

Saswata Bhattacharya

Professor,

Department of Materials Science and Metallurgical Engineering

Indian Institute of Technology Hyderabad, Kandi, Sangareddy – 502284, Telangana, India

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[Google Scholar profile](#)

Education

- **Doctor of Philosophy (Materials Engineering)**, 2008
Indian Institute of Science, Bangalore, India
Thesis: Evolution of Multivariant Microstructures with Anisotropic Misfit: A Phase Field Study
- **Master of Science (Eng.) (Metallurgy)**, 2002
Indian Institute of Science, Bangalore, India
Thesis: Ternary Spinodal Decomposition: Effect of Interfacial Energy
- **Bachelor of Science (Tech.) (Ceramic Technology)**, 1999
Calcutta University, Kolkata, India
First class with Honours.

Professional Experience

- **Professor**, Department of Materials Science and Metallurgical Engineering
Indian Institute of Technology Hyderabad, India (August 2023 – Present)
- **Associate Professor**, IIT Hyderabad (February 2019 – August 2023)
- **Assistant Professor**, IIT Hyderabad (July 2013 – January 2019)
- **Materials Scientist**, GE Global Research, Bangalore (2011 – 2013)
- **Postdoctoral Research Associate**, Pennsylvania State University, USA (2008 – 2011)

Research Interests

- Phase Transformations in Materials; Computational Modeling of Phase Transformations
- Phase-Field Models of Microstructural Evolution
- Microstructure-informed Micromechanical Modeling – Elastic Stress Effects, Dislocation Dynamics, Crystal Plasticity
- Integration of Mesoscale Microstructural Evolution Models with Deformation and Fracture Models: Multiphysics Coupling (e.g., phase-field coupled with discrete dislocation plasticity or crystal plasticity models)
- Prediction of process-microstructure-property relations: development and implementation of high-performance integrated computational materials engineering (ICME) tools for materials design
- Accelerating physics-based models of microstructural evolution using machine learning and deep learning techniques

- Development of physics-informed machine learning models

Expertise

- Development of Phase-Field codes for simulating microstructural evolution in alloys and oxides
- Development of Discrete Dislocation Dynamics codes (developed modules in Paradis code to implement dislocation-particle interactions), development of 2D DDD code to study particle strengthening
- High Performance Computing: GPU-accelerated phase-field codes using CUDA parallel programming environment, massively parallel PDE solvers using multiple GPUs and CPUs (CUDA + MPI + Threads)
- Development of numerical inverse methods using physics-informed neural networks, multi-objective optimization - extraction of mobility data in multicomponent alloy systems from experimental diffusion profiles
- Development of FFT-based microelasticity and crystal plasticity solvers

Publications

Peer-reviewed

- [1] Tanmay Dutta, Dasari Mohan, Saurav Shenoy, Nasir Attar, Abhishek Kalokhe, Ajay Sagar, Swapnil Bhure, Swaroop S. Pradhan, Jitendriya Praharaj, Subham Mridha, Anshika Kushwaha, Vaishali Shah, M.P. Gururajan, V. Venkatesh Shenoi, Gandham Phanikumar, [Saswata Bhattacharyya](#), Abhik Choudhury. "MicroSim: A high-performance phase-field solver based on CPU and GPU implementations". **Computational Materials Science** 246 (2025), p. 113438.
- [2] Sourav Ghosh, Hemanth Kumar, Christian Brandl, Abhik N Choudhury, [Saswata Bhattacharyya](#), Rajdip Mukherjee. "Effect of molybdenum addition on precipitate coarsening kinetics in Inconel 740H: A phase-field study". **Intermetallics** 175 (2024), p. 108513.
- [3] Suman Sadhu, Anindita Chakraborty, Monojit Dutta, Surendra Makineni, [Saswata Bhattacharyya](#), Alope Paul. "Introducing concepts of estimating tracer and intrinsic diffusion coefficients in a ternary system: a case study in the FCC Fe-Mn-Cr solid solution". **Philosophical Magazine** (2024), pp. 1–26.
- [4] Suman Sadhu, Anindita Chakraborty, Surendra Makineni, [Saswata Bhattacharyya](#), Alope Paul. "An experimental estimation method of diffusion coefficients in ternary and multi-component systems from a single diffusion profile". **Acta Materialia** 274 (2024), p. 120000.
- [5] Digvijay Narayan Singh, Ram Prakash Singh, [Saswata Bhattacharyya](#), Rajeev Ranjan. "Critical analysis of the isosymmetric transition and phase diagram of BiFeO₃-PbTiO₃". **Physical Review B** 110.13 (2024), p. 134112.
- [6] Soumya Bandyopadhyay, Vaishnavi SM, Tushar Jogi, Ranjith Ramadurai, [Saswata Bhattacharyya](#). "Role of electrostriction on domain switching near the morphotropic phase region in a ferroelectric solid solution: Thermodynamic analysis and phase-field simulations". **Physical Review B** 108.13 (2023), p. 134116.

