

DIMITRIOS MAROUDAS – List of Publications

Journal Articles

1. 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).
2. 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).
3. 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).
4. D. Maroudas and R. A. Brown, "Model of Dislocation Locking by Oxygen Gettering in Silicon Crystals," *Applied Physics Letters* **58**, 1842-1844 (1991).
5. 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).
6. D. Maroudas and R. A. Brown, "Atomistic Calculation of the Self-Interstitial Diffusivity in Silicon," *Applied Physics Letters* **62**, 172-174 (1993).
7. 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).
8. S. T. Pantelides, D. Maroudas, and D. B. Laks, "Defects in Heterogeneous Solids: From Microphysics to Macrophysics," *Materials Science Forum* **143**, 1-8 (1994).
9. 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).
10. 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).
11. D. Maroudas, "Dynamics of Transgranular Voids in Metallic Thin Films Under Electromigration Conditions," *Applied Physics Letters* **67**, 798-800 (1995).
12. 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).
13. D. Maroudas and S. Shankar, "Electronic Materials Process Modeling," *Journal of Computer-Aided Materials Design* **3**, 36-48 (1996).
14. 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).
15. 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).
16. B. Meng, D. Maroudas, and W. H. Weinberg, "Structure of the Chemisorbed Acetylene on the Si(001)-(2 \times 1) Surface and the Effect of Coadsorbed Atomic Hydrogen," *Chemical Physics Letters* **278**, 97-101 (1997).
17. 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).

18. 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).
19. 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).
20. 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).
21. L. J. Gray, D. Maroudas, and M. N. Enmark, "Galerkin Boundary-Integral Method for Evaluating Surface Derivatives," *Computational Mechanics* **22**, 187-193 (1998).
22. 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).
23. 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).
24. S. Ramalingam, D. Maroudas, E. S. Aydil, and S. P. Walch, "Abstraction of Hydrogen by SiH₃ from Hydrogen-Terminated Si(001)-(2×1) Surfaces," *Surface Science* **418**, L8-L13 (1998).
25. 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).
26. 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).
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28. 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).
29. S. Ramalingam, D. Maroudas, and E. S. Aydil, "Visualizing Radical-Surface Interactions in Plasma Deposition Processes: Reactivity of SiH₃ Radicals with Silicon Surfaces," *IEEE Transactions on Plasma Science* **27**, 104-105 (1999).
30. 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).
31. 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).
32. B. Z. Nosh, 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).
33. S. Ramalingam, D. Maroudas, and E. S. Aydil, "Atomistic Simulation Study of the Interactions of SiH₃ Radicals with Silicon Surfaces," *Journal of Applied Physics* **86**, 2872-2888 (1999).

34. L. A. Zepeda-Ruiz, B. Z. Nosh, 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).
35. S. Ramalingam, P. Mahalingam, E. S. Aydil, and D. Maroudas, "Theoretical Study of the Interactions of SiH₂ Radicals with Silicon Surfaces," *Journal of Applied Physics* **86**, 5497-5508 (1999).
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38. D. Maroudas, "Multi-Scale Modeling of Hard Materials: Challenges and Opportunities for Chemical Engineering," *AIChE Journal* **46**, 878-882 (2000).
 - **Invited Perspective Article**
39. 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).
40. 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).
41. 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).
42. 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).
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45. J. Zhao, D. Maroudas, and F. Milstein, "Thermal Activation of Shear Modulus Instabilities in Pressure-Induced bcc→hcp Transitions," *Physical Review B* **62**, 13799-13802 (2000).
46. 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).
47. 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).
48. 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).

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51. D. Maroudas, "Modeling of Radical-Surface Interactions in the Plasma-Enhanced Chemical Vapor Deposition of Silicon Thin Films," *Advances in Chemical Engineering* **28**, 251-296 (2001).
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57. S. Sriraman, E. S. Aydil, and D. Maroudas, "Atomic-Scale Analysis of Deposition and Characterization of a-Si:H Thin Films Grown from SiH Radical Precursor," *Journal of Applied Physics* **92**, 842-852 (2002).
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61. L. A. Zepeda-Ruiz, W. H. Weinberg, and D. Maroudas, "Combined Effects of Substrate Compliance and Film Compositional Grading on Strain Relaxation in Layer-by-Layer Semiconductor Heteroepitaxy: The Case of InAs/In_{0.50}Ga_{0.50}As/GaAs(111)A," *Surface Science* **540**, 363-378 (2003).
62. S. Sriraman, P. Mahalingam, E. S. Aydil, and D. Maroudas, "Mechanism and Energetics of Dimerization of SiH₂ Radicals on H-Terminated Si(001)-(2×1) Surfaces," *Surface Science* **540**, L623-L630 (2003).

63. S. Agarwal, B. Hoex, M. C. M. van de Sanden, D. Maroudas, and E. S. Aydil, "Absolute Densities of N and excited N₂ in an N₂ Plasma," *Applied Physics Letters* **83**, 4918-4920 (2003).
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80. 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).
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82. S. Agarwal, M. S. Valipa, B. Hoex, M. C. M. van de Sanden, D. Maroudas, and E. S. Aydil, "Interaction of SiH₃ Radicals with Amorphous Deuterated (Hydrogenated) Silicon Surfaces," *Surface Science* **598**, 35-44 (2005).
83. F. Milstein, J. Zhao, S. Chantasiriwan, and D. Maroudas, "Applicability of Born's Stability Criterion to Face-Centered-Cubic Crystals in [111] Loading," *Applied Physics Letters* **87**, Article No. 251919, 3 pages (2005).
84. M. S. Valipa and D. Maroudas, "Atomistic Analysis of the Mechanism of Hydrogen Diffusion in Plasma Deposited Amorphous Silicon Thin Films," *Applied Physics Letters* **87**, Article No. 261911, 3 pages (2005).
85. K. Kolluri, L. A. Zepeda-Ruiz, C. S. Murthy, and D. Maroudas, "Kinetics of Strain Relaxation in Si_{1-x}Ge_x Thin Films on Si(100) Substrates: Modeling and Comparison with Experiments," *Applied Physics Letters* **88**, Article No. 021904, 3 pages (2006).
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104. V. Tomar, M. R. Gungor, and D. Maroudas, "Theoretical Analysis of Texture Effects on the Surface Morphological Stability of Metallic Thin Films," *Applied Physics Letters* **92**, Article No. 181905, 3 pages (2008).
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Patents

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