Ab initio based growth simulations of thin films

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A challenge in performing crystal growth simulations is the large range of relevant length and time scales. While eventually being interested in a description on a mesoscopic/macroscopic scale (the size of typical defect or surface features is in the order of 10 to 100 nm and the growth time is in order of seconds up to hours) the mechanisms leading to these structures (adatom adsorption, diffusion, desorption, island nucleation) require a resolution in the length scale of atomic bonds (0.1 nm) and in the time scale of atomic vibrations (10^{-13} s^{-1}). Therefore, common approaches to simulate growth have been restricted on specific properties (on the meso/macro scale) and included microscopic information only indirectly by empirical/adjustable parameters. Examples are rate equations or continuum models. While these approaches give valuable insight into qualitative aspects of growth a quantitative analysis requires to include the microscopic mechanisms directly.

A new approach to describe microscopic growth mechanisms is the application of *ab initio* methods such as density-functional theory (DFT). The key idea of these methods is to describe nature of the most fundamental level: the growing crystal and its structural elements are decamped into the most elementary building blocks such as atomic nuclei and electrons and the interactions between them is described by the fundamental laws of electrodynamics and quantum mechanics.

In the present lecture I will discuss how by combining density-functional theory with concepts of thermodynamics statistical physics simulations can be performed which allow to bridge between microscopic and mesoscopic scales. Such multiscale simulations which couple methods developed for various length and time scales provide the unique opportunity to combine the advantages of *ab initio* methods (universality and predictive power) with the efficiency of mesoscopic models to address a wide range of crystal growth and doping problems. While this approach is still in its infancy first results are very promising and future improvements in the methods and in computers will allow to perform these types of studies routinely.