- [7] [Saswata Bhattacharyya](#), Soumya Bandyopadhyay. "Strain Engineering in Functional Materials and Devices". Ed. by Ranjith Ramadurai and Saswata Bhattacharyya. AIP Publishing LLC, 2023. Chap. Chapter 7. Phase-field Modeling of Ferroic Domains in Strained Structures.
- [8] Anuj Dash, [Saswata Bhattacharyya](#), Alope Paul. "Concepts for estimating all types of diffusion coefficients of NiCoFeCr multi-principal element alloys using two dissimilar or a combination of ideal and non-ideal pseudo-ternary diffusion couples". **Scripta Materialia** 237 (2023), p. 115719.
- [9] Anuj Dash, [Saswata Bhattacharyya](#), Alope Paul. "Estimation of diffusion coefficients in NiCoFeCrAl multi-principal element alloy following an inventive design strategy of diffusion couples". **Acta Materialia** 260 (2023), p. 119296.
- [10] Hemanth Kumar, Neelamegan Esakkiraja, Anuj Dash, Alope Paul, [Saswata Bhattacharyya](#). "Utilising physics-informed neural networks for optimisation of diffusion coefficients in pseudo-binary diffusion couples". **Philosophical Magazine** 103.18 (2023), pp. 1717–1737.
- [11] Ranjith Ramadurai, [Saswata Bhattacharyya](#). "Strain Engineering in Functional Materials and Devices". Ed. by Ranjith Ramadurai and Saswata Bhattacharyya. AIP Publishing LLC, 2023. Chap. Chapter 1. Strain Engineering in Crystalline Solids.
- [12] Ranjith Ramadurai, [Saswata Bhattacharyya](#). *Strain Engineering in Functional Materials and Devices*. AIP Publishing LLC, 2023.
- [13] M Verma, S Sugathan, S Bhattacharyya, R Mukherjee. "Effect of concurrent thermal grooving and grain growth on morphological and topological evolution of a polycrystalline thin film: Insights from a 3D phase-field study". **Acta Materialia** 261 (2023), p. 119393.
- [14] Pravallika Bandaru, [Saswata Bhattacharyya](#), Shourya Dutta-Gupta. "Insights into propagating surface plasmons in Ag–Cu alloy thin films: Enhancement of spin angular momentum of light". **Journal of Applied Physics** 132.18 (2022).
- [15] Hemanth Kumar, Anuj Dash, Alope Paul, [Saswata Bhattacharyya](#). "A physics-informed neural network-based numerical inverse method for optimization of diffusion coefficients in NiCoFeCr multi principal element alloy". **Scripta Materialia** 214 (2022), p. 114639.
- [16] P Pankaj, [Saswata Bhattacharyya](#), Subhradeep Chatterjee. "Competition of core-shell and Janus morphology in bimetallic nanoparticles: Insights from a phase-field model". **Acta Materialia** 233 (2022), p. 117933.
- [17] P Pankaj, [Saswata Bhattacharyya](#), Subhradeep Chatterjee. "Surface-directed and bulk spinodal decomposition compete to decide the morphology of bimetallic nanoparticles". **Modelling and Simulation in Materials Science and Engineering** 31.1 (2022), p. 015003.
- [18] M Verma, S Sugathan, S Bhattacharya, R Mukherjee. "A computational analysis of universal behavior of thermal groove in a moving grain boundary". **Scripta Materialia** 209 (2022), p. 114383.
- [19] Tushar Jogi, [Saswata Bhattacharya](#). "Interfacial dislocation network in precipitation strengthened alloys during creep: a discrete dislocation dynamics (DDD) study in three dimensions". **Modelling and Simulation in Materials Science and Engineering** 29.3 (2021), p. 035010.
- [20] P Kasirajan, S Bhattacharya, A Rajagopal, JN Reddy. "Phase field modeling of fracture in quasi-brittle materials using natural neighbor Galerkin method". **Computer Methods in Applied Mechanics and Engineering** 366 (2020), p. 113019.
- [21] Sanket Sarkar, Yan Gao, Shenyan Huang, [Saswata Bhattacharya](#), Swapnil Patil, Ramkumar Oruganti. "Back-stress and its evolution during primary creep in particle strengthened nickel superalloys". **Crystals** 10.4 (2020), p. 306.

