Curriculum Vitae: Doyl E. Dickel

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Education

PhD: Clemson University, *Physics*, December 2011, Advisor: Dr. Apparao M. Rao

Dissertation Title: Electrical Detection of Mechanical Resonance in Nanotubes and Semiconducting Nanowires

B.S.: California Institute of Technology, *Physics with honors*, May 2007

Teaching Experience

1. Lecturer, ME 4123: Failure of Engineering Materials. Mississippi State University, 2020.
2. Lecturer, ME 8373: Integrated Computational Materials Engineering. Mississippi State University, 2019.
3. Lecturer, Physics 2213: Physics I. Mississippi State University, 2016.
4. Lab Instructor, Physics 124: Physics Lab I. Clemson University, 2009-2010.
5. Lab Instructor, Physics 223: Physics Lab II. Clemson University, 2007.
6. Physics 207: General Physics I (assisted Prof. Apparao Rao), 2007.

Academic Experience and Appointments

August 2007-August 2008: Graduate Research Fellow (Clemson University)

August 2008-May 2010: Graduate Teaching Assistant (Clemson University)

June 2010-June 2012: Graduate Research Assistant (Clemson University)

August 2012-July 2014: Research Associate (Karlsruhe Institute of Technology)

September 2014-May 2018: Postdoctoral Associate (Mississippi State University)

June 2018-August 2020: Assistant Research Professor (Mississippi State University)

August 2020-Present: Assistant Professor, Mechanical Engineering (Mississippi State University)

Most cited papers:

1. K. Schulz, **D. Dickel**, S. Schmitt, S. Sandfeld, D. Weygand, and P. Gumbsch (2014): Analysis of Dislocation Pileups using a Dislocation based

Continuum Theory. *Modelling Simul. Mater. Sci. Eng.* **22**, 025008. (55 citations)

2. **D. Dickel**, M. I. Baskes, I Aslam, C. D. Barrett (2018): New interatomic potential for MgAlZn alloys with specific application to dilute Mg-based alloys system. *Model. Simul. Mater. Sci. Eng.* **26** (4), 045010 (47 citations)
3. **D. Dickel**, C. D. Barrett, R. L. Carino, M. I. Baskes, M. F. Horstemeyer (2018): Mechanical Instabilities in the Modelling of Phase Transitions in Titanium. *Model. Simul. Mater. Sci. Eng.* **26**, 065002 (22 citations)
4. **D. Dickel**, D. K. Francis, and C. D. Barrett (2020): Neural network aided development of a semi-empirical interatomic potential for titanium. *Computational Materials Science* 171, 109157. (17 citations)
5. D. Saini, H. Behlow, R. Podila, **D. Dickel**, B. Pillai, M. J. Skove, S. M. Serkiz, and A. M. Rao (2014): Mechanical Resonances of Helically Coiled Carbon Nanowires. *Scientific Reports* **4**, 5542. (16 citations)

