciences Division (MESD), American Institute of Chemical Engineers (AIChE), 11/2010 – 12/2012.
- Member, 2012 CoMSEF Impact Award Committee, Computational Molecular Science and Engineering Forum (CoMSEF), AIChE.

Editorial Boards

- Subject Editor, *Mathematical Methods*, *Handbook of Materials Modeling*, edited by Sidney Yip, Springer (2005).
- Member, Editorial Advisory Board, *Surface Science* (published by Elsevier), 1/1/2013 – present.
- Member, Editorial Advisory Board, *Materials Research Express* (published by Institute of Physics), 10/1/2013 – present.

Conference Organization

- Member, International Advisory Committee, 3rd International Conference on *Computational Modeling and Simulation of Materials*, May-June 2004, Acireale (Catania), Sicily, Italy.
- Member, International Advisory Committee, 6th Panhellenic Conference in *Chemical Engineering*, May-June 2007, Athens, Greece.
- Member, Program Committee, The IASTED International Conference on *Nanotechnology and Applications*, September-October 2008, Crete, Greece.
- Member, International Advisory Committee, 6th International Workshop on *Modeling in Crystal Growth* (IWMCG-6), August 2009, Lake Geneva, Wisconsin.
- Member, International Advisory Committee, 8th International Workshop on *Modeling in Crystal Growth* (IWMCG-8), November 2015, Spa, Belgium.

- Member, International Advisory Board, 2nd MiFuN Workshop on *Microstructural Functionality at the Nanoscale*, October 2017, Duisburg, Germany.

Educational and Mentoring Activities

- Founding Director, Materials Engineering Certificate Program, UMass Amherst College of Engineering, 9/2008 – 8/2023
- Chair, Interdisciplinary Graduate Program in Materials Science and Engineering Steering Committee, 4/2016 – 9/2017
- Member, Interdisciplinary Graduate Program in Materials Science and Engineering Task Force and Steering Committee, 1/2019 – present
- Graduate Program Director, Department of Chemical Engineering, UMass Amherst, 9/2005–8/2007 and 9/2009–8/2011
- Advised/co-advised 27 Ph.D. students, 13 postdoctoral research scholars, and 12 undergraduate researchers (since 7/1994)
- Served on 81 Ph.D. and 15 M.S. thesis committees in Chemical Engineering, Materials Science and Engineering, Chemistry, Physics, Mathematics, Mechanical Engineering, and Electrical Engineering (since 7/1994)

Membership in Professional Societies

- Technical Chamber of Greece; Member since 1987
- Materials Research Society (MRS); Member since 1989
- American Institute of Chemical Engineers (AIChE); Member since 1991, Senior Member since 2009; Fellow since 2020
- American Physical Society (APS); Member since 1992
- American Association for the Advancement of Science (AAAS); Member since 1994, Fellow since 2018

Publications

[234 refereed journal articles, 35 refereed symposium proceedings papers, 2 book chapters, and 3 U.S. patents, resulting in 6942 citations with h-index of 43 and i-10 index of 165 (Google Scholar; 11/18/2023)]

Invited Review/Perspective Articles

1. D. Maroudas, "Multi-Scale Modeling of Hard Materials: Challenges and Opportunities for Chemical Engineering," *AIChE Journal* **46**, 878–882 (2000).
   - **Invited Perspective Article**
2. D. Maroudas, "Surface Morphological Response of Crystalline Solids to Mechanical Stresses and Electric Fields," *Surface Science Reports* **66**, 299–346 (2011).
   - **Invited Review Article**
3. D. Maroudas, X. Han, and S. C. Pandey, "Design of Semiconductor Ternary Quantum Dots with Optimal Optoelectronic Function," *AIChE Journal* **59**, 3223–3236 (2013).
   - **Invited article** for special *AIChE J*. issue on *Tribute to Founders*: *Neal R. Amundson*
4. D. Maroudas, S. Blondel, L. Hu, K. D. Hammond, and B. D. Wirth, "Helium Segregation on Surfaces of Plasma-exposed Tungsten," *Journal of Physics*: *Condensed Matter* **28**, Article No. 064004, 13 pages (2016).
   - **Invited research article** for special issue on *Surface Segregation*
5. D. Maroudas and B. D. Wirth, "Atomic-Scale Modeling toward Enabling Models of Surface Nanostructure Formation in Plasma-Facing Materials," *Current Opinion in Chemical Engineering* **23**, 77–84 (2019).
   - **Invited review article** for special issue on *Frontiers of Chemical Engineering*: *Molecular Modeling*
6. D. Maroudas, A. R. Muniz, and A. Ramasubramaniam, "Structure-Properties Relations in Graphene Derivatives and Metamaterials Obtained by Atomic-Scale Modeling," *Molecular Simulation* **45** (14-15), 1173–1202 (2019).
   - **Invited review article** for special issue on *Recent Advances in Molecular Simulation*
7. A. Kumar, C.-S. Chen, and D. Maroudas, "Fabrication of Ordered Arrays of Quantum Dot Molecules Based on the Design of Pyramidal Pit Patterns on Semiconductor Surfaces," *Industrial & Engineering Chemistry Research* **59**, 2536–2547 (2020).
   - **Invited article** for special issue on *Christos Georgakis Festschrift*

Articles that have received recognition (selected papers, Editor's picks, etc.)

8. S. Sriraman, S. Agarwal, E. S. Aydil, and D. Maroudas, "Mechanism of Hydrogen-Induced Crystallization of Amorphous Silicon," *Nature* **418**, 62–65 (2002).
   - Articles and commentaries for this article were featured in numerous journals and newspapers, including *Nature*, *Chemical & Engineering News*, and the *Boston Globe*.
9. S. Sriraman, E. S. Aydil, and D. Maroudas, "Growth and Characterization of a-Si:H Thin Films from SiH_2 Radical Precursor: An Atomic-Scale Analysis," *Journal of Applied Physics* **95**, 1792–1805 (2004).
   - **selected paper** on *Nanotechnology – Theory and Modeling* (a collection of 50 outstanding papers focusing on the theory and modeling of nanoscale materials and

structures), ***Milestone Series of Selected Reprints***: *Collections of Outstanding papers from the world literature on optical and optoelectronic science, engineering, and technology*, edited by F. Wang and A. Lakhtakia (SPIE Press, Bellingham, Washington USA, 2006).

