National Institute of Technology Rourkela

Departmental Seminar

Seminar Title	: Molecular Dynamics Study on Bending Creep Characteristics of BaPd2 Crystal using Developed Embedded-Atom Method Potential of Palladium-Barium Alloy
Speaker	: Sankhasubhra Mukhopadhyay
Supervisor	: 9564266381
Venue	: M.Tech class room (MM 202E), MM Annex building
Date and Time	: 03 Jan 2025 (4:30 pm)
Abstract	: Molecular dynamics (MD) simulation has been performed to study the bending creep characteristics of BaPd2 crystal (C15 laves phase compound) using our developed embedded-atom method (EAM) potential for Palladium-Barium alloy. The force-matching method has been implemented to develop the EAM potential first, and then optimization to converged density-functional theory (DFT) data sets has been done to generate the accurate and reliable potential for the Pd-Ba alloy system. Density, elastic properties, and thermal expansion coefficient have been calculated using MD simulation and validated these properties with the help of DFT analysis to examine the performance of the potential. Then, using a force of around 2 pN applied in the Y direction with both ends held stationary, bending creep simulations have been carried out on BaPd2 crystal at 100 K, 490 K, 600 K, and 900 K. Tertiary region has been observed above 490 K. Creep rate increases with increase in temperature.