Epitaxial crystal growth with adatoms

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Surface diffusion is one of the most important mechanisms driving crystal growth. When bulk diffusion is much faster than the surface one, the evolution of the profile of the crystal is described by the so called Einstein–Nernst relation. According to this law, the normal velocity of the profile is related to the chemical potential. This evolution equation has a variational flavor, in that it can be obtained as a gradient flow of a suitable free energy.

Albeit usually neglected, adatoms (atoms freely diffusing on the surface of the crystal) seem to play a fundamental role in the description of the behaviour of a solid-vapor interfaces. For this reason, some years ago Fried and Gurtin introduced a system of evolution equations to describe such a situation, where adatoms are treated as a separate variable of the problem. Also such system of evolution equations can be seen as the gradient flow of an energy.

In this talk a first step in the programme of studying the above mentioned evolution equations from a variational point of view is presented. In particular, the focus is on the static problem in the small mass regime, where the elastic energy is negligible. Ground states, effective energy, and phase filed approximation suitable for numerical purposes are discussed. This latter is embedded in a general framework that allows to treat similar problems for a large class of functionals.

The talk is based on works in collaboration with Marco Caroccia (Roma Tor Vergata), and Laurent Dietrich (Lycée Fabert).