Aoyan Liang

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EDUCATION

University of Southern California   8/2020-Present
Ph.D. in Materials Science, GPA: 4.0/4.0

University of Southern California   1/2022-5/2024
M.S. in Computer Science (Data Science), GPA: 4.0/4.0

University of Southern California   8/2018-5/2020
M.S. in Materials Science, GPA: 4.0/4.0

Southwest Jiaotong University, China   9/2014-6/2018
B.Eng. in Materials Science (Mao Yisheng Honors College), GPA: 3.64/4.0

Certifications
AI for Science on Supercomputers (Argonne National Laboratory)   12/2022
Fundamentals of Deep Learning (NVIDIA)   6/2021

RESEARCH INTERESTS

Large-scale molecular dynamics (MD) simulations and machine learning (ML) methods for investigating nanoscale dynamical behavior, synthesis processes, structural correlations, and properties of advanced materials such as ceramics, high entropy alloys and metallic glasses.

RESEARCH EXPERIENCE

Lawrence Livermore National Laboratory   6/2024-present
Research Collaborator & CCMS Graduate Intern, Mentor: Dr. Vasily Bulatov & Dr. Sylvie Aubry
Main Projects:

- **Alloy Strengthening Mechanisms: Size Mismatch vs. Stiffness Mismatch**: Conduct extensive large-scale MD simulations to investigate the fundamental mechanisms of alloy strengthening through "alchemical" modifications of embedded atom method (EAM) potentials.

University of Southern California   8/2020-present
Graduate Research Assistant, Advisor: Prof. Paulo Branicio
Main Projects:

- **High Entropy Alloy (HEA) Films Phase Formation during Physical Vapor Deposition**: Combine MD simulations, molecular statics calculations, experiments, and ML methods to elucidate structure-property relationships in HEA thin films. Interpret and reveal the influence of atomic size differences on phase formation.
- **Energy Landscapes for Disordered Materials:** Utilize the activation relaxation technique (ART) to explore the energy landscapes of metallic glasses, particularly focusing on how heat treatment and strain influence activation processes.
- **Colloid Transport in Nanoporous Media**: Perform dissipative particle dynamics (DPD) simulations to study the colloid transport behavior in complex nanoporous media. Explore the effects of colloid concentration, flow rate, colloid-colloid and colloid-collector interactions.
- **Hot-press Sintering for Nanoceramics**: Conducted large-scale MD simulations using Fortran+MPI codes to investigate the effects of temperature, pressure, and particle size on the

densification process and microstructural evolution of AlN nanoceramics.

Southwest Jiaotong University, China   4/2016-6/2018
Research Assistant, Advisor: Prof. Xiaosong Jiang
Main Project:

- **Microstructure and Properties of Graphene Reinforced Copper Matrix Composites**: Prepared three graphene strengthened copper matrix composites based on the $Cu-Ti_3SiC_2-C$ system, and further processed high pressure torsion. Improved the mechanical properties of copper matrix through fine grain strengthening mechanism. Published a literature reviewed on dispersion methods and mechanisms of graphene.

TEACHING EXPERIENCE

University of Southern California
Teaching Assistant
Courses:

- MASC 575 - Basics of Atomistic Simulation of Materials   Spring 2022
- MASC 110L - Materials Science (Lab section)   Fall 2022
- MASC 520 - Mathematical Methods for Deep Learning   Spring 2023
- MASC 503 - Thermodynamics of Materials   Fall 2023
- CHE 499 - Confectionary Manufacturing - Science and Technology   Spring 2024

PUBLICATIONS

ORCID: https://orcid.org/0000-0001-5100-6232
Google Scholar Profile: https://scholar.google.com/citations?user=OHhN9N_f6JoC&hl=en
Web of Science Profile: https://www.webofscience.com/wos/author/record/HKM-4861-2023

