National Institute of Technology Rourkela

Progress Seminar

Seminar Title	: Parameterization of Interatomic Potentials for Metallic Systems
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Venue	: MME Annex Building :M.Tech. Classroom (Room No MM 202)
Date and Time	: 05 Feb 2025 (04:00 PM)
Abstract	: Molecular Dynamics (MD) simulation helps to investigate different aspects of an alloy system, starting from scratch. In this regard, interatomic potential plays an important role. We are carrying out our research in the direction of parameterization of interatomic potentials, particularly Embedded Atom Method (EAM) potentials, and implementing these potentials in MD simulations to investigate several aspects of different metallic systems. The force-matching approach was first taken to fit the EAM potentials. Then the optimization to converged Density Functional Theory (DFT) data sets was carried out to make reliable and appropriate potentials for BaPt 2 and BaRh 2 crystals because of their importance in high-temperature structural applications. Density, elastic properties, cohesive energy, and lattice thermal conductivity have been calculated through MD simulations using those parameterized EAM potentials and validated these properties with DFT-based results in order to examine the accuracy and performance of these potentials. Discrepancies in some places have been observed because of the difficulty in fitting procedures. Thereafter, these EAM potentials have been used to investigate some fundamental aspects.