10. M. R. Gungor and D. Maroudas, "Relaxation of Biaxial Tensile Strain in Ultra-Thin Metallic Films: Ductile Void Growth versus Nanocrystalline Domain Formation," *Applied Physics Letters* **87**, Article No. 171913, 3 pages (2005).
    - **selected paper** for the 10/31/2005 issue of the *Virtual Journal of Nanoscale Science and Technology*

11. S. Sriraman, M. S. Valipa, E. S. Aydil, and D. Maroudas, "Hydrogen-Induced Crystallization of Amorphous Silicon Thin Films. I. Simulation and Analysis of Film Post-Growth Treatment with H_2 Plasmas," *Journal of Applied Physics* **100**, Article No. 053514, 11 pages (2006).
    - **selected paper** for the 9/25/2006 issue of the *Virtual Journal of Nanoscale Science and Technology*

12. V. Tomar, M. R. Gungor, and D. Maroudas, "Current-Induced Stabilization of Surface Morphology in Stressed Solids," *Physical Review Letters* **100**, Article No. 036106, 4 pages (2008).
    - Articles and commentaries for this article were featured in *Physical Review Focus* (see story on this article: http://focus.aps.org/story/v21/st4), *United Press International*, *Materials World*, *Materials Performance*, *Advanced Materials and Processes*, and most physics and engineering newsletters and websites.

13. K. Kolluri, M. R. Gungor, and D. Maroudas, "Atomic-Scale Analysis of Defect Dynamics and Strain Relaxation Mechanisms in Biaxially Strained Ultra-thin Films of Face-Centered Cubic Metals," *Journal of Applied Physics* **103**, Article No. 123517, 11 pages (2008).
    - **selected paper** for the 6/30/2008 issue of the *Virtual Journal of Nanoscale Science and Technology*

14. K. Kolluri, M. R. Gungor, and D. Maroudas, "Comparative Study of the Mechanical Behavior Under Biaxial Strain of Prestrained Face-centered Cubic Metallic Ultrathin Films," *Applied Physics Letters* **94**, Article No. 101911, 3 pages (2009).
    - **selected paper** for the 3/23/2009 issue of the *Virtual Journal of Nanoscale Science and Technology*

15. A. R. Muniz, T. Singh, and D. Maroudas, "Effects of Hydrogen Chemisorption on the Structure and Deformation of Single-walled Carbon Nanotubes," *Applied Physics Letters* **94**, Article No. 103108, 3 pages (2009).
    - **selected paper** for the 3/23/2009 issue of the *Virtual Journal of Nanoscale Science and Technology*

16. A. R. Muniz, T. Singh, E. S. Aydil, and D. Maroudas, "Analysis of Diamond Nanocrystal Formation from Multiwalled Carbon Nanotubes," *Physical Review B* **80**, Article No. 144105, 12 pages (2009).
    - **selected paper** for the 10/19/2009 issue of the *Virtual Journal of Nanoscale Science and Technology*

- **featured in** *Physical Review Focus* (10/2/2009); See story on this article: http://focus.aps.org/story/v24/st13

17. A. R. Muniz, M. Meyyappan, and D. Maroudas, "On the Hydrogen Storage Capacity of Carbon Nanotube Bundles," *Applied Physics Letters* **95**, Article No. 163111, 3 pages (2009).
    - **selected paper** for the 11/2/2009 issue of the *Virtual Journal of Nanoscale Science and Technology*

18. K. Kolluri, M. R. Gungor, and D. Maroudas, "Atomistic Analysis of Strain Relaxation in [110]-Oriented Biaxially Strained Ultrathin Copper Films," *Journal of Applied Physics* **106**, Article No. 103519, 8 pages (2009).
    - **selected paper** for the 12/7/2009 issue of the *Virtual Journal of Nanoscale Science and Technology*

19. D. J. Beltran-Villegas, R. M. Sehgal, D. Maroudas, D. M. Ford, and M. A. Bevan, "Fokker-Planck Analysis of Separation Dependent Potentials and Diffusion Coefficients in Simulated Microscopy Experiments," *Journal of Chemical Physics* **132**, Article No. 044707, 8 pages (2010).
    - chosen as a **research highlight** featured on the journal website home page
    - selected as a 2010 *Journal of Chemical Physics* Editor's Choice in the area of Surfaces, Interfaces, and Materials

20. A. R. Muniz and D. Maroudas, "Hydrogenation Effects on the Structure and Morphology of Graphene and Single-walled Carbon Nanotubes," *Journal of Applied Physics* **108**, Article No. 113532, 10 pages (2010).
    - **selected paper** for the 12/20/2010 issue of the *Virtual Journal of Nanoscale Science and Technology*

21. S. C. Pandey, G. I. Sfyris, and D. Maroudas, "Theory of Surface Segregation in Ternary Semiconductor Quantum Dots," *Applied Physics Letters* **98**, Article No. 091907, 3 pages (2011).
    - **selected paper** for the 3/14/2011 issue of the *Virtual Journal of Nanoscale Science and Technology*

22. S. C. Pandey and D. Maroudas, "Equilibrium Compositional Distribution in Freestanding Ternary Semiconductor Quantum Dots: The Case of $In_xGa_{1-x}As$," *Journal of Chemical Physics* **135**, Article No. 234701, 12 pages (2011).
    - **selected paper** for the 1/9/2012 issue of the *Virtual Journal of Nanoscale Science and Technology*

23. C. Carpenter, A. Ramasubramaniam, and D. Maroudas, "Analysis of Vacancy-induced Amorphization of Single-Layer Graphene," *Applied Physics Letters* **100**, Article No. 203105, 4 pages (2012).
    - **selected paper** for the 5/28/2012 issue of the *Virtual Journal of Nanoscale Science and Technology*.

24. A. R. Muniz and D. Maroudas, "Opening and Tuning of Band Gap by the Formation of Diamond Superlattices in Twisted Bilayer Graphene," *Physical Review B* **86**, Article No. 075404, 11 pages (2012).

- **selected paper** as Editors' Suggestion for reading in *Physical Review B*

25. D. Dasgupta, G. I. Sfyris, and D. Maroudas, "Current-driven Morphological Evolution of Single-layer Epitaxial Islands on Crystalline Substrates," *Surface Science* **618**, L1–L5 (2013).
    - **Highlighted** in volume **618** of *Surface Science* with a **perspective article** (by I. G. Kevrekidis) on the subject and findings of our article.

26. L. Du and D. Maroudas, "Theory of Multiple Quantum Dot Formation in Strained-Layer Heteroepitaxy," *Applied Physics Letters* **109**, Article No. 023103, 4 pages (2016).
    - **Editor's Pick**; one of five articles highlighted on the journal homepage for the week of 7/17/2016

27. A. Weerasinghe, A. R. Muniz, A. Ramasubramaniam, and D. Maroudas, "Mechanical Properties of Hydrogenated Electron-Irradiated Graphene," *Journal of Applied Physics* **120**, Article No. 124301, 6 pages (2016).
    - **Featured Article** for the (weekly) issue of 9/28/2016 (No. 12 of volume 120) of the *Journal of Applied Physics*
    - A figure from this article was used for the **issue cover** for the journal's issue of 9/28/2016

28. L. Du and D. Maroudas, "Current-Induced Surface Roughness Reduction in Conducting Thin Films," *Applied Physics Letters* **110**, Article No. 103103, 5 pages (2017).
    - **Editor's Pick**; one of five articles highlighted on the journal homepage for the week of 3/6/2017
    - American Institute of Physics (AIP) **press release** for this article posted on 3/7/2017; news articles also appeared in most physics and science news websites.

