James A. Stewart

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Research Interests

Materials Theory and Modeling – Thermodynamics and kinetics of materials, nanoscale phenomena and microstructure evolution, kinetic surface roughening, matter and radiation at extremes, shock wave and detonation physics, radiation effects and defects, light-matter interactions, materials design and optimization, 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 properties of energetic materials and related devices: microstructures, equations-of-state, constitutive models, reaction kinetics.

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 **2021**

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

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

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

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

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

Peer Review:

Applied Mathematical Modelling, Computational Materials Science, Journal of Vacuum Science & Technology A, Materials Letters, Vacuum

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, Gnuplot, ImageMagick, ImageJ, OpenSCAD

Scientific and Technical:

Materials Modeling and Simulation

- Electronic structure (Quantum ESPRESSO, Socorro, VASP), molecular statics and dynamics (LAMMPS), phase-field and mesoscale methods (MEMPHIS), shock hydrodynamics and multiphysics (ALEGRA, CTH), deterministic and stochastic cluster dynamics

Mathematical and Numerical Modeling

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

Data Science, Analytics, and Statistics

- Linear least-squares regression, Gaussian process regression, principal component analysis, variance-based sensitivity analysis (Sobol' method)

Awarded Grants and Funding

2. A Theoretical Analysis on the Dynamic Behavior and Electromechanical Response of PZT. Funding Source: Sandia National Laboratories LDRD, Funding Period: 01/2024 – 09/2024, Awarded Amount: $150,000.

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

Research Profiles and Identifiers: Google Scholar, Semantic Scholar

17. **J.A. Stewart**, J.K. Startt, and R. Dingreville (2023) A molecular dynamics study on the Mie-Grüneisen equation-of-state and high strain-rate behavior of equiatomic CoCrFeMnNi. *Materials Research Letters*, **11**(12), 1055 – 1062.

16. J.M. Monti, **J.A. Stewart**, J.O. Custer, D.P. Adams, D. Depla, and R. Dingreville (2023) Linking simulated polycrystalline thin film microstructures to physical vapor deposition conditions. *Acta Materialia*, **245**, 118581.

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.

Presentations, Posters, and Talks

12. **J.A. Stewart**, D.E. Kittell, A.S. Tappan, R. Knepper, D.L. Damm, W.P. Bassett, and L.W. Tuttle (2024) Reactive Burn Model Calibration for Vapor Deposited HNS and PETN Films Using XHVRB. *Poster at the International Detonation Symposium.* Kansas City, MO.

11. **J.A. Stewart**, J. Monti, W. Bassett, R. Knepper, and D.L. Damm (2024) Effects of Microstructure and Surface Roughness on Initiation Behavior in Vapor-Deposited Explosives. *Presentation at the International Detonation Symposium.* Kansas City, MO.

10. **J.A. Stewart**, M. Sakano, J. Brown, M. Wood, D. Kittell, R. Knepper, and D.L. Damm (2023) Mesoscale Simulations on the Effects of Rate-Dependent Strength and the Shock-to-Detonation Behavior of Explosive Materials. *Poster at the APS SCCM Meeting.* Chicago, IL.

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

8. **J.A. Stewart**, J.D. Olles, R.R. Wixom, and R. Dingreville (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.

7. **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. *Poster at the EFRC NEES Meeting.* Albuquerque, NM.

6. **J.A. Stewart** and R. Dingreville (2018) Characterizing Displacement Cascade Damage in Bulk Si via Virtual Diffraction Techniques. *Presentation at the TMS Annual Meeting & Exhibition.* Phoenix, AZ.

5. **J.A. Stewart** and D.E. Spearot (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 (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 (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 (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 (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.