

VIR KARAN

Education

Indian Institute of Technology Madras

2019-23

B.Tech, Metallurgical and Materials Engineering

Major GPA: 9.67/10, CGPA: 9.24/10

Areas of Interest

- Computational Study of Condensed Matter Systems (ICME)
- Data-Driven Multi-Scale Modelling of Materials
- Deep Materials Informatics

Scholastic Achievements

- Selected for the coveted **Young Research Fellowship** at IIT Madras amongst **200+** applicants
- o Ranked in top 0.1% in EAMCET 2019 among 200,000 candidates in the state of Telangana
- Secured a percentile of 99.85% in JEE Mains 2019 among 1.4 million candidates

Research Experience

Data-Driven Solution of a Coupled Phase Field Problem using GANs

(July 2021 - Present)

Guide: Dr. Saswata Bhattacharya, Computational Materials Science Group, IIT Hyderabad

- Presently working on *drafting a Manuscript* for this work.
- Built a **Custom Generative Adversarial Network (GAN) Architecture** using Convolutional-LSTM layers for solving coupled temporal PDEs by training on Phase Decomposition sequences of Binary and Ternary alloys
- Set a Benchmark MSE of 0.0002% for a non-physics informed solution to the Coupled Cahn-Hilliard equations
- o Analyzed the Efficiency, Scalability & Accuracy of the trained model as a replacement for numerical solvers

Reduced Order Model for Damage Assessment in DP Steels

(August 2021 - Present)

Guide: Dr. Anand K Kanjarla, Mechanics of Microstructures Group, IIT Madras

- Presently working on *drafting a Manuscript* for this work.
- Built a reduced order model using a **Random Forest Regressor** to predict the damage initiation stress in DP steel microstructures of 6 different morpholiges and 3 work hardening rates and achieved an R^2 **score of 97**%
- Implemented a StyleGAN to generate two-phase microstructures with the maximum damage resistance
- \circ Achieved an \mathbb{R}^2 score of 90% on damage initiation stress of generated microstructures using reduced order model

CALPHAD-Coupled Phase Field Modelling of Al-Zn Alloys

(May 2021 - August 2021)

Guide: Dr. Abhik Choudhary, Materials Modelling Group, IISc Bangalore

- Extracted and analysed thermodynamic properties of Al-Zn system using the pyCALPHAD library
- Solved the coupled Phase Field PDEs numerically using a **Finite Difference discretization scheme**
- Used GSL Scientific Library to fit and incorporate thermodynamic data into custom phase field solvers
- o Successfully Simulated Microstructure evolution undergoing Phase Separation and Precipitate Growth

Generation of Synthetic Microstructures using GANs

(December 2020 - July 2021)

Guide: Dr. Anand K Kanjarla, Mechanics of Microstructures Group, IIT Madras

- o Implemented Generative Adversial Networks (GANs) on 70 classes of 2D two-phase microstructural data
- Achieved a **Mean Structural Similarity Measure(SSIM) of 99.1**% on the 2-point correlations of the generated data and an **SSIM >95**% for all classes of microstructural data generated using a **StyleGAN** architecture
- **Discovered 3 Physically-Significant directions** in the StyleGAN latent space that can be used for **controlling the morphology** of the generated microstructures & can potentially be applied in **Microstructural Design**

Academic Projects

First Principles Modelling of FCC Aluminium

(September 2021 - October 2021)

Guide: Dr. Satyesh Kumar Yadav, Atomistic Modelling of Materials Course

- o Applied DFT codes written in VASP to model Primitive cell and Unit cell of FCC-Aluminium
- o Analyzed the relation between K-Points sampled, SMEAR parameter and computational time of the simulations
- Used the points computed using DFT to calculate Lattice parameter, Bulk Modulus and Vibration Frequency
- Visualized the computed equilibrium structure of FCC Aluminum using VESTA

Theoretical Design of Wind Turbines for Powering a Campus of 10,000 Students Guide: Dr. Prathap Haridoss, Materials in Renewable Energy Tech. Course Project (May 2021)

- Estimated the power demanded by taking the IITM campus as reference, used weather data from around Chennai in the wind turbine power equation to calculate the dimensions required for the turbine
- Performed a simplified mechanical analysis of stresses on the tower and blades and suggested materials to be used in the turbine, while minimizing costs and environmental impact of the turbines

Competitions

TechSoc Deep Learning Hack-a-thon

(April 2021)

Ranked 2nd on the Leader-board

- Built a Deepfake Detector using transfer learning of a pretrained Convolutional Neural Network(VGG16)
- o Achieved a log-loss of 0.2 on a test set which was made using techniques to spoof deepfake detectors
- Fine-tuned a pretrained GPT-2 model for conditional open ended text generation
- Achieved a log-loss of 0.17 on the generation of abstracts given the titles of papers taken from ArXiv

Technical Skills

- **Programming Languages:** Python, C, JavaScript (Fundamentals)
- o Frameworks and Libraries: TensorFlow, Keras, NumPy, Sci-kit Learn, Open-CV, SciPy
- Materials Modelling: VASP, Abaqus(Fundamentals), DREAM.3D, pyCALPHAD, VESTA, ParaView
- Scientific Tools: MATLAB, GNU Octave, LATEX

Relevant Courses

* - Ongoing, c - Certified Online Course

- $\hbox{\bf Computation:} \ A tomisite Modelling of Materials* | Introduction to C Programming | Computational Materials Engineering Lab* | Data Structures and Algorithms^c \\$
- Materials Science: Thermodynamics of Materials | Transport Phenomenon | Phase Transformations | Materials in Renewable Energy Tech | Physics of Materials* | Materials Characterization*
- Materials Chemistry: Chemistry: Structure, Bonding and Reactivity | Structure of Materials
- **Machine Learning & Artificial Intelligence:** Machine Learning^c | Deep Learning | Reinforcement Learning | Practical Machine Learning in TensorFlow^c | Browser-based Models with TensorFlow.js^c
- Mathematics: Multivariate Calculus | Linear Algebra for Engineers | Probability, Statistics and Stochastic Processes | Series and Matrices

Extra-Curricular Activities

- **Head, Shaastra**¹ **Mind Trials** (*Shaastra* 2021-22, *IIT Madras*): **Heading** a team of 8 to host awareness initiatives and a case-study competition on the application of Behavioural Sciences into solving pressing societal issues such as Sanitation, Road Safety, Nutrition and Fitness
- Part of the **Editorial Team** of the MME department magazine, **ETCH**: Co-authoring scientific articles on Sustainable practices in alloy design and processing, and on the Undergraduate Research culture
- **Student Mentor** (*Avanti Fellows* 2019-20): **Mentored** a student from JNV Pondicherry to prepare for the JEE Main and Advanced examinations, as part of the Avanti Fellows Pondicherry Chapter

^{1.} Shaastra is the annual technical fest of IIT Madras