Refereed Journal Publications

1. **D. Dickel**, M. J. Skove and A. M. Rao (2009): An Analytic Characterization of the Harmonic Detection of Resonance Method *J. Appl. Phys.* **106**, 044515.
2. **D. Dickel**, M. S. Daw (2010): Improved Calculation of Vibrational Mode Lifetimes in Anharmonic Solids – Part I: Theory" *Comp. Mat. Sci.* **47**, 698.
3. **D. Dickel**, M. S. Daw (2010): Improved Calculation of Vibrational Mode Lifetimes in Anharmonic Solids – Part II: Numerical Results. *Comp. Mat. Sci.* **49**, 445.
4. B. Elliott, H. Behlow, **D. Dickel**, G. Keskar, M. J. Skove, and A. M. Rao (2011).: Deconvolution of Damping Forces with a Nonlinear Microresonator. *Rev. Sci. Instr.* **82**, 055103
5. D. Saini, **D. Dickel**, R. Podila, M. J. Skove, S. Serkiz, and A. M. Rao (2012): Fundamental mechanism for electrically actuated mechanical resonances in ZnO nanowhiskers. *Phys. Rev. B*. **86**, 205312.
6. K. Lingam, J. Reppert, **D. Dickel**, R. Podila, P. Puneet, E. Sheftic, N. Kuthirummal, M. Skove, J. He, and A. M. Rao (2012): Reexamination of Infrared Spectra of Bi Nanorods: L-T Transition, Surface States or Extrinsic Phases. *ACS Nano* **07,** 1230003.
7. D. Saini, H. Behlow, R. Podila, **D. Dickel**, B. Pillai, M. J. Skove, S. M. Serkiz, and A. M. Rao (2014): Mechanical Resonances of Helically Coiled Carbon Nanowires. *Scientific Reports* **4**, 5542.
8. K. Schulz, **D. Dickel**, S. Schmitt, S. Sandfeld, D. Weygand, and P. Gumbsch (2014): Analysis of Dislocation Pileups using a Dislocation based Continuum Theory. *Modelling Simul. Mater. Sci. Eng.* **22**, 025008.
9. **D. E. Dickel**, K. Schulz, S. Schmitt, and P. Gumbsch (2014): A Continuum Formulation of Stress Correlations of Dislocations in Two Dimensions. *Technische Mechanik* **34**, 205-212.

10. Y. Gao, **D. Dickel**, D. Harrison, and M. S. Daw (2014): Improved Calculation of Vibrational Mode Lifetimes in Anharmonic Solids – Part III: Extension to Fourth Moment. *Comp. Mat. Sci.* **89**, 12-18.

11. **D. Dickel**, K. Schulz, S. Schmitt, and P. Gumbsch (2014): Dipole Formation and Yielding in a Two-Dimensional Continuum Dislocation Model. *Phys. Rev. B* **90** (9), 094118.

12. **D. Dickel**, T. G. Tenev, P. Gullett, M. F. Horstemeyer (2016): The Notion of Plastic Material Spin in Atomistic Simulations. *Model. Simul. Mater. Sci. Eng.* **24** (8), 085010.

13. B. D. Huddleston, **D. E. Dickel**, M. F. Horstemeyer, N. Williams, K. Danielson, K., and Y. Hammi (2017). Damage Progression and Fragmentation in Atomistic, Single Crystal Copper at High Strain Rates. *Solid State Phenomena* **258**, 49-52

14. **D. Dickel**, M. I. Baskes, I Aslam, C. D. Barrett (2018): New interatomic potential for MgAlZn alloys with specific application to dilute Mg-based alloys system. *Model. Simul. Mater. Sci. Eng.* **26** (4), 045010

15. H. Wang, **D. Dickel**, M. S. Daw (2018): Theoretical treatment of anharmonicity of vibrational modes of single-walled carbon nanotubes. *J Raman Spectrosc.* 2018;1-6.

16. **D. Dickel**, C. D. Barrett, R. L. Carino, M. I. Baskes, M. F. Horstemeyer (2018): Mechanical Instabilities in the Modelling of Phase Transitions in Titanium. *Model. Simul. Mater. Sci. Eng.* **26**, 065002

17. S. A. Brauer, W. R. Whittington, H. Rhee, P. G. Allison, **D. E. Dickel**, C. K. Crane, M. F. Horstemeyer (2018): Stress-state, Temperature, and Strain Rate Dependence of Vintage ASTM A7 Steel. *Journal of Engineering Materials and Technology* **141**(2), 021002

18. **D. Dickel**, S. R. Gwaltney, S. Mun, M. I. Baskes, M. F. Horstemeyer (2018): A Dispersion-Corrected Modified Embedded-Atom Method Bond Order Interatomic Potential for Sulfur. *Journal of Physical Chemistry A. 122(49),* 9572-9578.