29. D. Dasgupta, A. Kumar, and D. Maroudas, "Analysis of Current-Driven Oscillatory Dynamics of Single-Layer Homoepitaxial Islands on Crystalline Conducting Substrates," *Surface Science* **669**, 25–33 (2018).
    - **Selected for cover page image** of Volume **669** of *Surface Science*.

30. A. Kumar, C.-S. Chen, and D. Maroudas, "Design of Semiconductor Surface Pits for Fabrication of Regular Arrays of Quantum Dots and Nanorings," *Journal of Applied Physics* **125**, Article No. 045303, 12 pages (2019).
    - **Editor's Pick**; one of five articles highlighted on the journal homepage for the week of 1/28/2019

31. M. Chen, L. Hu, A. Ramasubramaniam, and D. Maroudas, "Effects of Pore Morphology and Pore Edge Termination on the Mechanical Behavior of Graphene Nanomeshes," *Journal of Applied Physics* **126**, Article No. 164306, 12 pages (2019).
    - **Editor's Pick**; one of five articles highlighted on the journal homepage for the week of 10/28/2019

32. D. Dasgupta, D. Maroudas, and B. D. Wirth, "Prediction of Temperature Range for the Onset of Fuzz Formation in Helium-Plasma-Implanted Tungsten," *Surface Science* **698**, Article No. 121614, 7 pages (2020).
    - **Selected for cover page image** of Volume **698** of *Surface Science*.

Other Journal Articles

33. D. Maroudas and R. A. Brown, "On the Prediction of Dislocation Formation in Semiconductor Crystals Grown from the Melt: Analysis of the Haasen Model for Plastic Deformation Dynamics," *Journal of Crystal Growth* **108**, 399–415 (1991).

34. D. Maroudas and R. A. Brown, "Analysis of Point Defect Diffusion and Drift in Cubic-Type Lattices: Constitutive Modeling," *Physical Review B* **44**, 2567–2581 (1991).

35. D. Maroudas and R. A. Brown, "Analysis of the Effects of Oxygen Migration on Dislocation Motion in Silicon," *Journal of Applied Physics* **69**, 3865–3877 (1991).

36. D. Maroudas and R. A. Brown, "Model of Dislocation Locking by Oxygen Gettering in Silicon Crystals," *Applied Physics Letters* **58**, 1842–1844 (1991).

37. D. Maroudas and R. A. Brown, "Constitutive Modeling of the Effects of Oxygen on the Deformation Behavior of Silicon," *Journal of Materials Research* **6**, 2337–2352 (1991).

38. D. Maroudas and R. A. Brown, "Atomistic Calculation of the Self-Interstitial Diffusivity in Silicon," *Applied Physics Letters* **62**, 172–174 (1993).

39. D. Maroudas and R. A. Brown, "Calculation of Thermodynamic and Transport Properties of Intrinsic Point Defects in Silicon," *Physical Review B* **47**, 15562–15577 (1993).

40. S. T. Pantelides, D. Maroudas, and D. B. Laks, "Defects in Heterogeneous Solids: From Microphysics to Macrophysics," *Materials Science Forum* **143**, 1–8 (1994).

41. R. A. Brown, D. Maroudas, and T. Sinno, "Modeling Point Defect Dynamics in the Crystal Growth of Silicon," *Journal of Crystal Growth* **137**, 12–25 (1994).

42. D. Maroudas and S. T. Pantelides, "Point Defects in Crystalline Silicon, Their Migration, and Their Relation to the Amorphous Phase," *Chemical Engineering Science* **49**, 3001–3014 (1994).

43. D. Maroudas, "Dynamics of Transgranular Voids in Metallic Thin Films Under Electromigration Conditions," *Applied Physics Letters* **67**, 798–800 (1995).

44. D. Maroudas, M. N. Enmark, C. M. Leibig, and S. T. Pantelides, "Analysis of Damage Formation and Propagation in Metallic Thin Films Under the Action of Thermal Stresses and Electric Fields," *Journal of Computer-Aided Materials Design* **2**, 231–258 (1995).

45. D. Maroudas and S. Shankar, "Electronic Materials Process Modeling," *Journal of Computer-Aided Materials Design* **3**, 36–48 (1996).

46. B. D. Wirth, G. R. Odette, D. Maroudas, and G. E. Lucas, "Energetics of Formation and Migration of Self-Interstitials and Self-Interstitial Clusters in α-Iron," *Journal of Nuclear Materials* **244**, 185–194 (1997).

47. M. E. Barone and D. Maroudas, "Defect-Induced Amorphization of Silicon as a Mechanism of Disordered Region Formation During Ion Implantation," *Journal of Computer-Aided Materials Design* **4**, 63–73 (1997).

48. B. Meng, D. Maroudas, and W. H. Weinberg, "Structure of the Chemisorbed Acetylene on the Si(001)-(2×1) Surface and the Effect of Coadsorbed Atomic Hydrogen," *Chemical Physics Letters* **278**, 97–101 (1997).

49. S. Ramalingam, D. Maroudas, and E. S. Aydil, "Atomistic Simulation of SiH Interactions with Silicon Surfaces During Deposition from Silane Containing Plasmas," *Applied Physics Letters* **72**, 578–580 (1998).

50. M. R. Gungor and D. Maroudas, "Electromigration-Induced Failure of Metallic Thin Films Due to Transgranular Void Propagation," *Applied Physics Letters* **72**, 3452–3454 (1998).

51. D. Maroudas, L. A. Zepeda-Ruiz, and W. H. Weinberg, "Interfacial Stability and Misfit Dislocation Formation in InAs/GaAs(110) Heteroepitaxy," *Surface Science* **411**, L865–L871 (1998).

52. D. Maroudas, L. A. Zepeda-Ruiz, and W. H. Weinberg, "Kinetics of Strain Relaxation through Misfit Dislocation Formation in the Growth of Epitaxial Films on Compliant Substrates," *Applied Physics Letters* **73**, 753–755 (1998).

53. L. J. Gray, D. Maroudas, and M. N. Enmark, "Galerkin Boundary-Integral Method for Evaluating Surface Derivatives," *Computational Mechanics* **22**, 187–193 (1998).

54. S. Ramalingam, D. Maroudas, and E. S. Aydil, "Interaction of SiH Radicals from a Silane Plasma with Silicon Surfaces: An Atomic-Scale Simulation Study," *Journal of Applied Physics* **84**, 3895–3911 (1998).

