

Rasool Ahmad

CONTACT INFORMATION	Postdoctoral Researcher Quantum Simulation Group Physics and Life Sciences Division Lawrence Livermore National Laboratory CA 94550, USA	e-mail: rasoolahmad1@llnl.gov e-mail: rasoolahmad.a@gmail.com Mobile: +1 408 384 2528 OrcID: 0000-0002-4154-6902 Google Scholar: ujjgd08AAAAJ
RESEARCH INTERESTS	Computational materials science, dislocation mechanics, atomistic simulation, plasticity, machine learning for science	
EDUCATION	École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland Ph.D. in Mechanics Advisor: Dr. William Curtin	Aug 1, 2016 - Oct 30, 2020
	Indian Institute of Technology, Kanpur, India B.Tech.-M.Tech. Dual Degree in Mechanical Engineering	Jul 15, 2011 - Jul 15, 2016
SELECT AWARDS AND HONORS	Recipient of the Early Postdoctoral Mobility Fellowship (2021-2022) awarded by the Swiss National Science Foundation. Selected for the Humboldt Postdoctoral Research Fellowship (2021). Received the Best Ph.D. Thesis Award by EDME (Mechanics) doctoral program, EPFL (2021). Nominated for the MSMSE Emerging Leader 2023 by the <i>Modelling and Simulation in Materials Science and Engineering</i> journal.	
PUBLICATIONS	<i>Total citations: 833</i> (Google Scholar, Jul 2024) J. Chung, R. Ahmad , W. C. Sun, W. Cai, T. Mukerji, “Prediction of effective elastic moduli of rocks using graph neural networks”, <i>Comp. Meth. in Appl. Mach. and Eng.</i> 421 (2024) 116780. X. Hua, R. Ahmad , J. Blanchet, W. Cai, “Accelerated Sampling of Rare Events using a Neural Network Bias Potential”, <i>37th Conference on Neural Information Processing Systems</i> (NeurIPS 2023). R. Ahmad , M. Liu, M. Ortiz, T. Mukerji, and W. Cai, “Computation of effective elastic moduli of rocks using hierarchical homogenization”, <i>J. Mech. Phys. Solids</i> 174 (2023) 105268. M. Liu, R. Ahmad , W. Cai, and T. Mukerji, “Hierarchical homogenization with deep-learning-based surrogate model for rapid estimation of effective permeability from digital rocks”, <i>J. Geophys. Research: Solid Earth</i> (2022) e2022JB025378 R. Ahmad , and W. Cai, “Free energy calculation of crystalline solids using normalizing flows”, <i>Model. Simul. Mater. Sci. Eng.</i> 30 (2022) 065007 R. Ahmad , S. Paul and S. Basu, “Characterization of entanglements in glassy polymeric ensembles using the Gaussian linking number”, <i>Phys. Rev. E</i> 101 (2020) 022503. R. Ahmad , Z. Wu and W. A. Curtin, “Analysis of double cross-slip of pyramidal I ($\langle c + a \rangle$) screw dislocations and implications for ductility in Mg alloys”, <i>Acta Mater.</i> 183 (2020) 228-241. R. Ahmad , B. Yin, Z. Wu and W. A. Curtin, “Designing high ductility in magnesium alloys”, <i>Acta Mater.</i> 172 (2019) 161-184. R. Ahmad , Z. Wu, S. Groh and W. A. Curtin, “Pyramidal II to basal transformation of $\langle c + a \rangle$ edge dislocations in Mg-Y alloys”, <i>Scr. Mater.</i> 155 (2018) 114-118. R. Ahmad , S. Groh, M. Ghazisaeidi and W. A. Curtin, “Modified embedded-atom method interatomic potential for Mg-Y alloys”, <i>Model. Simul. Mater. Sci. Eng.</i> 26 (2018) 065010. Z. Wu, R. Ahmad , B. Yin, S. Sandlöbes and W. A. Curtin, “Mechanistic origin and prediction of enhanced ductility in magnesium alloys”, <i>Science</i> 359 (2018) 447-452.	

MANUSCRIPTS
SUBMITTED

R. Ahmad, and W. Cai, “Accelerating force calculation for dislocation dynamics simulations”, submitted to *Model. Simul. Mater. Sci. Eng.*, arxiv preprint: arXiv:2308.09817,

R. Ahmad, M. Liu, M. Ortiz, T. Mukerji, and W. Cai, “Homogenizing elastic properties of large digital rock images by combining CNN with hierarchical homogenization method”, submitted to *International journal of Solids and Structures*, arxiv preprint: arXiv:2305.06519,

CONFERENCE/
INVITED TALKS

R. Ahmad, ”From atoms to rocks: multiscale modeling of materials”, *NASA-AMES*, (2023), Mountain View, CA, USA.

R. Ahmad, ”Microstructure and macroscopic properties of materials: Mg alloy, Si, and rocks”, *Quantum Simulation Group, LLNL*, (2023), Livermore, CA, USA.

R. Ahmad, and W. Cai, “Hierarchical homogenization method to find elastic properties of digital rocks”, *GeoDict User Meeting*, (2023).

R. Ahmad, and W. Cai, “Free energy calculation of crystalline defects using normalizing flows”, *Multiscale Materials Modeling (MMM)* (2022) Baltimore, MD, USA

R. Ahmad, and W. Cai, “Free energy calculation of crystalline solids using normalizing flows”, *Materials Research Society (MRS) Spring Meeting* (2022) Honolulu, USA

R. Ahmad, Z. Wu, and W. A. Curtin, “Pyramidal $\langle c+\alpha \rangle$ cross-slip mediated ductility in Mg alloys ductility”, *Mechanics and Computation Seminar, Stanford University* (2020), USA.