1. **Liang, A.**, Liu, C., & Branicio, P. S. (2024). Colloid Transport in Bicontinuous Nanoporous Media. *Langmuir*.
2. Alwen, A., **Liang, A.,** Branicio, P. S., & Hodge, A. M. (2024). Combinatorial and high-throughput investigation of growth nanotwin formation. *Acta Materialia*, 270, 119839.
3. Yuan, S., **Liang, A.**, Liu, C., Tian, L., Mousseau, N., & Branicio, P. S. (2023). The effect of heat treatment paths on the aging and rejuvenation of metallic glasses. *Physical Review Materials*, 7(12), 123603.
4. Yuan, S., **Liang, A.**, Liu, C., Nakano, A., Nomura, K., & Branicio, P. S. (2023). Uncovering hidden vacancy-like motifs in metallic glasses with machine learning. *Materials & Design*, 233, 112185.
5. **Liang, A.**, Goodelman, D. C., Hodge, A. M., Farkas, D., & Branicio, P. S. (2023). $CoFeNiTi_x$ and $CrFeNiTi_x$ high entropy alloy thin films microstructure formation. *Acta Materialia*, 257, 119163.
6. Guan, X., **Liang, A.**, & Branicio, P. S. (2022). High pressure shear induced microstructural evolution in nanocrystalline aluminum. *Computational Materials Science*, 203(15), 111105.
7. **Liang, A.**, Liu, C., & Branicio, P. S. (2021). Hot-press sintering of aluminum nitride nanoceramics. *Physical Review Materials*, 5(9), 096001.
8. **Liang, A.**, Jiang, X., Hong, X., Jiang, Y., Shao, Z., & Zhu, D. (2018). Recent developments concerning the dispersion methods and mechanisms of graphene. *Coatings*, 8(1), 33.

CONFERENCE PRESENTATIONS

1. **Liang, A.**, Liu, C., & Branicio, P. S., Nanoparticle Transport in Bicontinuous Nanoporous Media. Talk presented at: *2024 MFD Student Research Symposium*; March 2024; Los Angeles, CA, USA
2. **Liang, A.**, Goodelman, D. C., Hodge, A. M., Farkas, D., & Branicio, P. S., Exploring the

Composition-Structure Relationships of High Entropy Alloy Thin Films: Combining Experiments and Atomistic Simulations. Poster presented at: *2023 MFD Student Research Symposium*; March 2023; Los Angeles, CA, USA

3. **Liang, A.**, Hodge, A. M., Farkas D., & Branicio P. S., Atomistic modeling of physical vapor deposition and melt-quenching of $CoCrFeNiTi_x$ high entropy alloys. Poster presented at: *2023 TMS Annual Meeting & Exhibition*; March 2023; San Diego, CA, USA.

4. **Liang, A.**, & Branicio, P. S., Atomistic Modeling of Electric-field-assisted Sintering of AlN Nanoceramics. Poster presented at: *2022 MFD Student Research Symposium*; March 2022; Los Angeles, CA, USA

5. **Liang, A.**, Liu, C., & Branicio, P. S., Atomistic Modeling of Hot-press Sintering of AlN Nanoceramics. Poster presented at: *2022 TMS Annual Meeting & Exhibition*; February 2022; Anaheim, CA, USA.

6. **Liang, A.**, Liu, C., & Branicio, P. S., Atomistic Modeling of Hot-Press Sintering of AlN Ceramics. Poster presented at: *2021 MRS Fall Conference*; November 2021; Boston, MA, USA.

7. **Liang, A.**, & Branicio, P. S., Hot-Press Sintering of Aluminum Nitride Nanoceramics. Poster presented at: *2021 MFD Student Research Symposium*; February 2021; Los Angeles, CA, USA

SKILLS

- **Software:** LAMMPS, OVITO, Activation Relaxation Technique (ARTn), Adobe Illustrator, SAS, Origin, Visual Studio, Microsoft Office.
- **Programming Languages:** Python (with ML packages), Fortran (with MPI), C/C++ (with MPI/OpenMP), Java, Spark, SQL (MySQL), R.
- **Operation Systems:** Linux, MacOS, Windows.
- **Other:** Machine Learning, Molecular Dynamics

PROFESSIONAL SERVICE

Reviewer for International Journals (Total: 11 journals, 37 reviews)

Acta Materialia, Applied Surface Science, Chemical Papers**,** Computational Materials Science, Computer Physics Communications, Journal of Alloys and Compounds, Journal of Non-Crystalline Solids, Progress in Materials Science, Scientific Reports, Surface and Interface Analysis, Thin Solid Films.

AWARDS & HONORS

2024 Symposium – MFD Presentations Award Winner	2024
First Place, USC Data Mining Competition (Link)	2023
Rank 17/6714, Modeling Earthquake Damage (DrivenData Competition Leaderboard)	2023
Nominee for 2021 MRS Fall Meeting Best Poster (Materials Research Society)	2021
Master's Student Achievement Award (University of Southern California) (Link)	5/2020
SAS Certified Base Programmer for SAS 9	6/2019
Outstanding Graduate of Southwest Jiaotong University	2018
China National Scholarship (1%)	2016-2017
Grand Comprehensive Scholarship (Southwest Jiaotong University)	2016-2017
First-Class Comprehensive Scholarship (4 times)	2014-2016
Honorable Mention in MCM/ICM	2017
Third Prize in Asia and Pacific Mathematical Contest in Modeling	2016