Materials Science and Engineering Dissertation Defense

Structural and Chemical Characterization of Ultrawide Bandgap
Semiconductor Heterostructures

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Abstract

Emerging technologies require semiconductor devices capable of handling high voltages (HV, >1 kV), high frequencies (HF, >1 MHz), and extreme thermal loads in compact device footprints. Conventional semiconductors cannot meet the demanding requirements, especially current densities and thermal effects. Ultrawide bandgap (UWBG) semiconductors including diamond, cubic-BN, AlGaN, and β -Ga2O3, have superior electrical and thermal properties, offering great potential for HV-HF power electronics. However, their integration into high-performance devices remains underdeveloped due to challenges in synthesis, defect control, doping, and heterointegration. The research of this dissertation has focused on optimization of material growth and device fabrication for UWBG-based heterostructures based on structural and chemical characterization using electron microscopy.

A detailed study of heat-spreading layers of polycrystalline diamond grown on Si substrates with dielectric interlayers (SiO2 or SiC) examined atomic-scale structural and chemical transitions at the interfaces. High-resolution (scanning) transmission electron microscopy (HR(S)TEM) and electron-energy-loss spectroscopy (EELS) revealed chemically graded, non-abrupt interfaces resulting from interdiffusion during diamond layer growth. These transitions significantly influenced phonon transmission, causing deviations from expected thermal boundary resistance (TBR) versus interlayer thickness trends. The measured TBR reductions of up to 70% compared to abrupt interfaces demonstrated the benefit of interface engineering for thermal management of high-power devices.

The origin of texture and coherent interfaces in epitaxial β -Ga2O3 films grown on (100) diamond with β -(Al/Ga)2O3 buffer layers was investigated. The results showed that substrate orientation, morphology and crystallographic symmetry of the monoclinic epilayer governed film texture and interface characteristics, with implications for phonon and carrier transport. Dark-field and HRTEM imaging, combined with symmetry analysis of monoclinic C2/m structure, were used to characterize rotational domain variants and prevalent domain boundaries (DBs). Coherency of DBs was shown to be linked to inter-domain lattice mismatch, causing lattice distortions, rotations, and changes in DB character.

Additional characterization studies included III-nitride and β-Ga2O3-based heterostructures, multiply twinned particles formed through twin-mediated growth of polycrystalline diamond at low temperatures, and phase transformation in BN induced by high-pressure high-temperature treatment. The results emphasized the ongoing need for optimization of growth conditions, and careful selection and preparation of suitable substrate(s), coupled with strategies for doping control, interface engineering and thermal management.

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