On Nucleation and Growth of Liquid Droplets in Single Crystals

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This is a study on a mathematical model which describes an elaborate process in single crystal GalliumArsenide (GaAs), where stress assisted diffusion might lead to the formation of liquid droplets. The model consists of a coupled system of PDEs for the variables strain, concentration and a space-time dependent phase density, that gives the size distribution of droplets.

Single crystal GaAs is formed by two fcc sublattices, which are completely occupied by Ga-atoms and As-atoms, respectively. In order to fabricate semiconducting GaAs, a small amount, say 0.001

The mathematical model describes the dislocation induced stress distribution in the crystal by the quasistatic momentum balance. The interaction of the diffusing atoms with the resulting stress field leads to a coupling of the momentum balance with the diffusion equation, which is written down for those excess atoms that do not exist in droplets. Thus there is a source term in the diffusion equation describing the rate of droplet formation. Finally, the evolution of droplets is determined by the Becker/Doering system of rate equations.