Ab initio based Multiscale Growth Simulations of Group-III Nitrides

Jörg Neugebauer and, L. Lymperakis
Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1,
D-40237 Düsseldorf, Germany

A challenge in performing accurate simulations on crystal growth is the large range of relevant length and time scales. While eventually one is interested in a description on a mesoscopic scale (the size of typical surface features such as quantum dots, surface roughness, terrace length is in the order of 10..1000 nm and the characteristic time scale to form such features is in the order of seconds) the mechanisms leading to these structures (adatom adsorption, diffusion, desorption, island nucleation) require a atomic scale resolution, i.e., a resolution in the length scale of 10-1nm and in the time scale of $10^{-13}s^{-1}$. Therefore, commonly approaches to simulate growth have been restricted on specific properties (on the mesoscopic scale) and included microscopic information only indirectly by empirical/adjustable parameters. In the present talk I will discuss how by combining density-functional theory with concepts of thermodynamics, continuum elastic theory, and/or statistical physics simulations can be performed which allow to bridge between microscopic and mesoscopic scales. To discuss the applicability but also the present limitations of this approach the focus will be on various issues regarding doping [1,2], formation/properties of extended defects and growth of group-III nitrides (GaN, AlN, InN and their alloys) [3-5].

[1] C. G. Van de Walle and J. Neugebauer, Nature 423, 626 (2003).
[2] C.G. Van de Walle and J. Neugebauer, J. Appl. Phys. **95**, 3851 (2004).
[3] L. Lymperakis, J. Neugebauer, M. Albrecht, T. Remmele, and H. P. Strunk, Phys. Rev. Lett. **93**, 196401 (2004).
[4] J. Neugebauer, T.K. Zywietz, M. Scheffler, J.E. Northrup, H. Chen, and R.M. Feenstra, Phys. Rev. Lett. **90**, 056101 (2003).
[5] L. Mandreoli, J. Neugebauer, R. Kunert, and E. Scholl, Phys. Rev. B **68**, 155429 (2003).