भारतीय प्रौद्योगिकी संस्थान दिल्ली
Indian Institute of Technology Delhi

GIAN
GLOBAL INITIATIVE OF ACADEMIC NETWORKS

UNT
UNIVERSITY
OF NORTH TEXAS

ATOMISTIC SIMULATIONS OF MATERIALS

8th to 12th July, 2019

Overview

Materials science involves disparate length and time scales spanning Angstroms to meters and femtoseconds to years depending on the problem of interest. The instructor proposes an intensive twenty-hour course on computational materials science involving *lectures* and *hands-on tutorials* in atomistic simulations incorporating semi-empirical potentials. Computers will be needed for tutorials only and will be provided by the host institution (IIT-Delhi) with computational software pre-installed.

The instructor focus will be on the atomistic simulations of point, line, and planar defects, and study of elastic and plastic deformation properties in metallic materials. Knowledge of crystallographic structure and properties is a pre-requisite. The workhorse techniques of molecular statics (MS) and molecular dynamics (MD) will be covered in sufficient detail. Applications of these techniques to classical problems in materials science, e.g., mechanical deformation, dislocation motion and interactions, nucleation and growth, melting and solidification, point defect behaviour, etc., will be presented.

On completion of the course, all participants will have an appreciation of the atomistic simulations of defects in metallic materials through the lectures and the daily two-hour tutorials. The course will give participants a basic understanding of atomistic simulations to be able to read and understand research literature in this fast emerging field.

Modules	**DAY ONE** **Lecture 1: Review of Defects in Metallic Materials and Introduction to Concepts and Methods Used in Atomistic Simulations** *Tutorial 1:* (i) Creating and visualizing body-centered cubic (BCC), face-centered cubic (FCC), and hexagonal close-packed (HCP) crystals, (ii) Creating vacancies and interstitials in FCC Cu, (iii) Creating (100), (110), and (111) surfaces and Σ5 grain boundary in FCC Cu, and (iv) Setting up files to run basic molecular statics simulations using LAMMPS.

DAY TWO

Lecture 2: Introduction to pair potentials and their limitations, and make a case for the creation of many-body potentials, especially the Embedded-Atom Method (EAM) potential

Tutorial 2: (i) Investigate the elastic properties predicted by pair potentials in a model FCC copper.
(ii) Calculate the screened pair potential versus interatomic distance for a Lennard-Jones (LJ) and Morse potentials from the equilibrium lattice constant, bulk modulus, and cohesive energy.
(iii) Compare the bulk modulus obtained numerically from the pair potentials and from the analytic formulae and experiment.

DAY THREE

Lecture 3: Modeling elastic properties of metals

Tutorial 3: For BCC, FCC, DC, SC, HCP at T=0K, use LAMMPS in MS mode to calculate:
(i) cohesive energy vs. 1st nearest neighbor (1NN) distance for LJ, Morse, and EAM copper potentials,
(ii) the *equilibrium* 1NN distance and cohesive energy, and
(iii) the elastic constants for FCC at equilibrium using energy method and stress method.

DAY FOUR

Lecture 4: Modeling energetics of point, surface, and interfacial defects in metals

Tutorial 4: For FCC copper at T=0 K, use LAMMPS in MS mode to calculate:
(i) formation energies of a vacancy, di-vacancy, and interstitials,
(ii) the vacancy and [110] split interstitial energy as a function of simulation cell size and extrapolate the energies to infinite system size,
(iii) formation energies of (100), (110), (111) surfaces, and Σ5 grain boundary, and
(iv) observe defects using visualization tools.

	DAY FIVE **Lecture 5: Study deformation of perfect FCC Cu and Cu with an edge dislocation. Both tensile and shear strain conditions will be contrasted. This will also include simulating mechanical properties of copper bicrystals.** *Tutorial 5:* For FCC copper at T=0 K, use LAMMPS in MS mode to: (i) create and relax an edge dislocation in Cu, (ii) use local structure analysis to ID dislocation core atoms and visualize the dislocation/stacking fault (SF) before and after relaxation, (iii) apply a shear strain determine the minimum strain to move the dislocation and track its motion, (iv) visualize the dislocation.
You Should Attend If…	You are an engineer or scientist working in the area of materials science and engineering. You are expected to have an undergraduate degree in metallurgical engineering, materials science and engineering, mechanical engineering or chemical engineering.
Fees	The participation fees for taking the course is as follows: Participants from abroad: US $500 Industry/ Research Organizations: 20000 INR Academic Institutions Faculty: 10000 INR Students: 5000 INR Application Deadline: Register at: http://www.gian.iitkgp.ac.in/GREGN/index For any queries, please email to ----- gian.pml@gmail.com

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The Faculty

Dr. Srivilliputhur is an expert in atomistic modelling of deformation behaviour and defect physics, irradiation effects in materials, phase transformations, and structure-property relations in metals and alloys. He has co-authored numerous, well-cited publications in prestigious journals such as Nature, Physical Review Letters etc. He is also an Editor of the Journal Materials Research Letters.

Professor Rajesh Prasad's area of interest is physical metallurgy. He has three decades of experience of teaching materials science courses at both undergraduate and graduate levels. He has been awarded a Teaching Excellence Award in 2012 by the Indian Institute of Technology Delhi. In 2013 he received the Distinguished Alumnus Award of the Department of Metallurgical Engineering, IIT-BHU, Varanasi.

Course Coordinator

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