The epitaxial strain and stress relationships in the alpha and beta phases of (Al,Ga)2O3 and their effects onto phonon and electronic properties

Mathias Schubert[1,2], Rafal Korlacki[2], Megan Stokey[3], Alyssa Mock[4], Vanya Darakchieva[1]
[1] Lund University, [2] University of Nebraska-Lincoln, [3] Milwaukee School of Engineering, [4] Weber State University

Pseudomorphic heteroepitaxial growth in the alloy system (Al,Ga)2O3 with composition-dependent lattice mismatch produces layers with varying amounts of strain, which modifies their phonon and electronic properties due to lattice cell distortions and subsequent band structure variations. We derive a general theory for the epitaxial strain-stress relationship in monoclinic beta-phase (Al,Ga)2O3 for arbitrary growth surface orientations. This relationship permits determination of the strain parameters as a function of composition, for example, and provides insight into the alloy induced changes in phonon and electronic properties. For monoclinic phase (Al,Ga)2O3, for any given eigenenergy state, four deformation parameters are sufficient to render the effect of symmetry-conserving strain, while two are sufficient for the same in the rhombohedral alpha phase of (Al,Ga)2O3. We then use first principles calculations to obtain the deformation potential parameters for phonon and electronic level shifts in the monoclinic as well as the rhombohedral phase of (Al,Ga)2O3within the general framework of first order perturbation theory. We predict the changes in phonon modes and band to band transitions in heteroepitaxial growth depending on crystallographic surface plane orientation in monoclinic and rhombohedral (Al,Ga)2O3. We discuss consequences for band alignment and band gap shifts depending on surface orientation in heteroepitaxy in the (Al,Ga)2O3 system, as a function of the type, structure, and composition of (Al,Ga)2O3 templates. We compare our calculations with experimental data obtained from ellipsometry investigations of heteroepitaxial thin films. We also discuss changes in pattern and polarization properties of phonon modes and band to band transitions and their associated excitons. .