55. M. R. Gungor and D. Maroudas, "Nonlinear Analysis of the Morphological Evolution of Void Surfaces in Metallic Thin Films Under Surface Electromigration Conditions," *Surface Science* **415**, L1055–L1060 (1998).

56. S. Ramalingam, D. Maroudas, E. S. Aydil, and S. P. Walch, "Abstraction of Hydrogen by SiH_3 from Hydrogen-Terminated Si(001)-(2×1) Surfaces," *Surface Science* **418**, L8–L13 (1998).

57. L. A. Zepeda-Ruiz, D. Maroudas, and W. H. Weinberg, "Semicoherent Interface Formation and Structure in InAs/GaAs(111)A Heteroepitaxy," *Surface Science* **418**, L68–L72 (1998).

58. M. R. Gungor, D. Maroudas, and L. J. Gray, "Effects of Mechanical Stress on Electromigration-Driven Transgranular Void Dynamics in Passivated Metallic Thin Films," *Applied Physics Letters* **73**, 3848–3850 (1998).

59. L. J. Gray, D. Maroudas, M. N. Enmark, and E. F. D'Azevedo, "Approximate Green's Functions in Boundary Integral Analysis," *Engineering Analysis with Boundary Elements* **23**, 267–274 (1999).

60. M. R. Gungor and D. Maroudas, "Theoretical Analysis of Electromigration-Induced Failure of Metallic Thin Films Due to Transgranular Void Propagation," *Journal of Applied Physics* **85**, 2233–2246 (1999).

61. S. Ramalingam, D. Maroudas, and E. S. Aydil, "Visualizing Radical-Surface Interactions in Plasma Deposition Processes: Reactivity of SiH_3 Radicals with Silicon Surfaces," *IEEE Transactions on Plasma Science* **27**, 104–105 (1999).

62. L. A. Zepeda-Ruiz, D. Maroudas, and W. H. Weinberg, "Theoretical Study of the Energetics, Strain Fields, and Semicoherent Interface Structures in Layer-by-Layer Semiconductor Heteroepitaxy," *Journal of Applied Physics* **85**, 3677–3695 (1999).

63. M. R. Gungor and D. Maroudas, "Nonhydrostatic Stress Effects on Failure of Passivated Metallic Thin Films Due to Void Surface Electromigration," *Surface Science* **432**, L604–L610 (1999).

64. B. Z. Nosho, L. A. Zepeda-Ruiz, R. I. Pelzel, W. H. Weinberg, and D. Maroudas, "Surface Morphology in InAs/GaAs(111)A Heteroepitaxy: Experimental Measurements and Computer Simulations," *Applied Physics Letters* **75**, 829–831 (1999).

65. S. Ramalingam, D. Maroudas, and E. S. Aydil, "Atomistic Simulation Study of the Interactions of SiH_3 Radicals with Silicon Surfaces," *Journal of Applied Physics* **86**, 2872–2888 (1999).

66. L. A. Zepeda-Ruiz, B. Z. Nosho, R. I. Pelzel, W. H. Weinberg, and D. Maroudas, "Kinetics of Strain Relaxation through Misfit Dislocation Formation in InAs/GaAs(111)A Heteroepitaxy," *Surface Science* **441**, L911–L916 (1999).

67. S. Ramalingam, P. Mahalingam, E. S. Aydil, and D. Maroudas, "Theoretical Study of the Interactions of SiH_2 Radicals with Silicon Surfaces," *Journal of Applied Physics* **86**, 5497–5508 (1999).

68. B. D. Wirth, G. R. Odette, D. Maroudas, and G. E. Lucas, "Dislocation Loop Structure, Energy, and Mobility of Self-Interstitial Clusters in BCC Iron," *Journal of Nuclear Materials* **276**, 33–40 (2000).

69. R. I. Pelzel, L. A. Zepeda-Ruiz, B. Z. Nosho, Y. Li, W. H. Weinberg, and D. Maroudas, "Mechanical Behavior of Thin Buffer Layers in InAs/GaAs(111)A Heteroepitaxy," *Applied Physics Letters* **76**, 3017–3019 (2000).

70. S. Sriraman, S. Ramalingam, E. S. Aydil, and D. Maroudas, "Abstraction of Hydrogen by SiH Radicals from Hydrogenated Amorphous Silicon Surfaces," *Surface Science* **459**, L475–L481 (2000).

71. M. R. Gungor, D. Maroudas, and S. J. Zhou, "Molecular-Dynamics Study of the Mechanism and Kinetics of Void Growth in Ductile Metallic Thin Films," *Applied Physics Letters* **77**, 343–345 (2000).

72. M. R. Gungor and D. Maroudas, "Current-Induced Non-Linear Dynamics of Voids in Metallic Thin Films: Morphological Transition and Surface Wave Propagation," *Surface Science* **461**, L550–L556 (2000).

73. R. I. Pelzel, L. A. Zepeda-Ruiz, W. H. Weinberg, and D. Maroudas, "Effects of Buffer Layer Thickness and Film Compositional Grading on Strain Relaxation Kinetics in InAs/GaAs(111)A Heteroepitaxy," *Surface Science* **463**, L634–L640 (2000).

74. S. P. Walch, S. Ramalingam, E. S. Aydil, and D. Maroudas, "Mechanism and Energetics of Dissociative Adsorption of SiH_3 on the Hydrogen-Terminated Si(001)-(2×1) Surface," *Chemical Physics Letters* **329**, 304–310 (2000).

75. L. A. Zepeda-Ruiz, R. I. Pelzel, W. H. Weinberg, and D. Maroudas, "Interfacial Stability and Structure in InAs/GaAs(111)A: Effects of Buffer Layer Thickness and Film Compositional Grading," *Applied Physics Letters* **77**, 3352–3354 (2000).

76. J. Zhao, D. Maroudas, and F. Milstein, "Thermal Activation of Shear Modulus Instabilities in Pressure-Induced bcc$\rightarrow$hcp Transitions," *Physical Review B* **62**, 13799–13802 (2000).

77. S. Ramalingam, S. Sriraman, E. S. Aydil, and D. Maroudas, "Evolution of Structure, Morphology, and Reactivity of Hydrogenated Amorphous Silicon Film Surfaces Grown by Molecular-Dynamics Simulation," *Applied Physics Letters* **78**, 2685–2687 (2001).

78. M. R. Gungor and D. Maroudas, "Modeling of Electromechanically-Induced Failure of Passivated Metallic Thin Films Used in Device Interconnections," *International Journal of Fracture* **109**, 47–68 (2001).

79. S. Ramalingam, E. S. Aydil, and D. Maroudas, "Molecular-Dynamics Study of the Interactions of Small Thermal and Energetic Silicon Clusters with Crystalline and Amorphous Silicon Surfaces," *Journal of Vacuum Science and Technology B* **19**, 634–644 (2001).

