LIAM ANDREW MYHILL

Mechanical Engineer ~ Materials Researcher

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SUMMARY

A continuing graduate student/materials researcher at Clemson University interested in the fields of **Crystal Plasticity**, **Uncertainty Quantification**, and **Integrated Computational Material Engineering**. Collaborative developer on open-source modelling software MoDELIB (https://github.com/MoDELib2).

SKILLS

Languages: Python, C++, MATLAB, Bash

Technologies: Microsoft Suite, Pybind11, Pytorch.

Organizations: Graduate Student Advisory Board (Mechanical Engineering Representative & Acting Secretary)

PROJECTS

TRI-Austin — **Alloy Development for Armour Penetration** — **Unclassified Report**
Developed computational workflows to predict ballistic penetration and deformation behavior of novel tungsten-based alloys

SRNL — **Bayesian Calibration of Continuum Defect Models** — **Upcoming Publication**
Utilize state-of-the-art simulation calibration techniques to ensure model agreement between defect behavior observed in molecular dynamics and continuum models

LANL — **Exascale Computing of Material Defect Evolution** — **NPJ Computational Materials**
Facilitated the briding of computational scales between Molecular Dynamics (MD) and Discrete Dislocation Dynamics (DDD). Research consultant on dislocation behavior.

LANL — **Analysis of Thermally Activated Dislocation Behaviors** — **Clemson Thesis**
Developed computational workflow to capture the energy landscape of glissile dislocations in continuum DDD. Validated results with transition-state theory rate analysis.

Clemson — **Continuum Modeling of Dislocations in Polymer Crystals** — **Upcoming Publication**
Developing a novel DDD model to describe defect evolution in crystalline polymer matrices. Currently replicates macroscopic plasticity trends.

Clemson — **Analysis of Grain Boundary Solute Drag via Kinetic Monte Carlo Simulation** — **Upcoming Publication**
Conducted over 200 individual simulation cases to gather statistics on concentration gradients local to a mobile grain boundary. Presented results at REU poster symposium (Clemson 2021).

EDUCATION + SCHOLARSHIP

1/2024 - — **Doctor of Philosophy, Mechanical Engineering** — **Clemson University**
Established candidacy 10/2025-GPA 3.68/4.00

1/2022 - 12/2023 — **Masters of Science, Mechanical Engineering** — **Clemson University**
Successfully defended Masters thesis 11/2023 - GPA 3.59/4.00

8-2017/12-2021 — **Bachelors of Science, Mechanical Engineering** — **Clemson University**
Graduated Dec. 2021 - GPA 3.41/4.00

2021 — **NSF Funded Undergraduate Research Program** — **Clemson University**
Funded by NSF for KMC research

8-2017/12-2021 — **Palmetto Fellows State Scholarship** — **Clemson University**
Maintained GPA requirements for highest level of in-state scholarship (SC)

EXPERIENCE

2/2022 - — **Graduate Research Assistantship** — **Los Alamos National Laboratory / Clemson University**

- Collaborated on project to develop machine learning model to predict trajectories of line defects in crystalline materials.
- Lead the initiative to bridge computational scales through automation programming.
  `Python / C++`

5/2021 - 8/2021 **Undergraduate Research Assistant** **Clemson University**

- Sampled KMC simulations to gather statistics on local material concentration within a doped metallic crystal.
- Drafted manuscript detailing research practice and results. Awaiting advisor approval for submission to academic journal.

`Python / Excel`

5/2019 - 1/2021 **Manufacturing Engineer CO-OP** **Komatsu America Corp.**

- Completely remapped entire floor plan and facilitated restructuring of assembly areas.
- Developed active data-tracking workflow to automatically capture manufacturing process time.