19. **D. E. Dickel**, C. D. Barrett (2019): Methods for the Determination of Diffusionless Transformation Conditions from Atomistic Simulations. *Model. Simul. Mater. Sci. 27(2)*, 023001

20. Aslam, I., M. I. Baskes, **D. E. Dickel**, S. Adibi, B. Li, H. Rhee, M. Asle Zaeem, and M. F. Horstemeyer (2019): Thermodynamic and Kinetic Behavior of Low-Alloy Steels: An Atomic Level Study Using an Fe-Mn-Si-C Modified Embedded Atom Method (MEAM) Potential." *Materialia,* 100473.

21. **D. Dickel** & M. S. Daw (2019): First-principles electronic structure in second-moment calculation of mode frequencies: Failure of quasiharmonic approximation in silicon. *Phys. Rev. B*. ***100****(21)* 214314.

22. **D. Dickel**, D. K. Francis, and C. D. Barrett (2020): Neural network aided development of a semi-empirical interatomic potential for titanium. *Computational Materials Science* 171, 109157.

23. B. Huddleston, **D. Dickel**, N. Williams, K. Danielson, Y. Hammi, A. Bowman, M.I. Baskes, and M. F. Horstemeyer (2020): Correlating damage progression to fragmentation at high strain rates using molecular dynamics. *Model. Simul. Mater. Sci. 28(2),* 025009

24. G. Esteban-Manzanares, R. Alizadeh, I. Papadimitriou, **D. Dickel**, C. D. Barrett, and J. LLorca (2020): Atomistic simulations of the interaction of basal dislocations with MgZn2 precipitates in Mg alloys. *Materials Science and Engineering: A* 139555.

25. **D. Dickel**, M. S. Daw (2020): Calculation of Vibrational Mode Lifetimes in Simple Anharmonic Potentials Using Eigenstates of the Quasi-Harmonic Liouvillian. *Computational Materials Science 185,* 109918.

26. J. Reeves, E. Williams, C. Plouffe, C. Staples, W. Carlucci, R. Smith, Y. Hammi, W. Whittington, **D. Dickel**, and Y. Liu (2021) Combined Experimental and Computational Failure and Fatigue Analysis of a Socket Drive Adapter. *Journal of Failure Analysis and Prevention* 21(4), 1434-1444.

27. M. Nitol, **D. E. Dickel**, C. D. Barrett (2021): Artificial Neural Network Potential for pure Zinc. *Computational Materials Science 188*, 110207.

28. **Dickel, D.**, Nitol, M., & Barrett, C. D. (2021). LAMMPS implementation of rapid artificial neural network derived interatomic potentials. *Computational Materials Science*, *196,* 110481.

29. H. Zhou, **D. E. Dickel**, M. I. Baskes, & M. A. Zaeem (2021): A modified embedded-atom method interatomic potential for bismuth. *Model. Simul. Mater. Sci. 29(6),* 065008.

30. Nitol. M. **Dickel, D.**, & C. D. Barrett (2021): Unraveling Mg⟨ c+ a⟩ slip using neural network potential. *Philosophical Magazine*, 1-23.

31. Nitol, M., **Dickel, D.**, & C. D. Barrett (2022): Machine learning models for predictive materials science from fundamental physics: An application to titanium and zirconium. *Acta Materialia* 224, 117347.

32. Ababtin, S., Adibi, S., Mun, S., Carino, R. L., **Dickel, D. E.** Gwaltney, S. R., Novotny, M., Baskes, M. I., & Horstemeyer, M. F. (2022) Single-wall carbon nanotube mechanical behavior using the modified embedded atom method with bond order (MEAM-BO). *Model. Simul. Mater. Sci.*

33. Reeves, J., Liu, Y., Hammi, Y., **Dickel, D.**, Stone, T. & Bounds, C. (2022) Automation and High-Speed Forming of Thin Layer Composite. *IJESI*, **11** (3), 34-54.