80. S. P. Walch, S. Ramalingam, S. Sriraman, E. S. Aydil, and D. Maroudas, "Mechanisms and Energetics of SiH_3 Adsorption on the Pristine Si(001)-(2×1) Surface," *Chemical Physics Letters* **344**, 249–255 (2001).

81. L. A. Zepeda-Ruiz, R. I. Pelzel, B. Z. Nosho, W. H. Weinberg, and D. Maroudas, "Deformation Behavior of Coherently Strained InAs/GaAs(111)A Heteroepitaxial Systems: Theoretical Calculations and Experimental Measurements," *Journal of Applied Physics* **90**, 2689–2698 (2001).

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Book Chapters

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Patents

P1. Christos Dimitrakopoulos, Dimitrios Maroudas, André R. Muniz, and D. Kurt Gaskill, "Multilayer Graphene Structures with Enhanced Mechanical Properties Resulting from Deterministic Control of Interlayer Twist Angles and Chemical Functionalization," U.S. Patent No. US 10,562,278 B2, issued on 2/18/2020.

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P3. Christos Dimitrakopoulos, Dimitrios Maroudas, and Yuxi Wang, "Formation of Interlayer Covalent Bonds in Bilayer, Trilayer and Multilayer Graphene," U.S. Patent Application Publication No.: US 2019/0055129 A1. Publication Date: 2/21/2019.

Invited Talks at Conferences and Workshops

Major Invited/Plenary Talks

1. D. Maroudas, L. A. Zepeda-Ruiz, R. I. Pelzel, B. Z. Nosho, and W. H. Weinberg, "Strain Relaxation and Interfacial Stability in III-V Semiconductor Strained-Layer Heteroepitaxy: Atomistic & Continuum Modeling and Comparisons with Experiment," Symposium on Multiscale Materials Modeling, International Conference of the International Union of Materials Research Societies (IUMRS), July 2000, Hong Kong.
2. D. Maroudas, "Multiscale Modeling," National Research Council Workshop on *Challenges for the Chemical Sciences in the 21st Century*: *Information and Communications*, National Academies of Sciences, October/November 2002, Washington, D.C.
3. D. Maroudas, "Analysis of Electromigration-Driven Void Surface Dynamics and Failure in Metallic Thin Films", International Workshop on *Energy Dissipation at Surfaces*, September 2004, Wesseling, Germany.
4. D. Maroudas, "Thin Films and Nanostructures of Hard Materials: Progress Made and Current Challenges in the Computational Modeling of Their Processing and Function," Invited Centennial Session on *Applied Mathematics and Chemical Engineering – Past 100 Years and the Future*, AIChE Annual Meeting, November 2008, Philadelphia, Pennsylvania.
5. A. R. Muniz, A. S. Machado, and D. Maroudas, "Mechanical Behavior of Diamond Superlattices Generated by Interlayer Covalent Bonding in Twisted Bilayer Graphene," MRS Fall Meeting, December 2013, Boston, Massachusetts.
6. D. Maroudas, "Theoretical Studies of Structure-Property Relations in Graphene-based Carbon Nanostructures," APS March Meeting, March 2014, Denver, Colorado.
7. D. Maroudas, "Current-Driven Surface Morphological Stabilization and Surface Nanopatterning," Workshop on *Microstructural Functionality*: *Dynamics, Adaption, and Self-Healing at the Nanoscale*, April 2014, Duisburg, Germany.
8. D. Maroudas, "Analysis of External-field-driven Surface Morphological Evolution: Stabilization and Nanopatterning," AIChE Area 10D Plenary Session (*Future Directions in Applied Mathematics and Numerical Analysis*), AIChE Annual Meeting, November 2014, Atlanta, Georgia.
9. L. Du and D. Maroudas, "Pore-Pore and Pore-Edge Interactions in Graphene Sheets and Nanoribbons," AIChE CAST Area Plenary Session (*Future Directions in Applied Mathematics and Numerical Analysis*), AIChE Annual Meeting, November 2016, San Francisco, California.
10. D. Maroudas, "Defect Engineering and Patterning of Crystal Surfaces, Epitaxial Thin Films, and Two-Dimensional Materials: A Computational Materials Science Approach," Keynote Lecture, *The Second International Computational Science and Engineering Conference*, October 2017, Doha, Qatar.

11. D. Maroudas, D. Dasgupta, R. D. Kolasinski, and B. D. Wirth, "Modeling of Surface Morphological Evolution of Plasma-Facing Tungsten," 60th Annual Meeting of the APS Division of Plasma Physics, November 2018, Portland, Oregon.

12. D. Maroudas and A. R. Muniz, "2D Diamond Superstructures in Interlayer-Bonded Twisted Bilayer Graphene: Thermomechanical Properties from Atomic-Scale Simulations," Plenary Talk, *International Conference on New Carbon Nanomaterials*: *Ultrathin Diamond Films*, December 2021, Moscow, Russia (virtual conference).

Other Invited Talks at Conferences and Workshops

13. D. Maroudas and R. A. Brown, "Modeling of Impurity and Dislocation Dynamics in Czochralski Grown Silicon and Liquid-Encapsulated-Czochralski Grown III-V Compound Semiconductors," Gordon Conference on *Crystal Growth*, March 1990, Oxnard, California.

14. S. T. Pantelides, D. Maroudas, and D. B. Laks, "Defects in Heterogeneous Solids: From Microphysics to Macrophysics," International Conference on *Defects in Semiconductors*, July 1993, Gmunden, Austria.

15. R. A. Brown, D. Maroudas, and T. Sinno, "Modeling Point Defect Dynamics in the Crystal Growth of Silicon," Ninth American Conference on Crystal Growth, August 1993, Baltimore, Maryland.

16. S. T. Pantelides, D. Maroudas, and D. B. Laks, "Theory of Microstructure Evolution in Heterogeneous Materials. From Atoms to Continuum Mechanics," ASME International Congress and Exposition, November 1994, Chicago, Illinois.

17. D. Maroudas and S. T. Pantelides, "Theory and Computer Simulation of Grain-Boundary and Void Dynamics in Polycrystalline Conductors," Fifth Symposium on Materials Reliability in Microelectronics, Materials Research Society (MRS) Spring Meeting, April 1995, San Francisco, California.

18. D. Maroudas, E. F. d'Azevedo, L. J. Gray, and S. T. Pantelides, "Theory and Computer Simulation of Microstructure Evolution in Polycrystalline Metallic Thin Films," Fourth International Symposium on Process Physics and Modeling in Semiconductor Technology, Spring 1996 Meeting of the Electrochemical Society, May 1996, Los Angeles, California.

