National Institute of Technology Rourkela

Departmental Seminar

Seminar Title	: Conference Return Seminar on Molecular Dynamics Studies on Hetero-epitaxial Growth of AlInGaN on polar GaN [0 0 0 1] surface (Presented at IIChE-CHEMCON 2024, NIT Jalandhar)
Speaker	: Mr. Anuj Debnath (Phd, Roll No. 521ch1002)
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Venue	: New Seminar Hall, Chemical Engg. Department
Date and Time	: 08 Jan 2025 (10.30 A.M.)
Abstract	: One important issue restricting semiconductor material performance is atomic-scale imperfections. Understanding the effects of defects, as well as the process underlying their formation, is crucial to improving these materials. In this work, We carried out Molecular dynamics simulations to investigate the vapor deposition of AlInGaN on polar GaN [0 0 0 1] surface. The quaternary AlInGaN offers prospects for the development of III-nitrides devices, including quantum well engineering, high mobility transistor, and LED efficiency enhancement. In this paper, the first section contains the methodologies to simulate the molecular beam epitaxy, and for that, We have implemented time and position-dependent conditional boundary conditions in the vapor phase region, bulk solid region and solid surface-vapor region, which is the growing region of film of AlInGaN. We have used the optimized Stillinger-Weber (SW) potential to determine the interaction between Al-In-Ga-N atoms. Heterogeneous growth of AlInGaN is performed at two different temperatures 1800K and 2500K, to check the substrate temperature effect on quaternary alloy growth. We have performed some analysis to check the crystallinity and surface roughness. Our findings show that with increasing temperature, crystallinity increases and surface roughness decreases. Keywords: Epitaxial growth, surface morphology, Stillinger-Weber (SW) potential, molecular dynamics, surface roughness, crystallinity, AlInGAN