Rasool Ahmad

CONTACT Information Postdoctoral Fellow

(SNSF Early Postdoc Mobility Fellow) Micro and Nano Mechanics Group

Department of Mechanical Engineering

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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 Aug 1, 2016 - Oct 30, 2020

Advisor: Dr. William Curtin

Indian Institute of Technology, Kanpur, India

B.Tech.-M.Tech. Dual Degree in Mechanical Engineering

Jul 15, 2011 - Jul 15, 2016

- Cumulative Performance Index (M.Tech.) - 10 (on a scale of 10)

- Cumulative Performance Index (B.Tech.) - $\bf 8.2$ (on a scale of 10)

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 Modelling and Simulation in Materials Science and Engineering journal.

Publications

Total citations: 643 (Google Scholar, Jul 2023)

R. Ahmad, M. Liu, M. Ortiz, T. Mukerji, and W. Cai, "Computation of effective elastic moduli of rocks using hierarchical homogenization", J. Mech. Phys. Solids 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", *J. Geophys. Research: Solid Earth* (2022) e2022JB025378

R. Ahmad, and W. Cai, "Free energy calculation of crystalline solids using normalizing flows", Model. Simul. Mater. Sci. Eng. 30 (2022) 065007

R. Ahmad, S. Paul and S. Basu, "Characterization of entanglements in glassy polymeric ensembles using the Gaussian linking number", *Phys. Rev. E* 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", *Acta Mater.* 183 (2020) 228-241.

R. Ahmad, B. Yin, Z. Wu and W. A. Curtin, "Designing high ductility in magnesium alloys", *Acta Mater.* 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", *Scr. Mater.* 155 (2018) 114-118.

R. Ahmad, S. Groh, M. Ghazisaeidi and W. A. Curtin, "Modified embedded-atom method interatomic potential for Mg-Y alloys", *Model. Simul. Mater. Sci. Eng.* 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", *Science* 359 (2018) 447-452.

Manuscripts submitted

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 *Computer Methods in Applied Mechanics and Engineering*, 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 $\langle c+a \rangle$ 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 $\langle c+a \rangle$ 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 $\langle c+a \rangle$ 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 $\langle c + a \rangle$ edge dislocations in Mg-Y alloys and its implication for ductility", *Euromat* (2019) Stockholm, Sweden.

RESEARCH EXPERIENCES Postdoctoral Fellow

May 1, 2021 - current

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

- 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	Kinetic Monte Carlo simulation of screw dislocation mobility in BCC metals	Feb - Jun 2019
	Updated Lagrangian Finite Element Formulation	Aug - Nov 2014
	Static Equilibrium of a Red Blood Cell	Aug - Nov 2014
	Minimum Energy Path of a Reaction Using Nudge Elastic Band Method	Jan - Apr 2014

- \mathbf{SELECT} $\mathbf{COURSES}$ Computational Multiscale Modeling of Solid
 - Nature and Properties of Materials
 - Fracture mechanics
 - Theory of Elasticity
 - Mechanics of Biological Membrane
 - Non-Linear Vibration
 - Topics in Topology
 - Linear Algebra and Ordinary Diff Eqns
 - Real Analysis and Calculus

- Molecular Modeling in Chemistry
- Non-Linear Finite Element Method
- Finite Element Method
- Advanced Mechanics of Solid
- Wave Propagation in Elastic Solid
- Rheology and Structure of Complex Fluids
- Vibration and Control
- Complex Analysis and Partial Diff Eqns
- Fourier Analysis and Boundary Value Problems

TECHNICAL SKILLS

Programming Languages - Python, C, C++, FORTRAN, Matlab, PyTorch, JAX, DGL

Software - LAMMPS, ParaDis, Ovito, Abaqus, VASP

Teaching EXPERIENCES

Teaching Assistant, EPFL (Four semesters)

- Solid Mechanics
- Introduction to Structural Mechanics

Spring Semesters 2018, 2019, 2020

Spring Semester 2017

Teaching Assistant, IIT Kanpur (Two semesters)

- Basic Electrical Engineering
- Engineering Graphics and Design

Fall Semesters 2016

Spring Semester 2015

References

Wei Cai

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Zhaoxuan Wu

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Department of Materials Science and Engineering

City University of Hong Kong, China

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William Curtin

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Sumit Basu

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