Multiscale modeling of epitaxial growth

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A deep understanding of the fundamental physics underlying epitaxial growth techniques is a prerequisite for any significant success in semiconductor nanotechnology. The frontiers in developing novel electronic devices lie in the realm of the length scales from nanometers to microns. Controlling the surface morphology during epitaxial growth at such scales is a challanging task. In this regime kinetic effects on an atomistic scale strongly influence the morphology. Thus a continuum theory based on rational mechanics cannot describe the growth process appropriately. On the other hand the applicability of discrete models on an atomistic scale is limited due to its high computational cost if time and length scales related to device applications are considered.

As first pointed out by Burton, Cabrera and Frank [1] an intermediate regime between atomistic and continuum modeling can be used to combine the appropriate atomistic properties with the computational ease of continuum models. At crystalline surfaces the evolution of the steps, their advancement, nucleation and annihilation, can be used to describe the surface morphology of the growing film. This allows to break the model in a $2+1$-dimensional model, continuous in the lateral direction but discrete in height. The evolution of steps is implicitly connected to atomistic motion via attachment and detachment at step edges and therefore allows to incorporate essential kinetic effects on an atomistic scale. Various step flow models have been developed which incorporate more and more of the relevant atomistic effects. These models have proven to be extremely powerful in understanding surface morphologies and the formation of patterns at the nanometer and micrometer scales. However most of these models assume implicitly a close-to-equilibrium situation, which is not fullfilled in many applications related to Molecular Beam Epitaxy. We will develop a step flow model, which does not rely on the assumption of the system to be close to equilibrium. The model is a terrace-step-kink model. We consider densities of adatoms on terraces, densities of step adatoms and kinks on curved steps and define all fluxes between them through atomistic processes. Similar models have been introduced in [2, 3].

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References

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