`AutoCAD / SolidWorks / Excel`

PUBLICATIONS

Liam Myhill
ORCID: https://orcid.org/0000-0002-0767-3799

- **2025**
  Activation Entropy Helps Explain Anomalous Flow Stress Temperature Dependence in Copper
  Arxiv.org (Awaiting Publication)
  Mohammadhossein Nahavandian, Liam Myhill, Enrique Martinez.
  A comparison of techniques utilized to predict the rate of thermal activation for a dislocation dipole microstructure in copper.
  DOI: `https://doi.org/10.2139/ssrn.5390840`

- **2025**
  Atomistically-Informed Partial Dislocation Dynamics of Multi-Principal Element Alloys
  npj Computational Materials
  Xin Liu, Hyunsoo Lee, Yang Li, Liam Myhill, Nikhil Chandra Admal, Giacomo Po, Enrique Martinez, Yinan Cui
  DOI: `https://doi.org/10.2139/ssrn.5358125`

- **2024**
  Data-Driven Modeling of Dislocation Mobility from Atomistics using Physics-Informed Machine Learning
  NPJ Computational Materials
  Yifeng Tian, Soumendu Bagchi, Liam Myhill, Giacomo Po, Enrique Martinez Saez, Yen Ting Lin, Nithin Mathew, Danny Perez.
  Multiscale modeling approach whereby dislocation defects generated in Molecular Dynamics are populated into Dislocation Dynamics to train a Physically Informed Graph Neural Network on general trends of dislocation mobility.
  DOI: `https://doi.org/10.21203/rs.3.rs-4171499/v1`

- **2023**
  The Generation of a Physics Informed Machine Learning Model to Predict Defect Evolution in Materials & On the Thermally Activated Regime of Dislocation Motion: A Simulation Driven Study on the Mechanical Behavior of Crystals
  Masters Thesis
  Liam Myhill.
  A summary of the work published in NPJ Computational Materials and overview of individual research related to thermally activated dislocation mobility in FCC materials.
  URL: `https://open.clemson.edu/all_theses/4198`

PRESENTATIONS + POSTERS

- **2025**
  Verification and Validation of Appropriate Model Parameters for Mesoscale Dislocation Dynamics Simulations of Thermally Activated Dislocation Motion
  Dislocations 2025 Conference Poster
  Outlined the use of gaussian process surrogate models to facilitate the calibration of mesoscale materials models to atomistic observations.

- **2024**
  Material Design: Strength by Diversity
  Winner of Clemson's Fall 2024 π-Minute Thesis Competition
  Highlighting unexplored design space of engineering materials through composition diversity and improved mechanical properties.

- **2024**
  Information Dynamics in Continuum Dislocation Models: Provision and Extraction
  Clemson University Graduate Seminar Series
  Overview of information exchange between atomistic models and continuum models pertaining to both solid solution strengthening and spectral analysis of dislocations.

- **2023**
  Material Defects: Because nothing is perfect!
  Clemson University π-Minute Thesis Competition
  Brief discussion of line defects in materials and their implications on crystal plasticity, including simulation techniques used to study dislocation mobility in atomistics and continuum frameworks.

- **2023**
  Improving Dislocation Dynamics Mobility Laws through Convolutional Neural Network
  Clemson University Graduate Seminar Series
  Overview of computational and analytical methods utilized to generate a physics informed machine learning model for the study of dislocation mobility.
  URL: `https://cecas.clemson.edu/gsrseminar/wp-content/uploads/2023/01/Spring-2023-Myhill.pdf`

- **2023**
  Improving Dislocation Dynamics (DD) Mobility Laws via Graph Neural Network (GNN)
  Clemson University Graduate Research Poster Competition
  Demonstration of information forwarding from the microscale to mesoscale and coarse-graining of atomistic data to improve upon phenomenolgical mobility laws in continuum dislocation dynamics.
  URL: `https://muexly.github.io/team/liam/PosterWorkFinalResized.pdf`

- **2021**
  Analyzing Grain Boundary Dynamics via Kinetic Monte Carlo Simulation
  Clemson University Research Experience for Undergraduates Poster Symposium
  Demonstration about generating mobile grain boundaries with solute atoms and application of kinetic monte carlo simulation to study boundary dynamics and composition gradients in proximity to the grain boundary.
  URL: `https://muexly.github.io/team/liam/REUPosterFinalDraft.pdf`