

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, microstructure-property relationships, materials in extreme environments, shock and detonation physics, radiation effects, light-matter interactions, 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	
<ul style="list-style-type: none">• 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	
<ul style="list-style-type: none">• 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	
<ul style="list-style-type: none">• 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	
<ul style="list-style-type: none">• 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 (MoS₂) 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.

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 (NWChem, Quantum Espresso, Socorro), molecular statics and dynamics (LAMMPS), phase-field and mesoscale methods (MEMPHIS), shock hydrodynamics and multiphysics (ALEGRA, CTH, LGR), 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, Web of Science

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.

POSTERS, PRESENTATIONS, AND TALKS

14. **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.
13. **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.
12. **J.A. Stewart** (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.
11. **J.A. Stewart** (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.
10. **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.

9. **J.A. Stewart** (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.
8. **J. Stewart**, 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.
7. **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.
6. **J.A. Stewart** (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 (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.