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Abstracts

Constitutive and FE modeling of Residual Stresses and Kirkendall Effect in Semiconductor Structures

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The interdiffusion of chemical components coupled with vacancy movement can cause void formation and/or spinodal decomposition in crystal growth. In the case of SiC growth on Si, the higher mobility of Si atoms compared to C results in the migration of SiC/Si interface and formation of voids in the substrate in some thermodynamic conditions. In the case of In-rich InGaN layers deposited on GaN a precipitation of metallic indium bordering with voids is observed.

In the current approach we consider interdiffusion, lattice distortion and chemical maps extracted from HRTEM images of SiC/Si and InGaN/GaN. Dislocations and void surface are treated as local regions of nucleation and annihilation of the vacancies transporting the mass in FE mesh. In result, the interface and FE mesh are convected with the crystal lattice drift. In the constitutive modeling applied [1] the lattice strain and the atom fraction of chemical component are used as two independent thermodynamic variables. Due to climbing of misfit dislocations the plastic distortion tensor field is taken into account in the form of additional nodal variables. This tensor field is spanned on corner nodes of Lagrangian finite elements (FE) which gives the possibility for reconstruction of the atomistic model of dislocation network interpenetrating the considered FE mesh [2,3].

The chemo-mechanical coupling is based on the use of Vegard's law formulated in terms of Biot strain. Due to the logarithmic strain applied in hyperelastic modeling, some transformation rule is considered for Vegard's law. This rule allowed us to eliminate artificial residual stresses yielding from incompatibe fields of the atom fraction and plastic distortions spanned on nodes by means of shape functions [2]. In the case of single finite elements, the mentioned approach allowed us to reduce spurious stresses in integration points from the level 100 MPa to 10^-5 MPa, while at the same time holding the stress components yielding from Vegard's law at the level of 1 GPa (relaxed by plastic distortions).

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