34. Connor, M. B., Calhoun, M., Cohen, M., Lum, D., KaJuana, M., Toellner, S., and **Dickel, D.** (2022). Failure Analysis of a M7X1 High-Speed Steel Tap. *Journal of Failure Analysis and Prevention*. **22**, 1431-1441.

35. Nitol, M. S., Dang, K., Fensin, S. J., Baskes, M. I., **Dickel, D. E.**, & Barrett, C. D. (2023). Hybrid interatomic potential for Sn. *Physical Review Materials*, 7(4), 043601.

Book Chapters

1. J.D. Taylor, B. Elliott, **D. Dickel**, G. Keskar, J. Gaillard, M.J. Skove and A.M. Rao (2008) Harmonic Detection of Resonance Methods for Micro- and Nano-Cantilevers: Theory and Selected Applications. In: *Frontiers in Nanoscience and Nanotechnology*, Ed. Anant Narlikar, Oxford University Press, Oxford, England.
2. **D. Dickel**, S. Mun, M. Baskes, S. Gwaltney, R.K. Prabhu, M.F. Horstemeyer (2022) Density Functional Theory and Bridging to Classical Interatomic Force Fields. In: *Multiscale Biomechanical Modeling of the Brain*, Ed. Raj Prabhu, Mark Horstemeyer, Academic Press.

Books

1. "Physics for Realists: Quantum Mechanics" A. Rizzi (2018) IAP Press, Baton Rouge, LA (contributor)

Patents

1. J. Reppert, J. Gaillard, B. Elliot, **D. Dickel**, P. Menguc, and A.M. Rao (2007): Substrate Patterning by Electron Emission-Induced Displacement. *US Patent Pending*.

Contributed Talks

1. D. Dickel, G. Keskar, M. J. Skove, and A. M. Rao (2009): Determination of Intrinsic Damping in a Multi-walled Carbon Nanotube using the Harmonic Detection of Resonance Method. APS March Meeting, Pittsburgh, PA.
2. M. Daw, D. Dickel (2010): Improved Calculation of Vibrational Mode Lifetimes in Anharmonic Solids. APS March Meeting, Portland, OR.
3. D. Dickel, M.J. Skove, and A.M. Rao (2010): Harmonic Detection of Resonance as a Method to Characterize Cantilevered Carbon Structures. Carbon 2010, Clemson, SC.
4. D. Dickel, K. Schulz, S. Schmitt, and P. Gumbsch (2013): A Continuum Formulation of Stress Correlations of Dislocations in Two Dimensions. ICMM3, Warsaw, Poland.
5. D. Dickel, K. Schulz, S. Schmitt, and P. Gumbsch (2013): Stress correlations of dislocations in a double-pileup configuration: a continuum dislocation density approach. COMPLAS XII, Barcelona, Spain.
6. D. Dickel, K. Schulz, and P. Gumbsch (2014): Continuum Dislocation Dynamics Modeling in Two Dimensions. WCCM XI, Barcelona, Spain.
7. D. Dickel, M. I. Baskes, M. F. Horstemeyer (2015): Atomistic Modelling of Titanium Polymorphism Using the Modified Embedded Atom Method. MRS 2015 Fall Meeting, Boston, MA
8. D. Dickel (2016): Efficient Modeling of Continuum Deformation Variables in Atomistic Simulations. TMS Annual Meeting and Exhibition 2016, Nashville, TN.

