Alex Selimov

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Summary

I am a PhD candidate in Materials Science at the Georgia Institute of Technology working with Dr. David McDowell seeking appointment to a postdoctoral position in which I can apply my experience with atomistic modeling, atomic structure analysis, and simulation toolset development for discovery of novel high-entropy materials.

Education

- **Georgia Institute of Technology** (North Avenue, Atlanta, GA 30332)
  PhD in Materials Science and Engineering (August 2017 - December 2022 Expected)
- **University of Central Florida** (4000 Central Florida Blvd, Orlando, FL 32816)
  B.S. in Mechanical Engineering (August 2013 - December 2016)
  Bachelor's Thesis: Characterization of Dispersion and Residual Stress in Nanoparticle Reinforced Hybrid Carbon Fiber Composites

Publications:

- Selimov, A., Chu, K., & McDowell, D. (2022). Effects of interdiffusion on shear response of semi-coherent {111} interfaces in Ni/Cu, *in review*
- Selimov, A., Chu, K., & McDowell, D. L. (2022). Coarse-grained atomistic modeling of dislocations and generalized crystal plasticity. Journal of Micromechanics and Molecular Physics, 1-23.
- Selimov, A., Xu, S., Chen, Y., & McDowell, D. (2021). Lattice dislocation induced misfit dislocation evolution in semi-coherent {111} bimetal interfaces. Journal of Materials Research, 1-16.
- Selimov, A., Jahan, S. A., Barker, E., Dackus, P., Carolan, D., Taylor, A., Raghavan, S. (2018). Silane functionalization effects on dispersion of alumina nanoparticles in hybrid carbon fiber composites. Applied optics, 57(23), 6671-6678.
- Selimov, A. P., Hoover, R., Fouliard, Q., Manero, A. C., Dackus, P., Carolan, D., … Raghavan, S. (2017). Characterization of hybrid carbon fiber composites using photoluminescence spectroscopy. In 58th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference (p. 0123).
- Manero II, A., Selimov, A., Fouliard, Q., Knipe, K., Wischek, J., Meid, C., … Raghavan, S. (2017). Piezospectroscopic evaluation and damage identification for thermal barrier coatings subjected to simulated engine environments. Surface and Coatings Technology, 323, 30-38.
- Hanhan, I., Selimov, A., Carolan, D., Taylor, A. C., Raghavan, S. (2017). Quantifying alumina nanoparticle dispersion in hybrid carbon fiber composites using photoluminescent spectroscopy. Applied spectroscopy, 71(2), 258-266.
- Hanhan, I., Selimov, A. P., Carolan, D., Taylor, A., Raghavan, S. (2016). Characterizing mechanical properties of hybrid alumina carbon fiber composites with piezospectroscopy. In 57th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference (p. 1413).

Presentations

- Selimov, A., Xu, S., Chen, Y., McDowell, D. (2019). Concurrent Atomistic-Continuum Framework for Slip Transfer Across Phase Interfaces In Nanoscale Metallic Multilayer Composites. International Conference on Plasticity, Damage, and Fracture 2020.
- Selimov, A., Chen, Y., McDowell, D. (2019) Collective Dislocation-Interface Interactions using the Concurrent Atomistic-Continuum Method. International Mechanical Engineering Congress Exposition
- Selimov, A. P., Hoover, R., Fouliard, Q., Manero, A. C., Dackus, P., Carolan, D., … Raghavan, S. (2017). Characterization of hybrid carbon fiber composites using photoluminescence spectroscopy. In 58th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference

Grants

- Role: Co-PI (PI. David McDowell), Amount: 1,997,041 Service Units
  Funding Source: Extreme Science and Engineering Discovery Environment (XSEDE)
  Project Title: Concurrent atomistic-continuum simulations of extended scale defect interactions in heterogeneous microstructures (TG-MSS150010)
  Funding Period: Jan 1, 2019 - June 30, 2022

Research Experience

McDowell Research Group, Dr. David McDowell, Georgia Tech
Graduate Research Assistant (August 2017 – Present)

- Worked on the development and extension of the Concurrent Atomistic-Continuum method for running massively parallel coarse-grained atomistic simulations of dislocation interactions with interfaces and other defect structures in nanolaminate and stainless steel materials.
- Improved parallel implementation and tuned calculation algorithms of in-house simulation suite obtaining runtime reductions of 66%. Also contributed to a fork of LAMMPS implementing the CAC simulation method.
- Implemented the finite element method to solve conservation law field equations to enable reductions in degrees-of-freedom leading to reduced computational cost.
- Tested various metrics to numerically characterize atomic interface structure of metallic semi-coherent interfaces and applied machine learning methods to track the interface structure evolution with loading.
- Modeled solute distributions in diffuse Cu/Ni semi-coherent interfaces and their effect on the glide of interface misfit dislocations and overall interface properties.
- Investigated the sequential interactions between dislocations and obstacles in various systems to quantify evolving obstacle strength and interaction mechanisms.

Mechanics of Materials Organization, Dr. Xiaowang Zhou, Sandia National Lab
Intern - Engineering Sciences Summer institute (May 2021 – Aug 2021)

- Studied the barrier strength of grain boundaries with embedded helium bubbles to improve hardening predictions of irradiated stainless steel materials, collaboration continued beyond internship period.
- Extended molecular dynamics barostat algorithms to coarse-grained regions for pressure relaxation.
- Worked on CAC capabilities for high temperature dynamics simulations through development of new finite element types and extension of neighboring codes for cluster potentials.

AeroStructures Lab, Dr. Seetha Raghavan, UCF
Research Assistant (September 2013 – December 2016)

- Utilized photoluminescence spectroscopy and piezospectroscopy for the characterization of material and mechanical properties in ceramic and composite materials.
- Worked on collaborative project with Imperial College London (Dr. Ambrose Taylor's Research Group) for the testing and characterization of novel hybrid carbon fiber reinforced polymer (HCFRP) composites.
- Worked on collaborative project with German Aerospace Center (DLR) to study stress development in thermally grown oxide layers of thermal barrier coatings.

Pollock Research Group, Dr. Tresa Pollock, UCSB
RISE Undergraduate Intern, NSF funded REU (June – August 2015)

- Studied Magnesium-zinc alloys to determine methods for texture weakening for improvement of material properties through analyzing presence of intermetallic particles.
- Utilized scanning electron microscopy to take secondary electron images, backscatter electron images, and to analyze crystallographic texture through electron backscatter diffraction
- Prepared image analysis tools to determine volume fraction of intermetallic particles from SEM images for comparison to grain size distribution of samples with Matlab.

Skills

- Programming in Fortran, C, and C++ with additional expertise utilizing the Message Passing Interface (MPI) for implementation of parallel and scalable simulation tools.
- Programming in MATLAB, HTML, and CSS.
- Data analysis and pipeline creation using Python with Numpy, Scipy, Scikit-Learn, Pandas, and Tkinter modules. Additional familiarity with Jupyter Notebooks.
- Expertise in atomistic simulations using LAMMPS with Molecular Statics, Molecular Dynamics, and Monte-Carlo methods.
- Expertise with Linux software environment and building applications for use with computing cluster architectures.
- Familiarity with software development methodologies including test case design and CI/CD pipelines.