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Three-Dimensional Lattice Matching of Epitaxially Embedded Nanoparticles[1] BRELON MAY, PETER ANDERSON, ROBERTO MYERS, The Ohio State University — Since Mathews and Blakeslee developed a theory of atomic lattice matched thin films in 1974, epitaxy has been modeled using 2D lattice-matching considering only the in-plane strain (ε^*_{IP}). Here, we present a 3D model to predict the conditions at which epitaxially encased nanoparticles relax by plastic deformation, including the out-of-plane lattice mismatch (ε^*_{OP}). The critical particle length (L_C) at which defect formation proceeds is determined by balancing the resulting reduction in strain energy from a dislocation, with the corresponding increase in the energy of formation. Our results use a modified Eshelby inclusion technique for an embedded nanoparticle, shedding new light on the epitaxy of nanostructures. By tailoring ε^*_{IP} and ε^*_{OP}, L_C can be increased to 70% beyond the case of encapsulation in a homogenous matrix. An InAs nanoparticle embedded in GaN ($\varepsilon^*_{IP} = \varepsilon^*_{OP} = -0.072$) results in $L_C = 10.8$ nm. However, it can be increased to 16.4 nm when grown on GaAs and surrounded by InSb ($\varepsilon^*_{IP} = -0.072, \varepsilon^*_{OP} = +0.065$), and a maximum of 18.4 nm if the particle is capped by an alloy with $\varepsilon^*_{OP} = +0.037$. This effect, which we term "3D Poisson-stabilization", provides a means to increase the strain tolerance and modify the strain state in epitaxial heterostructures through the engineering of ε^*_{OP}.

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