Aoyan Liang

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Updated on October 20, 2024

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

My research interests lie at the intersection of machine learning (ML) and materials science, particularly in using AI-driven techniques, generative models, and atomistic simulations (including both density functional theory (DFT) and molecular dynamics (MD)) to explore and design advanced materials, with a focus on accelerating materials discovery and innovation.

RESEARCH EXPERIENCE

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

- **Alloy Strengthening Mechanisms: Size Misfit vs. Stiffness Misfit**: 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**: Combine ML methods, MD simulations, DFT calculations, molecular statics calculations, and experiments to elucidate structure-property relationships in HEA thin films.
- **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. Bulatov, V. V., Bertin, N., Aubry, S., Zepeda-Ruiz, L. A., Zhou, X., **Liang, A.,** Oppelstrup, T., Sadig, B. (2024) Network aspects of single crystal plasticity (*Under review*)
2. Carvalho, A. P., **Liang, A.,** Kawasaki, Cupertino-Malheiros, L., Branicio, P. S., & Figueiredo, R. B. (2024) Dynamic recovery as a strengthening mechanism in nanostructured metals (*Under review*)
3. **Liang, A.,** Liu, C., & Branicio, P. S. (2024). Colloid Transport in Bicontinuous Nanoporous Media. *Langmuir*.
4. Alwen, A., **Liang, A.,** Branicio, P. S., & Hodge, A. M. (2024). Combinatorial and high-throughput investigation of growth nanotwin formation. *Acta Materialia*, 270, 119839.
5. 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.
6. 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.
7. **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.
8. Guan, X., **Liang, A.**, & Branicio, P. S. (2022). High pressure shear induced microstructural evolution in nanocrystalline aluminum. *Computational Materials Science*, 203(15), 111105.
9. **Liang, A.**, Liu, C., & Branicio, P. S. (2021). Hot-press sintering of aluminum nitride nanoceramics. *Physical Review Materials*, 5(9), 096001.
10. **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:** VASP, LAMMPS, OVITO, VESTA, 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, Density Functional Theory.

PROFESSIONAL SERVICE

Reviewer for International Journals (Total: 11 journals, 43 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