19. D. Maroudas, L. A. Zepeda-Ruiz, and W. Henry Weinberg, "Interfacial Stability and Misfit Dislocation Formation in Semiconductor Strained-Layer Heteroepitaxy," Workshop on *Quantitative Methods in Materials Research*, Institute for Theoretical Physics, University of California, Santa Barbara, February 1997, Santa Barbara, California.

20. D. Maroudas, L. A. Zepeda-Ruiz, and W. Henry Weinberg, "Interfacial Stability and Misfit Dislocation Formation in Semiconductor Heteroepitaxy," Seventh Conference on *Computational Research on Materials*, May 1997, Morgantown, West Virginia.

21. D. Maroudas, "Theoretical Analysis and Computer Simulation of Electromigration-Induced Failure of Metallic Thin Films," Eighth Conference on *Computational Research on Materials*, May 1998, Morgantown, West Virginia.

22. M. R. Gungor, L. J. Gray, and D. Maroudas, "Self-Consistent Theoretical Analysis of Electromigration-Induced Failure of Metallic Thin Films," Gordon Research Conference on *Thin Film Mechanical Behavior*, June 1998, Plymouth, New Hampshire.

23. D. Maroudas, S. Ramalingam, and E. S. Aydil, "Atomic-Scale Modeling of Plasma-Surface Interactions in the PECVD of Silicon," Symposium on Fundamental Gas-Phase and Surface Chemistry of Vapor-Phase Synthesis, The 194th Meeting of the Electrochemical Society, November 1998, Boston, Massachusetts.

24. D. Maroudas, "Multiscale Modeling of Failure Mechanisms in Metallic Thin-Film Interconnects," Workshop on *Mesoscale Investigations of Materials and Materials Processing Using X-Ray Microbeams*, April 1999, San Francisco, California.

25. D. Maroudas, L. A. Zepeda-Ruiz, and W. H. Weinberg, "Strain Relaxation and Interfacial Stability in III-V Semiconductor Heteroepitaxy: Continuum Theory, Atomistic Simulations, and Experimental Measurements," Mardi Gras Conference on *Materials Design*: *Experimental and Computational Challenges*, March 2000, Baton Rouge, Louisiana.

26. D. Maroudas, L. A. Zepeda-Ruiz, and W. H. Weinberg, "Strain Relaxation and Interfacial Stability in III-V Semiconductor Heteroepitaxy: Continuum Theory, Atomistic Simulations, and Experimental Measurements," Twelfth American Conference on Crystal Growth and Epitaxy (ACCGE-12), August 2000, Vail, Colorado.

27. D. Maroudas, "Multiscale Modeling of Electromechanically-Induced Failure in Metallic Thin Films Used in Microelectronics," Minisymposium on *Multiscale Modeling*: *Fundamentals and Applications*, SIAM Conference on *Computational Science and Engineering*, September 2000, Washington, D.C.

28. D. Maroudas, "Multiscale Theory and Simulation of Electromechanically-Induced Failure in Ductile Metallic Thin Films," APS Division of Computational Physics Annual Meeting, June 2001, Cambridge, Massachusetts.

29. D. Maroudas, "Challenges and Recent Advances in the Modeling of Plasma Deposition of Silicon Thin Films," Centre Europeen pour le Calcul Atomique et Moleculaire (CECAM) Workshop on *Multiscale Modeling of Materials*: *Methods, Algorithms, and Unsolved Problems*, July 2001, Heraklion, Crete, Greece.

30. D. Maroudas, "Plasma Deposition of Silicon Thin Films: Atomic-Scale Modeling of Radical-Surface Interactions," Symposium on Modeling of Plasma-Surface Interactions, American Vacuum Society (AVS) 48th International Symposium and IUVSTA 15th International Vacuum Congress & 11th International Congress on Solid Surfaces, October 2001, San Francisco, California.

31. S. Sriraman, E. S. Aydil, and D. Maroudas, "Understanding Radical-Surface Interactions in Plasma-Enhanced Chemical Vapor Deposition of Silicon Thin Films through Atomistic Simulations," New Mexico Local Section of the AVS, May 2002, Albuquerque, New Mexico.

32. D. Maroudas, "Recent Contributions of Molecular Simulation to the Modeling of Electronic Materials Processing and Reliability," *Foundations of Molecular Modeling and Simulation* (FOMMS) 2003 Meeting, July 2003, Keystone, Colorado.

33. S. Agarwal, S. Sriraman, A. Takano, M. C. M. Van de Sanden, D. Maroudas, and E. S. Aydil, "Understanding Radical-Surface Interactions in the Plasma-Assisted Deposition of Amorphous Hydrogenated Silicon," AVS 50th International Symposium, November 2003, Baltimore, Maryland.

34. D. Maroudas, "Multiscale Modeling: Status and Opportunities in Research and Education," Computing and Systems Technology (CAST) Division Plenary Talk, AIChE Annual Meeting, November 2003, San Francisco, California.

35. D. Maroudas, S. Sriraman, S. Agarwal, M. S. Valipa, and E. S. Aydil, "Atomic-Scale Modeling of Plasma Deposition of Silicon Thin Films," Session on *Plasma Processing I*, AIChE Annual Meeting, November 2003, San Francisco, California.

36. D. Maroudas, M. S. Valipa, S. Sriraman, and E. S. Aydil, "Atomistic Modeling of Nanocrystalline Silicon Synthesis," 3rd International Conference on *Computational Modeling and Simulation of Materials*, May-June 2004, Acireale (Catania), Sicily, Italy.

37. D. Maroudas, "Multiscale Modeling of Materials Processing and Function," Session on Simulation and Control of Multiscale Processes, American Control Conference, June 2004, Boston, Massachusetts.

38. D. Maroudas, "Analysis of Electromechanically-Induced Defect Dynamics and Failure in Metallic Thin Films," Stratis V. Sotirchos Memorial Session, AIChE Annual Meeting, November 2004, Austin, Texas.

39. T. Bakos, M. S. Valipa, and D. Maroudas, "Chemical Reactions and Diffusion of Growth Precursors on Plasma-Deposited Silicon Thin-Film Surfaces," Minisymposium on *The Impact of Materials Chemistry on Materials Performance*, U. S. National Congress on Computational Mechanics (USNCCM8), July 2005, Austin, Texas.

40. D. Maroudas, "Multiscale Modeling of Materials Processing and Function," AIChE Annual Meeting, November 2005, Cincinnati, Ohio.

41. V. Tomar, J. S. Cho, M. R. Gungor, and D. Maroudas, "Electromechanically-Driven Complex Morphological Evolution of Void Surfaces in Metallic Thin Films," CAST Division Plenary Talk, AIChE Annual Meeting, November 2006, San Francisco, California.

42. D. Maroudas, "Materials Surface Engineering by Simultaneous Action of Multiple External Forces," AIChE CAST Division Web Seminar, September 2007.

