National Institute of Technology Rourkela

Progress Seminar

Seminar Title	: Investigation of anomaly phase transition of Gallium, and effect of doping on its composite materials (InGaN, AlInGaN)
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Venue	: New Seminar Room(Chemical Engineering)
Date and Time	: 23 Jan 2025 (4:30 PM)
Abstract	: Gallium with exceptional properties, has applications in thermal energy transport, wearable soft electronics, micro-fluidic transport, drug delivery, and its composites fall in III-nitrides family and are important materials in electronic devices. Phase transition studies are important for elemental gallium for its efficient application, and also for its composite (III-nitrides) to identify the typical defects observed in the growth composite, which include threading and misfit dislocation, stacking fault, grain and domain boundaries, surface roughness. Molecular Dynamics (MD) simulations are a powerful tool for optimizing process conditions in material growth processes because they provide detailed, atomic-level insights into the dynamic interactions and behaviors of atoms and molecules. We have performed MD simulation of solid&ndashliquid phase transition study for elemental gallium and vapor deposition of AlInGaN film growth on solid GaN substrate. To predict the solid&ndashliquid phase transitions of gallium, we calculated free energy by employing the &ldquoconstrained *&lambda* integration&rdquo method, coupled with multiple histogram reweighting (MHR). Our findings indicate that the solid-liquid phase coexistence temperature of gallium is 305.2± 1.2 K. The solid&ndashliquid coexistence line is determined through the Gibbs&ndashDuhem integration technique. Our vapour deposition of AlInGaN film on polar GaN [0001] surface reveals different defects that formed with a change in the Al to In ratio and impact of substrate temperature on the growth film. We found crystallinity and surface roughness improve upon increasing substrate temperature and Al to In ratio. Low temperature and lower Al to In ratio promote the formation of highly polytypic columnar structures which reduce crystallinity, and domain size and increase surface roughness. From the dislocation study, we found dislocation with Buger vector 1/3[1□ 10] and 1/3[1□ 00] are primarily formed, which release lattice mismatch strain in the x and y directions.

Keywords: MD simulation, phase transition, vapor deposition