Aaditya Valliyur Rau

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Education

- **Massachusetts Institute of Technology** — Cambridge, MA
  Ph.D., Computational Science and Engineering — *May 2024 - Present*
- **Massachusetts Institute of Technology** — Cambridge, MA
  S.M., Computational Science and Engineering — *August 2022 - May 2024*
- **Johns Hopkins University** — Baltimore, MD
  B.S., Engineering Mechanics, Applied Mathematics & Statistics, Mathematics Minor — *August 2018 - May 2022*

Research Experience

- **Massachusetts Institute of Technology** — Cambridge, MA
  Graduate Research Assistant — *Aug 2022 – Present*

  Contributed to sumMIT finite element software for research in micromechanics, including phase transformation, compatibility stresses, grain boundary diffusion, and chemoelastic fracture.

- **Princeton Plasma Physics Laboratory** — Princeton, NJ (Remote)
  DOE SULI Intern — *Jun 2020 – May 2022*

  Simulated graphite under boron bombardment for fusion reactor design using LAMMPS on PPPL and NERSC clusters

- **Johns Hopkins University, Mechanical Engineering** — Baltimore, MD
  Undergraduate Research Assistant — *Jan 2019 – May 2022*

  Performed molecular dynamics simulations of nanotwinned Ni–Mo–W alloys for MEMS using LAMMPS; studied 3D-printed polymer welds via mechanical testing and microscopy

- **University of Alabama–Birmingham, Physics** — Birmingham, AL
  NSF REU Student — *May – Jul 2019*

  Synthesized and characterized novel "superhard" Ta-B compounds using CVD, XRD, XPS, Raman, and nanoindentation.

- **University of Nebraska–Lincoln, Mechanical & Materials Engineering** — Lincoln, NE
  High School Research Intern — *May – Aug 2016, 2017*

  Optimized graphene growth using chemical vapor deposition; characterized samples with Raman and AFM; assembled graphene/boron-nitride heterostructures for transistor applications

Publications

1. A. Rau, D. Pickard (2025). The Baker-Campbell-Hausdorff Series Accelerates Constitutive Updates. *Journal of Computational Physics*, *540*, 114256
2. T.A. Rulko, A. Rau, G. Chomette, L. Wheeler, D. Mathias, J. Dotson, R. Radovitzky (2025). Stress analysis of asteroids during atmospheric entry and implications for the breakup criterion. *Icarus*, *434*, 116526
3. A. Rau, C.A. Schuh, R. Radovitzky (2024). Quantification of elastic incompatibilities at triple junctions via physics-based surrogate models. *Mechanics of Materials*, *199*, 105163
4. A. Rau, S. Jubin, J.R. Vella, I.D. Kaganovich (2022). Simulations of graphite boronization: A molecular dynamics study of amorphization resulting from bombardment. *Frontiers in Physics*, *10*, 933494
5. S. Jubin, A. Rau, Y. Barsukov, S. Ethier, I. Kaganovich (2022). Boron adatom adsorption on graphene: A case study in computational chemistry methods for surface interactions. *Frontiers in Physics*, *10*, 908694.

6. A. Rau, K. Chakrabarty, W. Gullion, P.A. Baker, I. Bikmukhametov., R.L. Martens, G.B. Thompson, S.A. Catledge (2020). A diffusion approach for plasma synthesis of superhard tantalum borides. *Journal of Materials Research*, *35*(5), 481-490.

Presentations

1. A. Rau, R. Radovitzky. *Simulations of Fracture in Polycrystals Accounting for Grain Boundary Energy Anisotropy.* US National Congress on Computational Mechanics, Chicago, IL, Jul 2025. Oral.
2. A. Rau, R. Radovitzky. *Quantification of Elastic Incompatibilities at Triple Junctions via a Physics-Based Surrogate Model.* Engineering Mechanics Institute and Probabilistic Mechanics and Reliability Conference, Chicago, IL, May 2024. Oral.
3. S. Jubin, A. Rau, A. Harges, Y. Barsukov, I. Kaganovich. *Modeling the Interaction of Atomic Boron with Graphene Surfaces.* APS Division of Plasma Physics, Virtual, Nov 2021. Poster.
4. A. Rau, S. Jubin, I. Kaganovich. *Surface Evolution in Long-Term Simulations of Graphite Boronization.* APS Division of Plasma Physics, Virtual, Nov 2021. Poster.
5. A. Rau, S. Jubin, O. Dwivedi, I.D. Kaganovich. *Large-Scale Simulations of Plasma-Facing Component Boronization.* APS Division of Plasma Physics, Virtual, Nov 2020. Poster.

Teaching Assistant Experience

Massachusetts Institute of Technology

- Unified Engineering: Materials and Structures *Fall 2023*

Johns Hopkins University

- Mechanics-Based Design *Spring 2022*
- Introduction to Fluid Mechanics Laboratory *Fall 2021*
- Mechanical Engineering Thermodynamics Laboratory *Fall 2020*
- Gateway Computing: MATLAB *Spring 2020*

Awards and Honors

- AeroAstro Graduate Teaching Assistantship Award *May 2024*
- James F. Bell Award *November 2021*
- Barry Goldwater Scholar *March 2021*
- Charles A. Miller Award *November 2020*
- Provost's Undergraduate Research Award *November 2020*