9. D. Dickel, M. F. Horstemeyer, M. Tschopp (2018): Calibration of a Titanium MEAM Potential to High Temperature Behavior. TMS Annual Meeting and Exhibition 2018, Phoenix, AZ.
10. D. Dickel, M. F. Horstemeyer (2018): Plastic Material Spin in Atomistic Simulations. TMS Annual Meeting and Exhibition 2018, Phoenix, AZ.
11. D. Dickel, D. Francis, C. D. Barrett (2018): Toward a Machine Learning Aided Interatomic Potential for Multi-element Alloys: Application to Binary Compounds. MMM 2018, Osaka, Japan.
12. D. Seely, B. Huddleston, S. Mun, A. Vo, N. Lee, D. Dickel, K. Limmer (2022): Atomistic Study on Diffusion and Trapping of Hydrogen in Nanocrystalline Steel. TMS Annual Meeting and Exhibition 2022.
13. C. D. Barrett, D. Dickel, M. Nichols, K. Sebeck, M. Conner (2022): Materials design of polycarbonates at the atomistic scale with machine learning. Automotive Research Center Annual Meeting 2022.
14. C. Jouhari, Y. Liu, and D. Dickel (2023): Phase-Field Modeling of Aluminum Foam Based on Molecular Dynamics Simulations. TMS Annual Meeting and Exhibition 2023.
15. C. Jouhari, Y. Liu, and D. Dickel (2023): Molecular Dynamics Study of Gradient Energy Coefficient and Grain-Boundary Migration in Aluminum Foam

Invited Talks

1. “Stress Determination in a Continuum Formulation of Dislocation Dynamics” **D. Dickel**. Clemson University, April 2nd 2014
2. “Quantum Mechanics- Hydrodynamic Analogs” **D. Dickel**, S. Strickland. Institute for Advanced Physics 13th Annual Summer Conference, July 31st 2015
3. “Quantum Dynamics of a Superball” **D. Dickel**, Institute for Advanced Physics Annual Summer Conference 14th Annual Summer Conference, July 29th 2016
4. “Bouncing Droplets: A Hydrodynamic Analog of Quantum Mechanics” **D. Dickel**, S. Strickland. Institute for Advanced Physics 14th Annual Summer Conference, July 29st 2016
5. “Bouncing Oil Droplets: A Macroscopic Model of “Quantum” Phenomena” **D. Dickel**. Clemson University, August 22nd 2017
6. “Bridging Length Scales: Machine Learning of Density Functional Theory” **D. Dickel**. Mississippi State University, March 6th, 2021.
7. “Machine Learned Interatomic Potentials for Molecular Dynamic Simulation of Metal Systems” **D. Dickel**. Clemson University, February 2nd 2022.

Student Mentoring

1. Denver Seely, PhD. Fall 2018. Thesis Topic: “The Process-Structure-Property Relations of a Laser Engineered Net Shaping (LENS) Titanium-Aluminum-Vanadium Alloy that is Functionally Graded with Boron”
2. Yangqing Dou, PhD. Fall 2018. Thesis Topic: “Multiscale Modeling of Copper/Nickel Impact”
3. Imran Aslam, PhD. Fall 2018. Thesis Topic: “Atomistic Investigation of Inhibition Layers in Galvanized Steel”
4. Bradley Huddleston, PhD.Fall 2019. Thesis Topic: “Multiscale Modeling of Fragmentation”
5. Mashroor Nitol, PhD Fall 2021. Thesis Topic: “Predictive Computational Materials Modeling with Machine Learning: Creating the Next Generation of Atomistic Potential Using Neural Networks”
6. Henan Zhou, PhD. Expected graduation: Fall 2023. Thesis Topic: “Atomistic Investigation of Shape Memory Behavior in Ferroelectric Perovskites”

Honors and Awards

1. Nominated for outstanding graduate researcher award for the College of Engineering and Science at Clemson University for the year 2009-2010.
2. Nominated for the Oak Ridge Associated Universities (ORAU) travel award to attend 61st Lindau Meeting of Nobel Laureates and Students in Lindau, Germany, 2011.
3. IOP Publishing Outstanding Reviewer Award 2019.
4. Mechanical Engineering Outstanding Junior Faculty Research Award 2021. Mississippi State University, Department of Mechanical Engineering

Society Memberships

1. American Physical Society
2. American Society for Metals
3. Materials Research Society
4. Minerals, Metals, and Materials Society (TMS)