Rasool Ahmad

Contact Information

Postdoctoral Fellow
(SNSF Early Postdoc Mobility Fellow)
Micro and Nano Mechanics Group
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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.) - **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).

Publications

Total citations: 528 (Google Scholar, Nov 2022)

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 $\langle \boldsymbol{c}+\boldsymbol{a} \rangle$ 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 $\langle \boldsymbol{c}+\boldsymbol{a} \rangle$ 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, "Computation of effective elastic moduli of rocks using hierarchical homogenization", submitted to *J. Mech. Phys. Solids*, arXiv preprint *arXiv:2208.02320*

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", submitted to *J. Geophys. Research - Solid Earth*, eossoar priprint *essoar.10512161.1*

Conference/ Invited Talks

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 $\langle \boldsymbol{c}+\boldsymbol{a} \rangle$ 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 $\langle \boldsymbol{c}+\boldsymbol{a} \rangle$ 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 $\langle \boldsymbol{c}+\boldsymbol{a} \rangle$ 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 $\langle \boldsymbol{c}+\boldsymbol{a} \rangle$ 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

Select 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, DGL,

Software - LAMMPS, ParaDis, Ovito, Abaqus, Gaussian

Teaching Experiences

Teaching Assistant, EPFL (Four semesters)

- Solid Mechanics — Spring Semesters 2018, 2019, 2020
- Introduction to Structural Mechanics — Spring Semester 2017

Teaching Assistant, IIT Kanpur (Two semesters)

- Basic Electrical Engineering — Fall Semesters 2016
- Engineering Graphics and Design — Spring Semester 2015

References

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Zhaoxuan Wu
Assistance Professor
Department of Materials Science and Engineering
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Sumit Basu
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