43. D. Maroudas, "Surface Engineering by Simultaneous Action of Multiple External Fields," First Program Meeting on *Physical Behavior of Materials*, U.S. Department of Energy, Office of Basic Energy Sciences, March 2008, Warrenton, Virginia.

44. E. S. Aydil, M. J. Behr, T. Singh, A. R. Muniz, and D. Maroudas, "Hydrogen Induced Transformation of Carbon Nanotubes to Diamond and New Carbon Allotropes at Room Temperature," Gordon Research Conference on *Plasma Processing Science*, July 2008, South Hadley, Massachusetts.

45. D. Maroudas, "Modeling Plasma-Surface Interactions and Their Role in Inducing Structural Transitions in Materials," Special session to honor Professor Herbert H. Sawin, AIChE Annual Meeting, November 2008, Philadelphia, Pennsylvania.

46. V. Tomar, K. Kolluri, M. R. Gungor, and D. Maroudas, "Surface Morphological Response of Crystalline Solids to Mechanical Stresses and Electric Fields," Symposium on *Multiphysics Materials Modeling from Atoms to Continuum* in honor of Professor Sidney Yip, 10th U.S. National Congress for *Computational Mechanics*, July 2009, Columbus, Ohio.

47. A. R. Muniz, T. Singh, and D. Maroudas, "Effects of Hydrogen Chemisorption on the Structure and Deformation of Carbon Nanotubes," Symposium on *Multiphysics Materials Modeling from Atoms to Continuum* in honor of Professor Sidney Yip, 10th U.S. National Congress for *Computational Mechanics*, July 2009, Columbus, Ohio.

48. D. Maroudas, "Surface Engineering by Simultaneous Action of Multiple External Fields," Second Program Meeting on *Physical Behavior of Materials*, U.S. Department of Energy, Office of Basic Energy Sciences, March 2011, Warrenton, Virginia.

49. D. Maroudas, "Surface Morphological Response of Crystalline Solids to Mechanical Stresses and Electric Fields," 7th GRACM International Congress on *Computational Mechanics*, Greek Association of Computational Mechanics (GRACM), June-July 2011, Athens, Greece.

50. D. Maroudas, "Design of New Nanomaterials with Optimal Electronic Function Using Computational Nanoscience," Symposium to honor the 2010 Wilhelm Award Recipient (Prof. I. G. Kevrekidis), AIChE Annual Meeting, October-November 2012, Pittsburgh, Pennsylvania.

51. D. Maroudas, "Surface Engineering by Simultaneous Action of Multiple External Fields," Third Principal Investigators' Meeting on *Physical Behavior of Materials*, U.S. Department of Energy, Office of Basic Energy Sciences, April 2013, Potomac, Maryland.

52. D. Maroudas, "External-Field-Driven Surface Stabilization and Patterning," 2015 *Physical Behavior of Materials* Principal Investigators' Meeting, Division of Materials Sciences and Engineering, DOE Office of Basic Energy Sciences, March-April 2015, Gaithersburg, Maryland.

53. D. Maroudas, "External-Field-Driven Stabilization and Patterning of Materials Surfaces," Minisymposium on *Growth, Instabilities and Evolutions of Thin Films and Micro/Nanostructures*, SIAM Conference on *Mathematical Aspects of Materials Science*, May 2016, Philadelphia, Pennsylvania.

54. D. Maroudas, "Physically Driven Patterning of Surfaces, Thin Films, and Two-Dimensional Materials," 2017 *Physical Behavior of Materials* Principal Investigators' Meeting, Division of Materials Sciences and Engineering, DOE Office of Basic Energy Sciences, May 2017, Gaithersburg, Maryland.

55. L. Du, M. Khenner, and D. Maroudas, "Kinetics of Nanoring Formation on Surfaces of Stressed Thin Films," Minisymposium on *Models and Mechanisms for Nanoscale Crystal Growth*, SIAM Conference on *Mathematical Aspects of Materials Science*, July 2018, Portland, Oregon.

56. D. Maroudas, "Pattern Formation on Surfaces of Strained Thin Films," Session *in Honor of Yannis Kevrekidis' 60th Birthday*, AIChE Annual Meeting, November 2019, Orlando, Florida.

57. D. Maroudas, M. Chen, A. Ramasubramaniam, and A. R. Muniz, "Graphene Derivatives and Metamaterials: Structure-Properties Relations Obtained by Atomic-Scale Modeling," Innovation Award Lecture 2020, Advanced Materials Lecture Series, International Association of Advanced Materials (IAAM), October 2020, Virtual lecture.

58. D. Dasgupta, C.-S. Chen, B. D. Wirth, and D. Maroudas, "Continuum-scale Modeling of Surface Morphological Response of Plasma-Facing Tungsten," 63rd Annual Meeting of the APS Division of Plasma Physics, November 2021, Pittsburgh, Pennsylvania.

59. A. R. Muniz and D. Maroudas, "Superlattices of Finite Interlayer-Bonded Domains in Twisted Bilayer Graphene – Structural, Electronic, and Some Thermodynamic Properties," Plenary Talk, *International Conference on New Carbon Nanomaterials*: *Ultrathin Diamond Films*, December 2021, Moscow, Russia (virtual conference).

60. D. Dasgupta, S. Blondel, A. Weerasinghe, C.-S. Chen, D. Maroudas, and B. D. Wirth, "On the Onset of 'Fuzz' Formation in Plasma-Facing Materials: A Hierarchical Multiscale Modeling Approach," 10th International Conference on Multiscale Materials Modeling, October 2022, Baltimore, Maryland.

Invited Seminars and Colloquia

1. Physical Sciences Seminar, IBM T. J. Watson Research Center, February 1992, Yorktown Heights, New York.

2. Chemical Engineering Departmental Seminar, University of Illinois at Urbana-Champaign, February 1992, Urbana-Champaign, Illinois.

3. Chemical Engineering Departmental Seminar, University of California, Santa Barbara, March 1992, Santa Barbara, California.

4. Chemical Engineering Departmental Seminar, University of California, Berkeley, March 1992, Berkeley, California.

5. Chemical Engineering Departmental Seminar, The Johns Hopkins University, March 1992, Baltimore, Maryland.

6. Chemical Engineering Departmental Colloquium, University of California, Berkeley, October 1995, Berkeley, California.

7. Solid-State Division Seminar, Oak Ridge National Laboratory, February 1996, Oak Ridge, Tennessee.

8. Division of Chemistry and Materials Science Seminar, Lawrence Livermore National Laboratory, March 1996, Livermore, California.

9. Chemical Engineering Departmental Seminar, University of California, Santa Barbara, May 1996, Santa Barbara, California.

10. Device & Process Modeling and Nanotechnology Seminar, NASA Ames Research Center, February 1997, Moffett Field, California.

11. Silicon Science and Technology Division Colloquium, IBM T. J. Watson Research Center, December 1997, Yorktown Heights, New York.

