Manuel Diehm

Characterisation of Surfaces by Atomistic Simulation

With the increasing tendency of new technologies to use materials with nanoscale sizes, the influence of surfaces on material properties becomes more and more important. However, the thermodynamical quantities which are used to characterize surfaces, namely surface energy and surface stress, are difficult to determine directly in experiment. Atomistic simulation offers a relatively easy way to determine these quantities for a wide range of material surfaces. In this contribution I will first outline the basics of Gibbsian surface thermodynamics, with a special emphasize on solid surfaces. The thermodynamical quantities of surface energy and surface stress and their interrelation will be derived and their physical interpretation will be discussed. I will then describe how these quantities can be caluclated from atomistic simulation. Finally, I will explain how surface phase diagrams are constructed and how they should be interpreted.