James A. Stewart

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Research Interests

Computational physics and materials science – Thermodynamics and kinetics of materials; nanoscale phenomena and microstructure evolution; kinetic surface roughening; processing-microstructure-property-performance relationships; materials in extreme environments; shock and detonation physics; radiation effects; atomistic and mesoscale simulation methods; numerical modeling and code development.

Academic Education

Ph.D. **Photonics**, University of Arkansas, Fayetteville, AR **05/2016**

M.S. **Photonics**, University of Arkansas, Fayetteville, AR **08/2012**

B.A. **Physics and Mathematics**, Alfred University, Alfred, NY **05/2009**

Professional Experience

Sandia National Laboratories, Albuquerque, NM **01/2020 – Present**

R&D S&E Computer Science, Explosives Research and Development Department

- Multiscale modeling to characterize the shock and detonation behavior of explosive materials and devices: microstructures, equations-of-state, constitutive models, reactions, etc.

Sandia National Laboratories, Albuquerque, NM **03/2017 – 01/2020**

Postdoctoral Appointee, Nanostructure Physics Department

- DFT and MD simulations of radiation damage and shock behavior in metals and semiconductors, phase-field modeling of processing-microstructure relationships in nanostructured materials.

University of Michigan, Ann Arbor, MI **06/2016 – 03/2017**

Research Fellow, Department of Materials Science and Engineering

- Mesoscale modeling of microstructural influences, such as grain boundaries and intermetallics, on the evolution of corrosion pit morphologies via phase-field and smoothed boundary methods.

University of Arkansas, Fayetteville, AR **08/2012 – 05/2016**

Senior Graduate Assistant, Department of Mechanical Engineering

- Advisor: Douglas E. Spearot, Dissertation: Phase-Field Models for Simulating Physical Vapor Deposition and Microstructure Evolution of Thin Films.

University of Arkansas, Fayetteville, AR **01/2010 – 08/2012**

Senior Graduate Assistant, Department of Mechanical Engineering

- Advisor: Douglas E. Spearot, Thesis: Atomistic Simulations of Defect Nucleation and Intralayer Fracture in Molybdenum Disulphide (MoS_2) During Nanoindentation.

Alfred University, Alfred, NY **06/2008 – 08/2008**

Summer Research Intern, Department of Physics and Astronomy (Stull Observatory)

- CCD imaging and photometry of cataclysmic variable star systems to elucidate outburst periods and provide light-curve data to the Center for Backyard Astrophysics.

Synergistic Activities

Honors and Awards:

Finalist, 3rd Rising Stars in Computational Materials Science **11/2021**

- Award to recognize the accomplishments and promise of early career researchers.

NSF Scholarship in STEM, University of Arkansas **01/2010**

- Award to allow graduate students in STEM fields to focus on coursework and research.

Natasha Goldowski Renner Prize in Physics, Alfred University **05/2009**

- Award to recognize a student who has shown excellence and promise in the study of physics.

Mentoring:

Interns and Graduate Students, Sandia National Laboratories

- Gabriel Brookman (Carleton College), Elton Chen (Georgia Tech), Skylar Grayson (Whitman College), Parker Hamilton (BYU), Elizabeth Herman (NC State), Christopher Nellis (Virginia Tech), Daniel Vizoso (Georgia Tech)

Research Communications Group Leader, University of Arkansas **08/2011 – 05/2013**

- Managed a small group of first- and second-year graduate students to promote and develop skills in technical communication and project planning.

Peer-Review:

Applied Mathematical Modelling, Computational Materials Science

Additional Skills and Experience

Computing and Software:

Systems, Document Preparation, and Project Planning

- macOS, Linux, Microsoft Office Suite, Microsoft Project, LaTeX

Programming Languages, Data Analysis, and Visualization

- Bash, Python, Fortran, C/C++, MPI, OpenMP, Make/CMake, ParaView, DAKOTA, OVITO, VTK, Gnuplot, ImageMagick, ImageJ

Scientific and Technical:

Materials Modeling and Simulation

- Electronic structure calculations (Quantum Espresso, Socorro), molecular statics and dynamics

