

Afnan Mostafa

125 Hopeman Building (Box 270132)
University of Rochester, Rochester, NY 14627
amostafa@ur.rochester.edu | afnanmostafa102@gmail.com

Ph.D. Student, Department of Mechanical Engineering

Research Interest

Computational Materials Science, Molecular and Multi-scale Modeling, Machine Learning, Deep Learning, Density Functional Theory, Metamaterials.

Education

Ph.D. in Mechanical Engineering (Expected) September, 2028
Specialization: **Molecular and Multi-scale Modeling, Nanomaterials**
University of Rochester, United States. GPA: 4/4

MS in Mechanical Engineering 09/01/2023
Specialization: **2D Materials, Molecular Simulations**
University of Massachusetts, Amherst, United States. GPA: 3.9/4 (overall)

B.Sc. in Mechanical Engineering 07/2014 - 10/2018
Specialization: **Molecular Modeling, Nanotechnology**
Bangladesh University of Engineering and Technology, Bangladesh. GPA: 3.71/4 (overall)

Professional Experience

Journal Article Reviewer 08/2024 - Present
Nature Communications, Nature Publishing Group, [ORCID](#)


Research & Teaching Assistant 09/2023 - Present
Department of Mechanical Engineering,
University of Rochester, Rochester, NY

Research & Teaching Assistant 01/2021 - 08/2023
Department of Mechanical and Industrial Engineering,
University of Massachusetts, Amherst, MA


HVAC Design Coordinator and Project Supervisor 07/2019 - 01/2021
MEP Design Studio, Dhaka, Bangladesh


Paid Co-op Internship, Engineering Division 03/2018 - 04/2018
Eskayef Pharmaceuticals Ltd., Dhaka, Bangladesh

Awards & Achievements

 MIE Departmental Fellowship, University of Massachusetts Amherst 2021

 University Dean's award for academic excellence in B.Sc. 2016-2018

 University Merit and Technical scholarships for academic excellence in B.Sc. 2014-2016

 National Education Board Scholarship for securing top 100 amongst 230,000 candidates 2011

Publications

Journal Articles (peer-reviewed)

- J1.** Mostafa, A., Vu, L., Guo, Z., Shargh, A. K., Dey, A., Askari, H., Abdolrahim, N., “Phase-transformation assisted twinning in molybdenum nanowires,” *Computational Materials Science*, vol. 244, p. 113 273, 2024.
- J2.** Mostafa, A., Ramasubramaniam, A., Maroudas, D., “Thermal conductivity of 2D diamond superstructures in interlayer-bonded twisted bilayer graphene,” *Applied Physics Letters*, vol. 122, no. 13, 2023.
- J3.** Mostafa, A., Weerasinghe, A., Ramasubramaniam, A., Maroudas, D., “Response of interlayer-bonded bilayer graphene to shear deformation,” *Journal of Applied Physics*, vol. 134, no. 15, 2023.

Journal Articles (under preparation)

- J4.** Li, F., Mostafa, A., Zimmerman, J., Liang, Z., Klinger, L., Yeom, J., Janczak-Rusch, J., Abdolrahim, N., Rabkin, E., “Solid-state dewetting of co-sputtered thin Mo-Cu films accompanied by phase separation,” 2024.
- J5.** Qian, S., Mostafa, A., Li, F., Rabkin, E., Abdolrahim, N., “Orientation-dependent phase transformation in Molybdenum nanowires under uniaxial and bi-axial bending deformation,” 2024.

Conference Proceedings

- C1.** Mostafa, A., Motalab, M., Faiyaz, A. R., Paul, R., “Uniaxial and cyclic stress-strain behavior of lead-free solders at nanoscale,” in *AIP Conference Proceedings*, AIP Publishing, vol. 2324, 2021.

Presentations

A. Mostafa, L. Vu, F. Li, A. Dey, H. Askari, E. Rabkin, and N. Abdolrahim, “Novel Methods for Phase-Transformation-Assisted Twinning in Molybdenum Nanomaterials: Simulation and Experimental Study”, *ASME International Mechanical Engineering Congress and Exposition (IMECE) 2024, Portland, OR (Scheduled)*.

S. Qian, A. Mostafa, F. Li, E. Rabkin, and N. Abdolrahim, “Influence of Non-Uniaxial Bending on Twinning and Phase Transformation in Molybdenum Nanowires”, *ASME International Mechanical Engineering Congress and Exposition (IMECE) 2024, Portland, OR (Scheduled)*.

A. Mostafa, L. Vu, F. Li, A. Dey, H. Askari, E. Rabkin, and N. Abdolrahim, “Atomistic insights on orientation-dependent deformation mechanisms in Molybdenum: Single-crystal nanowires and polycrystals”, *TMS Annual Meeting & Exhibition 2025, Las Vegas, NV (Scheduled)*.

F. Li, A. Mostafa, N. Abdolrahim, J. Zimmerman, Z. Liang, L. Klinger, J. Yeom, J. Janczak-Rusch, and E. Rabkin, “Solid state dewetting of co-sputtered thin Mo-Cu films accompanied by phase separation”, *TMS Annual Meeting & Exhibition 2025, Las Vegas, NV (Scheduled)*.

