Ab initio simulations of homoepitaxial SiC growth

M. C. Righi,[1] C. A. Pignedoli,[1] A. Catellani,[2] R. Di Felice,[1] and C. M. Bertoni[1]
[1] *INFM-National Research Center on nanoStructures and bioSystems at Surfaces (S^3), Dipartimento di Fisica, Università di Modena e Reggio Emilia, Via Campi 213/A, 41100 Modena, Italy*
[2] *CNR-IMEM, Parco Area delle Scienze 37a, 43010 Parma, Italy*

Understanding the modifications which occur in the surface local geometry during materials growth is mandatory to control and refine the process. We present first-principles total energy and force calculations of the initial stages of SiC growth on the β-SiC(111)$\sqrt{3} \times \sqrt{3}$ surface. We faced the problem of adsorption on a reconstructed, non stoichiometric surface by considering the potential energy surface (PES) experienced by one adatom, as a multilevel function: we studied the energy landscape both *above* and *within* the reconstruction layer. We found that C adsorption is favored *within* the superstructure rather than on its top. The origin of this less obvious adsorption mechanism is that weak surface bonds (Si-Si) are replaced by almost bulk-like Si-C bonds. We simulated the incorporation of C and Si atoms on SiC(111) following a step-by-step procedure according to which the adsorption processes take place one after the other. At each step the adatom binding energy was calculated as a function of the local surface geometry and the lateral coordination; the lowest energy configuration was chosen as the staring point for the next process. Proceeding in this way, without imposing any a-priori-determined evolution path, a precise unconstrained growth mechanism came out. From a thorough comparison of the evolution and energetics of the several computed structures, we were able to identify some peculiar behaviors which can act as driving factors during SiC growth. Our results reveal that the surface superstructure developing during growth, plays a fundamental role in favoring the stabilization of the deposited material into ordered crystal structure.