(LAMMPS), phase-field and mesoscale methods (MEMPHIS), hydrocodes and shock physics (CTH, LGR), deterministic and stochastic cluster dynamics

Mathematical and Numerical Modeling

- Finite difference methods with explicit and implicit solvers, smoothed boundary methods, parallel and distributed computing

Statistics and Data Analysis

- Variance-based sensitivity analysis (Sobol method), supervised machine learning (e.g., linear regression models, Gaussian processes), principal component analysis

Awarded Grants and Funding

1. Understanding Microstructure Variability in Vapor-Deposited Energetic Materials by Using Phase-Field Methods. Funding Source: Sandia National Laboratories LDRD, Funding Period: 03/2020 – 09/2020, Awarded Amount: $100,000.

Journal Articles and Publications

15. **J.A. Stewart** (2022) Recent progress on the mesoscale modeling of architected thin-films via phase-field formulations of physical vapor deposition. *Computational Materials Science*, **211**, 111503.

14. **J.A. Stewart**, J.D. Olles, and M.A. Wood (2022) Elucidating size effects on the yield strength of single-crystal Cu via the Richtmyer-Meshkov instability. *Journal of Applied Physics*, **131** (11), 114901.

13. M. Powers, **J.A. Stewart**, R. Dingreville, B.K. Derby, and A. Misra (2021) Compositionally-Driven Formation Mechanism of Hierarchical Morphologies in Co-Deposited Immiscible Alloy Thin Films. *Nanomaterials*, **11** (10), 2635.

12. D. Montes de Oca Zapiain, **J.A. Stewart**, and R. Dingreville (2021) Accelerating phase-field-based microstructure evolution predictions via surrogate models trained by machine learning methods. *npj Computational Materials*, **7** (1), 1 – 11.

11. E. Herman, **J.A. Stewart**, and R. Dingreville (2020) A data-driven surrogate model to rapidly predict microstructure morphology during physical vapor deposition. *Applied Mathematical Modelling*, **88**, 589 – 603.

10. **J.A. Stewart**, N.A. Modine, and R. Dingreville (2020) Re-examining the silicon self-interstitial charge states and defect levels: A density functional theory and bounds analysis study. *AIP Advances*, **10** (9), 095004.

9. C.W. Lee, **J.A. Stewart**, R. Dingreville, S.M. Foiles, and A. Schleife (2020) Multiscale simulations of electron and ion dynamics in self-irradiated silicon. *Physical Review B*, **102** (2), 024107.

8. **J.A. Stewart** and R. Dingreville (2020) Microstructure morphology and concentration modulation of nanocomposite thin-films during simulated physical vapor deposition. *Acta Materialia*, **188**, 181 – 191.

7. A.F. Chadwick, **J.A. Stewart**, R.A. Enrique, S. Du, and K. Thornton (2018) Numerical Modeling of Localized Corrosion Using Phase-Field and Smoothed Boundary Methods. *Journal of The Electrochemical Society*, **165** (10), C633 – C646.

6. **J.A. Stewart**, A.A. Kohnert, L. Capolungo, and R. Dingreville (2018) Design and analysis of forward and reverse models for predicting defect accumulation, defect energetics, and irradiation conditions. *Computational Materials Science*, **148**, 272 – 285.

5. **J.A. Stewart**, G. Brookman, P. Price, M. Franco, W. Ji, K. Hattar, and R. Dingreville (2018) Characterizing single isolated radiation-damage events from molecular dynamics via virtual diffraction methods. *Journal of Applied Physics*, **123** (16), 165902.

4. **J.A. Stewart** and D.E. Spearot (2018) Physical vapor deposition of multiphase materials with phase nucleation via a coupled phase-field approach. *Computational Materials Science*, **143**, 71 – 79.

3. **J.A. Stewart** and D.E. Spearot (2017) Phase-field simulations of microstructure evolution during physical vapor deposition of single-phase thin films. *Computational Materials Science*, **131**, 170 – 177.

2. **J.A. Stewart** and D.E. Spearot (2016) Phase-field models for simulating physical vapor deposition and grain evolution of isotropic single-phase polycrystalline thin films. *Computational Materials Science*, **123**, 111 – 120.