12. Computational Materials Physics Seminar, Department of Physics and Division of Engineering and Applied Sciences, Harvard University, December 1997, Cambridge, Massachusetts.

13. Chemical Engineering Departmental Seminar, Princeton University, February 1998, Princeton, New Jersey.

14. Chemical Engineering & Materials Science Departmental Seminar, University of Minnesota, April 1998, Minneapolis, Minnesota.

15. Chemical Engineering Departmental Seminar, Massachusetts Institute of Technology, April 1998, Cambridge, Massachusetts.

16. Chemical Engineering Departmental Colloquium, University of Illinois at Urbana-Champaign, September 1998, Urbana-Champaign, Illinois.

17. Mechanical & Environmental Engineering Departmental Seminar, University of California, Santa Barbara, November 1998, Santa Barbara, California.

18. Chemical Engineering Departmental Colloquium, Stanford University, November 1998, Stanford, California.

19. Chemical Engineering Departmental Colloquium, University of Wisconsin, April 1999, Madison, Wisconsin.

20. Chemical Engineering Departmental Seminar, California Institute of Technology, October 1999, Pasadena, California.

21. Materials Modeling Seminar, Massachusetts Institute of Technology, September 2000, Cambridge, Massachusetts.

22. Transport Phenomena Seminar, Massachusetts Institute of Technology, September 2000, Cambridge, Massachusetts.

23. Physical Mathematics Seminar, Massachusetts Institute of Technology, October 2000, Cambridge, Massachusetts.

24. Molecular Modeling & Simulation Seminar, Massachusetts Institute of Technology, November 2000, Cambridge, Massachusetts.

25. Chemical Engineering Departmental Seminar, University of Massachusetts, Amherst, February 2001, Amherst, Massachusetts.

26. Complex Materials Seminar, Princeton Materials Institute, March 2001, Princeton, New Jersey.

27. Materials Theory Seminar, Princeton Materials Institute, March 2001, Princeton, New Jersey.

28. Continuum Mechanics Seminar, Massachusetts Institute of Technology, May 2001, Cambridge, Massachusetts.

29. Chemical Engineering Departmental Seminar, Massachusetts Institute of Technology, May 2001, Cambridge, Massachusetts.

30. Chemical Engineering Departmental Seminar, Northwestern University, May 2001, Evanston, Illinois.

31. Chemical Engineering Departmental Seminar, University of Massachusetts, Amherst, October 2001, Amherst, Massachusetts.

32. Chemical Engineering Departmental Seminar, State University of New York at Buffalo, November 2001, Buffalo, New York.

33. Chemical Engineering Departmental Seminar, University of Delaware, November 2001, Newark, Delaware.

34. Chemical Engineering Departmental Seminar, University of California, Santa Barbara, December 2001, Santa Barbara, California.

35. Physics Departmental Seminar, California State University at Northridge, December 2001, Northridge, California.

36. Chemical Engineering Departmental Seminar, University of California, Los Angeles, January 2002, Los Angeles, California.

37. United Technologies Research Center Seminar, March 2003, E. Hartford, Connecticut.

38. Process Systems Engineering Consortium Seminar, University of Massachusetts, Amherst, June 2003, Amherst, Massachusetts.

39. Workshop on *Aging and Long-Term Reliability of Microelectronics Materials and Devices*, Vanderbilt University, October 2003, Nashville, Tennessee.

40. IBM T. J. Watson Research Center, Microelectronics Division Seminar, October 2004, Yorktown Heights, New York.

41. Chemical & Biomolecular Engineering Departmental Seminar, University of Pennsylvania, December 2004, Philadelphia, Pennsylvania.

42. Chemical Engineering & Materials Science Departmental Seminar, University of Minnesota, February 2005, Minneapolis, Minnesota.

43. Chemical Engineering & Materials Science Departmental Seminar, University of Minnesota, September 2005, Minneapolis, Minnesota.

44. Chemical Engineering Departmental Seminar, Stanford University, October 2005, Stanford, California.

45. Chemical and Biological Engineering Departmental Seminar, Tufts University, November 2005, Medford, Massachusetts.

46. Chemical Engineering Departmental Seminar, Iowa State University, March 2006, Ames, Iowa.

47. Computational Materials Physics Seminar, Department of Physics and Astronomy, Vanderbilt University, October 2006, Nashville, Tennessee.

48. Chemical and Biomolecular Engineering Departmental Seminar, University of Maryland, December 2006, College Park, Maryland.

49. United Technologies Research Center Seminar, March 2007, E. Hartford, Connecticut.

50. Applied Mathematics Seminar, University of Massachusetts Amherst, October 2007, Amherst, Massachusetts.

51. Chemical Engineering Departmental Seminar, Colorado School of Mines, November 2007, Golden, Colorado.

52. Connecticut River Valley Quantum Chemistry Group Seminar, December 2007, Amherst, Massachusetts.

53. Symposium on *Recent Advances in Materials Physics* in honor of Professor Sokrates T. Pantelides, Vanderbilt University, April 2009, Nashville, Tennessee.

54. Saint-Gobain Northboro Research Center Seminar, October 2009, Northboro, Massachusetts.

55. Materials Science and Engineering Departmental Seminar, Drexel University, January 2012, Philadelphia, Pennsylvania.

56. Materials Science and Engineering Departmental Seminar, University of Illinois at Urbana-Champaign, October 2013, Urbana-Champaign, Illinois.

57. Spring 2014 Polymer Event Seminar, University of Massachusetts, May 2014, Amherst, Massachusetts.

58. Division of Materials Science and Engineering Seminar, Boston University, October 2014, Boston, Massachusetts.

59. Cabot Corporation Business and Technology Center Research Seminar, January 2015, Billerica, Massachusetts.

60. High-Performance Computing Seminar, University of Massachusetts, April 2015, Amherst, Massachusetts.

61. Penn Institute for Computational Science (PICS) and Applied Mathematics and Computational Science (AMCS) Colloquium, University of Pennsylvania, March 2016, Philadelphia, Pennsylvania.

62. Chemical and Biomolecular Engineering Departmental Seminar, Rice University, April 2017, Houston, Texas.

63. Chemical and Biomolecular Engineering Departmental Seminar, New York University, March 2019, Brooklyn, New York.

64. Chemical and Biological Engineering Departmental Seminar, Iowa State University, February 2021, Ames, Iowa.

65. Chemical and Biological Engineering Departmental Seminar, Tufts University, November 2021, Medford, Massachusetts.

66. Computational Nuclear Engineering Seminar, University of Tennessee, Knoxville, October 2022, Knoxville, Tennessee.

67. Materials Colloquium and Materials Science and Engineering Seminar, UMass Amherst, October 2023, Amherst, Massachusetts.

Contributed Presentations: 583 contributed (oral and poster) presentations in national and international conferences.