S. Qian, A. Mostafa, F. Li, E. Rabkin, and N. Abdolrahim, “Influence of Non-Uniaxial Bending on Twinning and Phase Transformation in Molybdenum Nanowires”, *TMS Annual Meeting & Exhibition 2025, Las Vegas, NV (Scheduled)*.

A. Mostafa, A. Ramasubramaniam, and D. Maroudas, “Thermal conductivity of interlayer-bonded bilayer graphene”, *AICHE Annual Meeting 2023, Orlando, FL*.

A. Mostafa, A. Ramasubramaniam, and D. Maroudas, “Atomistic study of thermal and mechanical properties of graphene-nanodiamond composites”, *MSE Poster Symposium 2023, University of Massachusetts, Amherst*.

M. Chen, A. Mostafa, A. Weerasinghe, A. R. Muniz, A. Ramasubramaniam, and D. Maroudas, “2D diamond superstructures in interlayer-bonded twisted bilayer graphene: Mechanical response and thermal transport from molecular-dynamics simulations”, *AICHE Annual Meeting 2022, Phoenix, AZ*.

M. Chen, A. Weerasinghe, A. R. Muniz, **A. Mostafa**, A. Ramasubramaniam, and D. Maroudas, “Thermomechanical properties of nanodiamond superstructures in interlayer-bonded twisted bilayer graphene”, *AICHE Annual Meeting 2021, Boston, MA*.

A. Mostafa, M. Motalab, A. R. Faiyaz, and R. Paul, “Uniaxial and cyclic stress-strain behavior of lead-free solders at the nanoscale”, *AIP Conference Proceedings, 2019, Dhaka, Bangladesh*.

Graduate Thesis

Afnan Mostafa 2023, “Thermal conductivity and mechanical properties of interlayer-bonded graphene bilayers”, University of Massachusetts, Amherst, MA, US.

- Addressed two major bottlenecks in graphene-based bilayers (*i.e.*, brittle failure and reduction in thermal conduction)
- Investigated and compared various types of graphene bilayers for thermal management and shear applications
- [MS Thesis DOI: 10.7275/35901268.0](#)

Selected Academic Projects

FEM formulation in MATLAB and ABAQUS for Hertzian contact

Course Instructor: Hesam Askari, Asst. Professor, ME

Fall 2023, **ME441**

- o Formulated finite element methods from scratch in MATLAB
- o Generated stress and displacement profiles for a Hertzian contact problem
- o Compared such results with ABAQUS-simulated results and theoretical predictions
- o [Report DOI: 10.13140/RG.2.2.32394.48328](#)

Machine learning and neural network models across different programming platforms

Course Instructor: Brendan Mort, Director, CIRC

Fall 2023, **DSCC401**

- o Developed machine learning and neural network models for various test cases
- o Compared accuracy among models written in Python and R
- o Analyzed big data using SPARK
- o [GitHub Repository](#)

Undergraduate Thesis

Afnan Mostafa, et al. **2018**, “Uniaxial and cyclic stress-strain behavior of lead-free solders at nanoscale”, Department of ME, Bangladesh University of Engineering and Technology, Dhaka, Bangladesh.

- Investigated cyclic life of environment-friendly lead-free solder materials through atomistic simulations
- Developed atomistic models to predict the lifetime of such solder alloys
- [DOI: 10.1063/5.0037536](#)

Skills (*ordered by decreasing fluency)

Programming*:	Python, Matlab, C/ C++, Bash, SPARK, R, Go, Fortran, MySQL, SPSS, SAS
Simulation Tools*:	LAMMPS, AtomsK, VMD, ANSYS, ABAQUS
Visualization:	Ovito, Vesta, VMD
3D CAD*:	SolidWorks, AutoCAD, OnShape, Adobe Illustrator
Document Preparation:	L ^A T _E X, MathCAD, Vi, Nano, Microsoft Office Suite
Info-graphic:	Gnuplot, Origin, Plot Digitizer
Job-Scheduling Utility:	Slurm, PBS
Build-Automation:	Make
Others:	Git, High-performance computing, Cluster computing

References

Niaz Abdolrahim, Ph.D.

Associate Professor, Department of Mechanical Engineering,
Scientist, Laboratory for Laser Energetics (LLE),

404 Hopeman Engineering Building, University of Rochester, Rochester, NY 14627.
Tel: (585) 276-7817
E-mail: niaz@rochester.edu
Website: [Advanced Computational Mechanics and Materials Laboratory](#)

Ashwin Ramasubramaniam, Ph.D.

Professor, Mechanical and Industrial Engineering,
Adjunct, Chemical Engineering,
Director, Materials Science & Engineering Graduate Program,
Engineering Lab (ELab), Room 208C,
160 Governors Drive,
University of Massachusetts Amherst, MA 01003, United States.
E-mail: ashwin@umass.edu
Website: [Computational Nanomaterials Laboratory](#)

Dimitrios Maroudas, Ph.D.

Professor and Department Head, Chemical Engineering,
Affiliated Faculty, Materials Science & Engineering,
Adjunct Professor, Chemistry,
Goessmann Laboratory, Room 154A,
Chemical Engineering Department,
686 N Pleasant St., Amherst, MA 01003-9303, United States.
Tel: (413) 545-3617
E-mail: maroudas@ecs.umass.edu
Website: [D. Maroudas Laboratory](#)