1. **J.A. Stewart** and D.E. Spearot (2013) Atomistic simulations of nanoindentation on the basal plane of crystalline molybdenum disulphide (MoS_2). *Modelling and Simulation in Materials Science and Engineering*, **21** (4), 045003.

Posters, Presentations, and Talks

14. **J.A. Stewart**, R. Knepper, and D.L. Damm (July 2022) Effects of Microstructure and Binder on the Shock-to-Detonation Behavior of Hexanitrostilbene (HNS). *Poster at the APS SCCM Meeting.* Anaheim, CA.

13. **J.A. Stewart** (Dec 2019) Atomistic Insights of Materials in Extreme Environments via Virtual Characterization. *Seminar in the Materials Science in Radiation & Dynamics Extremes Group at Los Alamos National Laboratory.* Los Alamos, NM.

12. **J.A. Stewart** (Dec 2019) Microstructure Morphology and Concentration Modulation of Nanocomposite Thin-Films During Simulated PVD. *Seminar in the Energetic Materials Dynamic & Reactive Science Department at Sandia National Laboratories.* Albuquerque, NM.

11. **J.A. Stewart**, J.D. Olles, R.R. Wixom, and R. Dingreville (June 2019) Shock Hugoniot Relationships for Crystalline and Amorphous HNAB: Insights from Atomistic Simulations and Virtual Diffraction Calculations. *Poster at the APS SCCM Meeting.* Portland, OR.

10. **J.A. Stewart** (Jan 2019) Nanoscale to Mesoscale Materials Modeling and Simulation: Shock Behavior and Materials Processing. *Seminar in the Energetics Characterization Department at Sandia National Laboratories.* Albuquerque, NM.

9. **J. Stewart**, A. Kohnert, L. Capolungo, and R. Dingreville (May 2018) Design and Analysis

of Forward and Reverse Models for Predicting Defect Accumulation, Defect Energetics, and Irradiation Conditions. *Poster at the EFRC NEES All-Hands Meeting.* Albuquerque, NM.

8. **J.A. Stewart** and R. Dingreville (Mar 2018) Characterizing displacement cascade damage in bulk Si via virtual diffraction techniques. *Presentation at the TMS Annual Meeting & Exhibition.* Phoenix, AZ.

7. **J. Stewart**, P. Price, K. Hattar, and R. Dingreville (Sep 2017) A Virtual Diffraction Method for Guiding the Characterization of Isolated Radiation-Induced Nanoscale Damage Events. *Poster at the CINT Annual User Meeting.* Santa Fe, NM.

6. **J.A. Stewart** (Dec 2016) Phase-Field Models for Simulating Physical Vapor Deposition and Microstructure Evolution in Polycrystalline Thin Films. *Seminar in the Structural & Thermal Analysis Department at Sandia National Laboratories.* Albuquerque, NM.

5. **J.A. Stewart** and D.E. Spearot (Feb 2016) Phase-Field Models for Simulating Microstructure Development During Physical Vapor Deposition of Single-Phase Polycrystalline Thin Films. *Presentation at the TMS Annual Meeting & Exhibition.* Nashville, TN.

4. **J.A. Stewart** and D.E. Spearot (Nov 2015) A Phase-Field Model for Simulating Microstructure Development During Physical Vapor Deposition of Isotropic Polycrystalline Thin Films. *Presentation at the MRS Fall Meeting & Exhibit.* Boston, MA.

3. **J.A. Stewart** and D.E. Spearot (Oct 2015) A Phase-Field Model for Simulating Microstructure Development During Physical Vapor Deposition of Isotropic Multiphase Thin Films. *Presentation at the SES Annual Technical Meeting.* College Station, TX.

2. **J.A. Stewart** and D.E. Spearot (Apr 2014) Development of a Multiphase Phase-Field Model for Simulating Vapor Deposition of Thin-Films. *Poster at the MRS Spring Meeting & Exhibit.* San Francisco, CA.

1. **J. Stewart** and D. Spearot (Oct 2012) Atomistic Simulations of Defect Nucleation and Intralayer Fracture in Molybdenum Disulphide (MoS_2) During Nanoindentation. *Presentation at the SES Annual Technical Meeting.* Atlanta, GA.