- [22] Sandeep Sugathan, [Saswata Bhattacharya](#). “A phase-field study of elastic stress effects on phase separation in ternary alloys”. **Computational Materials Science** 172 (2020), p. 109284.
- [23] Mariappan Anandkumar, [Saswata Bhattacharya](#), Atul Suresh Deshpande. “Low temperature synthesis and characterization of single phase multi-component fluorite oxide nanoparticle sols”. **RSC advances** 9.46 (2019), pp. 26825–26830.
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- [26] Sandeep Sugathan, [Saswata Bhattacharya](#). “Phase-Field Modelling of Evolution of Compact Ordered Precipitates in Ternary Alloy Systems”. **MRS Advances** 4.25-26 (2019), pp. 1457–1463.
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Teaching Experience

- Computational Methods in Materials Science
- Thermodynamics and Kinetics of Materials
- Metallic Materials
- Introduction to ICME Techniques and Tools
- Phase Equilibria
- Kinetics of Materials
- Introduction to Micromechanics of Solids
- Rate Phenomena in Process Metallurgy
- Transport Phenomena
- Machine Learning and Data Analytics in Materials Science
- Fundamentals of Scientific Computing
- Mesoscale Microstructural Modeling
- NPTEL course on “Thermodynamics and Kinetics of Materials”

Selected Training Courses and Workshops

- Certificate course on “Micromechanics: fundamental concepts and applications in the study of microstructural evolution” at TATA Steel
- A short course on “Discrete Dislocation Dynamics Simulations” at DMRL, Hyderabad
- Workshops on MicroSim (Microstructure Simulator): Modules taught – KKS-CuFFT, KKS-FD-CUDA, FFT-based microelasticity models (open-source GPU-accelerated modules of MicroSim developed at IIT Hyderabad using CUDA programming)
- Workshop on Phase-field modeling at NIT Srinagar
- NRC-M Lectures on “Phase-field modeling and its applications” at IISc, Bangalore
- NRC-M Lecture on “Examples of phase-field modeling in ICME” at IISc, Bangalore

PhD Guidance

Graduated Students:

Sl. No.	Name of PhD Student	Thesis Title	Year	Current Affiliation
1	Dr. Sandeep Sugathan	A Phase-Field Study of Elastic Stress Effects on Phase Separation in Ternary Alloy Systems	2019	Research Professor, Kookmin University, Korea
2	Dr. Soumya Bandyopadhyay	A Phase-Field Study of Electromechanical Effects on Domain Evolution and Polarization Switching in Bulk, Thin-film and Multilayer Ferroelectric Perovskite Oxides	2021	Postdoctoral Research Associate, University of Florida, USA
3	Dr. Tushar Jogi	Computational Modeling and Simulations of Process-Microstructure-Property Relations in Model Ni-base Superalloys	2021	Postdoctoral Researcher, Max-Planck Institute for Sustainable Materials
4	Dr. Pankaj	Morphology Development in Bimetallic Nanoparticles: A Phase Field Study (Jointly supervised with Prof. Subhradeep Chatterjee)	2023	Postdoctoral Researcher, Kookmin University

National Postdoctoral Fellow (NPfF):

- Dr. Anuj Dash (Currently Assistant Professor, IIT Bhubaneswar)

Ongoing PhD Students at IITH:

- Ms. Gaijinliu Gangmei
Thesis Title: Building Multiscale Surrogate Model of Process-Structure Linkages from Phase-field Simulations
JDP student (Deakin University), Research Proposal Seminar Completed: 3rd April 2023
Thesis Supervisors: Kishalay Mitra, Saswata Bhattacharya, Bernard Rolf, Santu Rana
- Mr. Shashikumar
Thesis Title: Accelerated Design of Novel Binder Alloys in WC-based Hardmetals
External PhD student from Kennametal India
Thesis Supervisors: Saswata Bhattacharya and Pinaki Prasad Bhattacharjee
- Mr. D. Atchyut Kumar
Thesis Title: Phase-field Modelling of Microstructure Evolution in Multicomponent Alloys
Thesis Supervisors: Saswata Bhattacharya
External Co-supervisor: Prof. Alope Paul, IISc

External Co-supervisor:

- Mr. Suman Sandhu, IISc (2023)
- Mr. Pushkar Pandit, IISc (2023)
- Mr. Ismail Kamil Worke, IISc (2023)
- Mr. Aravind K., IIT Kanpur (2023, jointly with Prof. Rajdip Mukherjee)

Projects (Sponsored/Consultancy)

