# Subhendu Chakraborty

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## --EDUCATION--

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| Ph.D. | **Johns Hopkins University** (JHU), Baltimore, USA<br>Department of Mechanical Engineering<br>Advisor: Prof. Somnath Ghosh | 2013–2020 |
| M.E. | **Indian Institute of Science** (IISc), Bangalore, India<br>Department of Aerospace Engineering.<br>Advisor: Prof. D. Roy Mahapatra | 2009-2011 |
| B.E. | **Jadavpur University** (JU), Kolkata, India<br>Department of Civil Engineering | 2005-2009 |

Course works: https://subhenduchakraborty.com/course-works/

## -- PROFESSIONAL EXPERIENCE--

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| Postdoc | **Los Alamos National Laboratory** (LANL), Los Alamos, USA<br>Theoretical Division (T-3).<br>Mentors: Dr. Darby J. Luscher, Dr. Abigail Hunter | 2021-Present |
| Postdoc | **Johns Hopkins University** (JHU), Baltimore, USA<br>Department of Civil and Systems Engineering.<br>Mentor: Prof. Somnath Ghosh | 2020-2021 |
| Project Assistant | **Indian Institute of Science** (IISc), Bangalore, India<br>Department of Aerospace Engineering<br>Mentor: Prof. D. Roy Mahapatra | 2011-2013 |

## -- RESEARCH EXPERIENCE

Research in detail: https://subhenduchakraborty.com/my-research/

1. **Development of dislocation-transport-based crystal plasticity model and it's implementation within MOOSE framework.** (Postdoc work, 2021 to Present)
   A. Developed a **dislocation-transport-based** crystal plasticity material model that incorporates the dislocation transport within the grain and across the grain boundary. A novel **dislocation-grain boundary interaction** model was developed to identify the dislocation flux transfer across the grain boundary. The novelty of this model is that dislocation transfer across the grain boundary can happen between different pairs of slip-systems as well as dislocation of opposite sign depending on the relative mis-orientation between grains. The material model is implemented within the open-source multi-physics code **MOOSE.** The model is used to study the interaction of **dislocations** with **grain boundary** in polycrystalline materials and it's macroscopic implication in the deformation behavior of the metallic material.
   B. The code is open-sourced and available in the LANL Github page with name DiscofluxM.

2. **Development of a coupled Thermo-Elastic - Molecular Dynamics model to study the defect nucleation and evolution during additive manufacturing process.** (Postdoc work, 2021 to 2022, Project: RR22CHAK)
    A. A concurrent multiscale model was developed by coupling continuum **thermos-elasticity** with **Molecular Dyanmics**(MD). The main objective of this project was to derive the constitutive laws related to the defect nucleation and evolution during the interaction of high energy laser with powder material.
    B. The open-source atomistic code **LAMMPS** was coupled with multi-physics code **MOOSE** in a concurrent fashion. In the coupling scheme, LAMMPS is used as library and MOOSE as the main driver code.
    C. The model is appropriate to study the localized material behavior during the **additive manufacturing** process where the physics of the impact of laser, subsequent melting, recrystallization and defect formation were captured using the Molecular Dynamic model and the already crystalized region is modelled as continuum(thermos-elasticity). The continuum region provides the temperature boundary condition for the atomistic domain and the atomistic domain provides the thermal flux as the boundary condition for the continuum domain at the interface. Strong displacement continuity is enforced at the interface between the atomistic and continuum domains.
    D. The interface between the atomistic and the continuum **domain is advanced** by converting the crystalized atomistic domain into continuum as simulation progresses. This keeps the computational cost almost constant even though new material is added in the powder form in the atomistic domain.

3. **Concurrent multiscale coupling of Molecular Dynamics(MD) and Crystal Plasticity(CPFE) to extend the spatial and temporal scale of the atomistic simulation.** (PhD work, 2016 to 2020)
    A. Development and application of atomistic (MD)-continuum (dislocation density based CPFE) **multiscale** coupled model to study the deformation mechanisms near the crack tip of metallic materials. **LAMMPS** was coupled with in-house FORTRAN based CPFE code for this model.
    B. **Meshless** method **(RKPM)** was used to propagate the dislocation within the continuum region once the dislocations are nucleated at the crack tip and reaches the atomistic-continuum interface.
    **C.** The model was used to extract the evolution laws for plastic variables e.g., dislocation nucleation rate from the crack-tip and free-energy functional for higher scale full-continuum simulation. The model was also used to construct some of the energy functional related to defects for full-continuum **phase-field** model.