R. Ahmad, Z. Wu, and W. A. Curtin, “Pyramidal $\langle c+\alpha \rangle$ cross-slip mediated ductility in Mg alloys ductility”, *Max Planck Institute for Iron Research* (2020) Düsseldorf, Germany.

R. Ahmad, Z. Wu, and W. A. Curtin, “Pyramidal $\langle c+\alpha \rangle$ cross-slip mediated ductility in Mg alloys ductility”, *The Minerals, Metals & Materials Society (TMS)* (2020) San Diego, USA.

W. A. Curtin, **R. Ahmad**, B. Yin and Z. Wu, “Design of Ductile Rare-Earth-Free Magnesium Alloys”, *Magnesium Technology 2020*, 19-24

R. Ahmad, Z. Wu, S. Groh and W. A. Curtin, “Pyramidal II to basal transformation of $\langle c + \alpha \rangle$ edge dislocations in Mg-Y alloys and its implication for ductility”, *Euromat* (2019) Stockholm, Sweden.

RESEARCH
EXPERIENCES

Postdoctoral Researcher Oct, 2022 - current
Quantum Simulation Group
Physics and Life Sciences Division
Lawrence Livermore National Laboratory.

Postdoctoral Fellow May, 2021 - Sep 2022
Swiss National Science Foundation (SNSF) Early Postdoc Mobility Fellow for the project titled *Investigation into finite temperature atomic-scale crystal plasticity through generative deep learning*.
Micro and Nano Mechanics Group,
Stanford University, California, USA
Advisor: Dr. Wei Cai

Graduate Student Researcher (Ph.D.) Aug 1, 2016 - Oct 30, 2020
Atomic Scale Investigations into the Origins of Ductility in Mg Alloys
École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
Advisor: Dr. William Curtin

Graduate Student Researcher (M.Tech.) Jul 15, 2015 - Jul 15, 2016
Investigation into disentanglement of polymer chains in a glassy amorphous polymer through molecular dynamics simulations
Indian Institute of Technology, Kanpur, India
Advisor: Dr. Sumit Basu

SERVICES	<ul style="list-style-type: none"> - Referee services for journals Acta Materialia, and CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry - Session-chair in conferences Multiscale Materials Modeling, 2022, Baltimore, MD, USA 	
ACADEMIC PROJECTS	<ul style="list-style-type: none"> Kinetic Monte Carlo simulation of screw dislocation mobility in BCC metals Updated Lagrangian Finite Element Formulation Static Equilibrium of a Red Blood Cell Minimum Energy Path of a Reaction Using Nudge Elastic Band Method 	<ul style="list-style-type: none"> Feb - Jun 2019 Aug - Nov 2014 Aug - Nov 2014 Jan - Apr 2014
SELECT COURSES	<ul style="list-style-type: none"> <li style="width: 50%;">- Computational Multiscale Modeling of Solid <li style="width: 50%;">- Molecular Modeling in Chemistry <li style="width: 50%;">- Nature and Properties of Materials <li style="width: 50%;">- Non-Linear Finite Element Method <li style="width: 50%;">- Fracture mechanics <li style="width: 50%;">- Finite Element Method <li style="width: 50%;">- Theory of Elasticity <li style="width: 50%;">- Advanced Mechanics of Solid <li style="width: 50%;">- Mechanics of Biological Membrane <li style="width: 50%;">- Wave Propagation in Elastic Solid <li style="width: 50%;">- Non-Linear Vibration <li style="width: 50%;">- Rheology and Structure of Complex Fluids <li style="width: 50%;">- Topics in Topology <li style="width: 50%;">- Vibration and Control <li style="width: 50%;">- Linear Algebra and Ordinary Diff Eqns <li style="width: 50%;">- Complex Analysis and Partial Diff Eqns <li style="width: 50%;">- Real Analysis and Calculus <li style="width: 50%;">- Fourier Analysis and Boundary Value Problems 	
TECHNICAL SKILLS	<p>Programming Languages - Python, C, C++, FORTRAN, Matlab, PyTorch, JAX, DGL</p> <p>Software - LAMMPS, ParaDis, Ovito, Abaqus, VASP</p>	
TEACHING EXPERIENCES	<p>Teaching Assistant, EPFL (Four semesters)</p> <ul style="list-style-type: none"> <li style="width: 50%;">- Solid Mechanics <li style="width: 50%;">- Introduction to Structural Mechanics <p style="text-align: right;">Spring Semesters 2018, 2019, 2020 Spring Semester 2017</p> <p>Teaching Assistant, IIT Kanpur (Two semesters)</p> <ul style="list-style-type: none"> <li style="width: 50%;">- Basic Electrical Engineering <li style="width: 50%;">- Engineering Graphics and Design <p style="text-align: right;">Fall Semesters 2016 Spring Semester 2015</p>	
REFERENCES	<div style="display: flex; justify-content: space-between;"> <div style="width: 45%;"> <p>Wei Cai Professor Department of Mechanical Engineering Stanford University, USA caiwei@stanford.edu</p> <p>Zhaoxuan Wu Assistance Professor Department of Materials Science and Engineering City University of Hong Kong, China zhaoxuwu@cityu.edu.hk</p> <p>Stanimir Bonev Staff Scientist Physics Division, Lawrence Livermore National Laboratory, USA bonev@llnl.gov</p> </div> <div style="width: 45%;"> <p>William Curtin Professor Institute of Mechanical Engineering EPFL, Switzerland william.curtin@epfl.ch</p> <p>Sumit Basu Professor Department of Mechanical Engineering Indian Institute of Technology (IIT) Kanpur, India sbasu@iitk.ac.in</p> <p>Fei Zhou Staff Scientist Physics Division, Lawrence Livermore National Laboratory, USA zhou6@llnl.gov</p> </div> </div>	