

Afnan Mostafa

Ph.D. Student, Department of Mechanical Engineering

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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., Sharq, 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](https://doi.org/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](https://doi.org/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](https://doi.org/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^AT_EX, 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.

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Scientist, Laboratory for Laser Energetics (LLE),

404 Hopeman Engineering Building, University of Rochester, Rochester, NY 14627.
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Ashwin Ramasubramaniam, Ph.D.
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Adjunct, Chemical Engineering,
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Dimitrios Maroudas, Ph.D.
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Affiliated Faculty, Materials Science & Engineering,
Adjunct Professor, Chemistry,
Goessmann Laboratory, Room 154A,
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