

Phase-Field Modeling of Nanowire Growth

T. Philippe

Normandie Université, Groupe de Physique des Matériaux (GPM), UMR CNRS 6634 BP 12, Avenue de l'Université, 76801 Saint Etienne du Rouvray, France
Email: thomas.philippe1984@gmail.com

We use the phase-field (PF) method to model nanowire growth by the vapor-liquid-solid (VLS) mechanism. As major advantages, the PF method operates on the same length and time scales as experiments and naturally accounts for the Gibbs-Thompson effect. Moreover, the PF method can also account for elastic deformation and anisotropic interfacial energy. We model nanowire growth in two-dimensions, see Fig.1. In this preliminary work, we investigate the role of tri-junctions on nanowire growth and compare our simulations to sharp-interface models, in the case of isotropic surface energies. We vary the difference in chemical potentials between the liquid and solid phases and compare growth velocity, shape and diameter of nanowires and morphology of triple junctions. We plan to include anisotropy in both surface energy and mobility so that to reproduce changes in growth direction such as wire kinking, as observed in experiments, and also to elucidate the role of tri-junctions in such mechanisms. Important features of nanowires such as facets of the sidewall and the shape of the nanowires cross section need modeling in three dimensions.

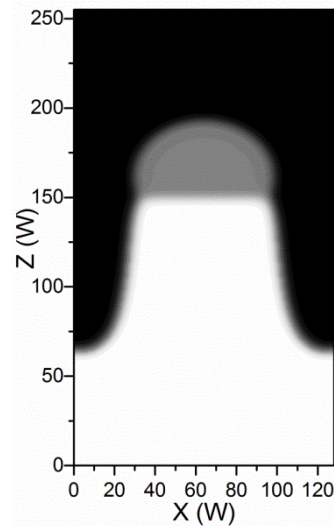


Figure 1: 2D Phase-Field simulation of nanowire growth by the VLS mechanism. Lengths are expressed in terms of the interface width (W).