4. **Atomic scale investigation of deformation mechanisms using Accelerated Molecular Dynamics.** (PhD work, 2013 to 2016)
    A. Accelerated Molecular Dynamics (Hyperdynamics) model was implemented within **LAMMPS** and used to study the strain rate dependent plastic deformation mechanisms in metallic materials.
    B. The model was able to **capture the transition** in the plastic deformation mechanism from **twin** at high strain rate to **dislocation** at low strain rate in fcc Nickel.

5. **Development of polygonal XFEM model to study the brittle crack propagation in honeycomb like structure.** (Master's work, 2009 to 2011)
    A. An optimization based numerical integration scheme was developed to integrate the stiffness terms for polygonal FEM and XFEM. The novelty of this scheme is that, the integration points are defined on an **unit circle**. Three-step mapping is used to map the integration points from unit circle to physical polygon. First, the **Schwarz–Christoffel conformal mapping** is used to map the integration points from unit circle to regular polygon and then **isoparametric** mapping is used to map those integration points onto the physical polygon. The benefit of this approach is that integration points are always defined on an unit circle, irrespective of the number of sides a polygonal element has.
    B. The eXtended Finite Element Method (**XFEM**) was incorporated within the polygonal finite element to study the propagation of crack in brittle materials. For the numerical integration of the stiffness term, the above-mentioned integration scheme was used. The main objective of this project was to study the **propagation of a preexisting crack** within a material with honeycomb like internal structure.

Highlights: **Crystal Plasticity, MOOSE, Molecular Dynamics, LAMMPS, Meshless RKPM, PFEM, XFEM**.

## -- PROJECTS AWARDED –

1. **Title**: Development of a concurrent coupled Atomistic – Continuum model to predict the defect and grain structure for Additive Manufacturing process.
   **PI**: Subhendu Chakraborty
   **Sponsor**: IMS Rapid Response 2022, LANL.
   **Project** Code: RR22CHAK
   **Budget**: $20,000
   **Duration**: Feb,2022 – Sept,2022

## -- AWARDS AND HONORS --

1. 3'rd place in the student poster competition at 13'th World Congress On Computational Mechanics (WCCM2018), New York, NY.
2. All India Rank 22 (out of 8854) in Graduate Aptitude Test in Engineering (GATE) held in 2009.

## -- PROFESSIONAL SERVICES--

1. Reviewer of journals: Metals, Polymers, Processes, Sustainability, Applied Science, Water.
2. Judge of Poster Session: Society of Engineering Science (SES) 2021.
3. Conference session chair: "Multiscale Behavior of Damage and Failure Mechanics", Engineering Mechanics Institute Conference (EMI), 2021.

## -- PROGRAMMING PROFICIENCY --

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| Programming skills: | C++, FORTRAN95, Python, MATLAB, Parallel Programming using MPI. |

Proficiency in open source code: MOOSE, LAMMPS,

Others: Git, Linux, Worked with different HPCs both institutional and commercial(LANL-HPC, MARCC, AWS).

## -- PUBLICATIONS--

**Peer Reviewed Journal Publications:** (citations:431, h-index:8)
Google Scholar, ORC ID: 0000-0002-5685-3630, Research Gate.

1. **S. Chakraborty** and A. Hunter and D. J. Luscher. “Development of a transport-based crystal plasticity model for inter and intra granular Dislocation transport.” (under preparation).
2. **S. Chakraborty** and S. Ghosh, “A concurrent atomistic-continuum model for augmenting crack phase-field model parameters”, J. of the Mechanics and Physics of Solids,104563 (2021). https://doi.org/10.1016/j.jmps.2021.104563
3. **S. Chakraborty** and S. Ghosh. "A Concurrent Atomistic-Crystal Plasticity Multiscale Model for Crack Propagation in Crystalline Metallic Materials", Computer Methods in Applied Mechanics and Engineering,379,113748 (2021). https://doi.org/10.1016/j.cma.2021.113748
4. **S. Chakraborty** and S. Ghosh. "Hyperdynamics accelerated concurrent atomistic-continuum model for developing crack propagation models in elastic crystalline materials", Computational Materials Science, 154:212-224 (2018). https://doi.org/10.1016/j.commatsci.2018.07.064 **[Editor's Choice]**
5. J. Zhang, **S. Chakraborty** and S. Ghosh. "Concurrent atomistic-continuum model for developing self-consistent elastic constitutive modeling of crystalline solids with crack", Int. J. Multiscale Comp. Eng. 15:99- 19 (2017). http://doi.org/10.1615/IntJMultCompEng.2017020072
6. ***S.* Chakraborty**, J. Zhang and S. Ghosh. Accelerated molecular dynamics simulations for characterizing plastic deformation in crystalline materials with cracks. Computational Material Science, 121, 23-34, (2016). http://dx.doi.org/10.1016/j.commatsci.2016.04.026 **[Editor's Choice]**
7. *C.S.Tiwary, **S Chakraborty**, D RoyMahaPatra, K Chattopadhyay*. Length-scale dependent mechanical properties of Al-Cu eutectic alloy: Molecular dynamics based model and its experimental verification. Journal of Applied Physics, 115, 203502 (2014). http://dx.doi.org/10.1063/1.4879249
8. C. S. Tiwary, J. Prakash, **S. Chakraborty**, D. R. Mahapatra & K.Chattopadhyay. "Subsurface deformation studies of aluminium during wear and its theoretical understanding using molecular dynamics", Philosophical Magazine, 98:29, 2680-2700 (2018), https://doi.org/10.1080/14786435.2018.1502481
9. *S. Natarajan, **S. Chakraborty,** M. Ganapathi, M.* Subramanian. A parametric study on the buckling of functionally graded material plates with internal discontinuities using the partition of unity method. European Journal of Mechanics - A/Solids, 44, 136-147 (2014). http://dx.doi.org/10.1016/j.euromechsol.2013.10.003
10. **S. Chakraborty**, S. Natarajan, S. Singh, D. Roy Mahapatra & S.P.A. Bordas, "Optimal Numerical Integration Schemes for a Family of Polygonal Finite Elements with Schwarz–Christoffel Conformal Mapping", International Journal for Computational Methods in Engineering Science and Mechanics, 19:4, 283-304 (2018). https://doi.org/10.1080/15502287.2018.1502218