1. **As PI:** Dislocation Dynamics based studies in Particle Strengthened Alloy Systems
Sponsoring Agency: General Electric India Technology Centre, JFWTC, Bangalore
Period: 2014-2016
2. **As PI:** Phase field modeling of eutectoid transformation in steel
Sponsoring Agency: Tata Steel Limited
Period: 2015-2016
3. **As PI:** Development of modeling techniques (Atomistic Monte Carlo and Phase-field simulations) to understand metallurgical phenomena in advanced high strength steels
Sponsoring Agency: Tata Steel Limited
Period: 2016-2019
4. **As PI:** Computational Microstructural Design of P/M Disk Superalloys using Phase Field Modeling towards Accelerated Alloy Design
Sponsoring Agency: CARS, DMRL (DRDO)
Period: 2017-2020
5. **As PI:** Accelerated Alloy Design and Processing Optimization Using Computational Thermodynamics and Kinetics-Based Tools
Sponsoring Agency: Mishra Dhatu Nigam Limited (MIDHANI)
Period: 2017-2020
6. **As PI:** Effect of Electromechanical Forces on Domain Evolution in Ferroelectric and Multiferroic Thin Films: Phase-Field Modeling and Simulations
Sponsoring Agency: DST-SERB (EMR)
Period: 2017-2020
7. **As Co-PI (multi-institute project):** National Centre for Clean Coal Research and Development (NCCCRD)
Sponsoring Agency: DST
Period: 2018-2023
8. **As PI (IITH):** Repository of high-performance phase field solvers for Microstructure Simulations (MicroSim) – Phase 1
Sponsoring Agency: DST-NSM (National Supercomputing Mission)
Period: 2021-2023
9. **As PI (IITH):** Repository of high-performance phase field solvers for Microstructure Simulations (Phase 2)
Sponsoring Agency: DST-NSM (National Supercomputing Mission)
Period: 2023-2024
10. **As PI:** Assessment of high-fidelity diffusion coefficients in ternary and multicomponent Ni-Al-X (X=Mo, Ta, Re, W) alloys and their effect on Ostwald ripening
Sponsoring Agency: DST-SERB (CRG)
Period: 2022-2025 (Ongoing)
11. **As PI:** Through-process modeling of DS/SC superalloy turbine blades processed using modified Bridgman route – Validation with CMSX-4 alloy
Sponsoring Agency: ARDB (GTMAP)
Period: 2022-2026 (Ongoing)

12. **As PI:** Computational Approach Using Machine Learning, CALPHAD and First Principles Calculations for Accelerated Development of Complex Concentrated Alloys
Sponsoring Agency: CARS (DMRL)
Period: 2022 - 2024 (Ongoing)

Technology Developed and Transferred

1. A set of programs to study grain growth in two and three dimensions using a large number of grain orientations (implementation of active parameter tracking algorithm) and study the topological and morphological characteristics of polycrystalline microstructures – **transferred to Tata Steel**.
2. A set of GPU-accelerated codes (developed using NVIDIA CUDA architecture) to study elastic stress effects on microstructural evolution in superalloys, in-house modified PARADIS discrete dislocation dynamics code to study the formation of interfacial dislocation network during creep – **transferred to DMRL**.
3. Indigenous open-source HPC software **MicroSim** to simulate microstructural evolution using Phase-field method – the complete GPU-based module (using NVIDIA CUDA architecture) developed by my group at IITH (KKS-CuFFT, KKS_FD_CUDA_MPI).
<https://github.com/ICME-India/MicroSim>
<https://microsim.co.in>
#atmanirbharbharat, National #Supercomputing Mission

Infrastructure Established

1. HPC Cluster (**Sukshma**) with 256 CPU cores, InfiniBand switch, and 5 Nvidia Tesla GPU cards (8x Tesla A100 cards, 2x Tesla V100 cards, 2x Tesla P100 cards, 1x Tesla K80 card – 40000 GPU cores).
Funding: DST-SERB, CARS (DMRL), GTMAP, DIA-RCOE.
2. Server for ThermoCalc software suite v2019A (Institute-wide access) with thermodynamic and mobility databases – Academic Network License.
Funding: MIDHANI.
3. Upgradation of ThermoCalc software suite (v2024A) (Institute-wide access).
Funding: Institute.
4. Teaching and Research Lab for Computational Materials Science.
Funding: GE, Tata Steel, Department.
5. VASP License Server for Materials Simulations Group.
Funding: CARS (DMRL).

Administrative Activities

- Coordinator for the Online M. Tech. Program on ICME.
- Coordination and Curriculum Development for the Interdisciplinary B. Tech. program of Computational Engineering (along with Prof. Raja Banerjee).
- Head of the Department, Materials Science and Metallurgical Engineering, IIT Hyderabad (November 2023 -)