

Kevin Chu, PhD Candidate Materials Science - Georgia Tech

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The online version is available at <https://kvnchv.github.io/cv>

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I am a graduate research assistant pursuing my PhD in Materials Science under [Dr. David L. McDowell](#) at the Georgia Institute of Technology. My expertise lies in molecular dynamics and scientific software development. My research focuses primarily on physics-based atomistic and coarse-grained atomistic modeling of multicomponent alloys and fundamental deformation processes at the nanoscale.

Education

- **Georgia Institute of Technology** -- PhD Materials Science and Engineering (Projected 2022)
- **University of California, Los Angeles** -- B.S. Materials Science and Engineering 2017

Publications

2020

- Chu, K., Foster, M. E., Sills, R. B., Zhou, X., Zhu, T., & McDowell, D. L. (2020). Temperature and composition dependent screw dislocation mobility in austenitic stainless steels from large-scale molecular dynamics. *npj Computational Materials*, 6(1), 1-10.
- Spataru, C.D., Chu, K., Sills, R.B. Zhou, X. (2020). Molecular Statics Analyses of Thermodynamics and Kinetics of Hydrogen Cottrell Atmosphere Formation Around Edge Dislocations in Aluminum. *JOM* 72, 3020–3027 .

2018

- Chu, K., Gruber, J., Zhou, X. W., Jones, R. E., Lee, S. R., & Tucker, G. J. (2018). Molecular dynamics studies of InGaN growth on nonpolar (11 $\bar{2}$ 0) GaN surfaces. *Physical Review Materials*, 2(1), 013402.

2017

- Zhou, X. W., Jones, R. E., & Chu, K. (2017). Polymorphic improvement of Stillinger-Weber potential for InGaN. *Journal of Applied Physics*, 122(23), 235703.

Conference presentations

Chu, K., Chen, D., Diaz, A., Selimov, A., Chen, Y., Zhu, T., McDowell, D. (2019). *Application of the concurrent atomistic-continuum (CAC) method to dislocation reaction pathway modeling in FCC metals*. at Materials Science and Technology, Portland, OR

Research experience

Georgia Institute of Technology Atlanta, GA

Graduate Research Assistant - David L. McDowell Group

Aug 2018 - Present

I design and execute multiscale modeling experiments using LAMMPS and custom simulation codes to elucidate novel nanoscale deformation mechanisms in multicomponent alloys. This comprises:

- software development activities to improve or extend existing methods relevant to the [Concurrent Atomistic-Continuum \(CAC\)](#) method
- co-development of [LAMMPS-CAC](#) integration and validation
- simulation/analysis pipelining using a combination of shell and Python scripted workflows, interfacing with high performance computing clusters
- compilation of resultant data for the writing of manuscripts.

education lammmps hpc python c++ fortran

Sandia National Laboratories Livermore, CA

Research & Development Graduate Intern

May 2019 - Aug 2019

Executed molecular dynamics modeling and data analysis activities to support the following projects:

- Cottrell atmosphere formation kinetics
- large scale dislocation mobility analysis in 3XX stainless steels

Highlights include the development/implementation of a continuum-scale diffusion model and fully pipelined execution and analysis of multi-parameter space molecular dynamics simulations.

lammmps matlab python hpc

Sandia National Laboratories Livermore, CA

Undergraduate Research Intern

May 2017 - Aug 2017

- Analyzed existing datasets from molecular dynamics simulations of InGaN film deposition to investigate threading dislocation nucleation mechanisms and derived critical film thickness relations and parameters.
- Designed and executed simulations to validate melting temperature of newly developed interatomic potentials
- Developed presentations for further internal dissemination and produced a number of visualizations for publication.

lammmps hpc

University of California, Los Angeles Los Angeles, CA

Undergraduate Research Assistant - Jaime Marian Group

Mar 2016 - May 2017

I assisted with general research tasks relating to computational materials analysis and modelling. Projects included translation of existing calculation/tools from Matlab into C++ (two temperature model, Green's function, and Lennard-Jones potential calculations)

c++ matlab