11. S*. Natarajan, **S. Chakraborty**, M. Thangavel, S. Bordas and T. Rabczuk*. Size-dependent free flexural vibration behavior of functionally graded nanoplates. Computational Materials Science. 65, 74-80 (2012). http://dx.doi.org/10.1016/j.commatsci.2012.06.031

**Presentation in Conferences and Workshops:**

1. **S. Chakraborty** and A. Hunter and D. J. Luscher. “A dislocation transport based Crystal Plasticity model to study Structure-Property relations in Polycrystalline materials”. USNCCM, 2023.
2. **S. Chakraborty** and A. Hunter and D. J. Luscher. “Development of dislocation transport based mesoscale crystal plasticity model”. TMS, 2022.
3. **S. Chakraborty** and S. Ghosh. “Development of the Phase Field Free-Energy Functional from a Self-consistent Coupled Atomistic Continuum Model to Study the Ductile Fracture in Metallic Materials”. EMI, 2021.
4. **S. Chakraborty** and S. Ghosh. “A Self-consistent Coupled Atomistic-Continuum Model to Study the Brittle and Ductile Fracture in Metallic Materials”. SES2020, 2020.
5. **S. Chakraborty** and S. Ghosh. “Concurrent Atomistic-Continuum Multiscale Model for Inelastic Modelling of Materials”. SES2019, St. Louis, MO, 2019.
6. **S. Chakraborty** and S. Ghosh. “Spatial and Temporal scale bridging of Atomistic-Continuum Concurrent Multiscale Models for Inelastic modelling of materials”. WCCM2018, New York City, NY,2018.
7. S. Ghosh, **S. Chakraborty** and J. Zhang. “Coupled Atomistic-Continuum Modelling for Crack Propagation”. NIST Workshop on Atomistic Simulations for Industrial Needs, Gaithersburg, USA,2018.
8. **S. Chakraborty**, J. Zhang and S. Ghosh. “Characterization and Quantification of Crack Tip Plasticity in Crystalline Materials at Experimentally Achievable Strain Rate”. TMS-2016, Nashville, USA, 2016.
9. **S. Chakraborty**, J. Zhang and S. Ghosh. “Near-Crack Phenomenon Modelling using Finite Temperature Atomistic-Continuum Self-consistent Method”. USACM Thematic Conference on Recent Advances in Computational Methods for Nanoscale Phenomena, U. of Michigan, Ann Arbor, USA, 2016.
10. **S. Chakraborty** and D. Roy Mahapatra. "Crystal Plasticity based Material Modelling for Lamellar Microstructure". SMiRT-22, San Francisco, USA, 2013.
11. **S. Chakraborty** and D. Roy Mahapatra. “Modeling of Polycrystalline Microstructure Using Polygonal FEM”. ICCMS-2012, Hyderabad, India. 2012.
12. **S. Chakraborty**, D. Roy Mahapatra, S. Natarajan and S. Bordas. "Optimal Integration Scheme for Polygonal Finite Element Method(PFEM) and eXtended Finite Element Method(XFEM) for Isotropic Homogeneous Material", XFEM-2011, Cardiff, UK, 2011.
13. **S. Chakraborty**, S. Singh and D. Roy Mahapatra. "Modeling of Polycrystalline Microstructure Using Polygonal FEM". SMiRT-21, New Delhi, India, 2011.

*Presenting author's name is underlined.

## -- REFERENCES --

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