Stepped 4H-SiC {0001} surfaces: a DFT study

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The wide band-gap semiconductor silicon carbide has attracted a great interest during the past decades because of number of properties which make it very attractive for many applications in electronic devices. For electronic applications purposes hexagonal 4H-SiC is the preferred polytype. One of the main problems in the development of the SiC-based electronics is still poor quality of the SiC crystals. There have been theoretical studies of both clean and adsorbed ideal 4H-SiC{0001} surfaces. However, real surfaces are stepped ones and chemical processes important for crystal growth can occur at steps or in their vicinity. In this paper we presents DFT calculations of clean steps along $\langle 10\bar{1}0\rangle$ and $\langle 11\bar{2}0\rangle$ directions on Si- and C-terminated 4H-SiC{0001} surfaces. DTF calculations can deal with relatively small number of atoms. Surface steps are large structures in atomic scale. Therefore, it is extremely important to choose a proper model describing stepped surface. In experiments, steps with a half or one cell height are observed. We applied two different models for steps with various heights (Fig. 1). For each model tests were performed aiming at finding a minimal step width by increasing the step width from 4 to 14 atomic layers. We searched for the sufficient step width to describe correctly flat terraces between steps. Our research shows that even for the widest steps examined the corrugation on terraces is still observed. It exists in both models and is especially pronounced on Si-terminated surfaces. It is an indication of strong long-range stress induced by steps. Our biggest calculations involved more 400 atoms which is at the limit of DFT. Therefore, we couldn't test wider steps. However, by comparison of a Si/C atom adsorption on the terraces and clean surfaces we can estimate the corrugation effect on the binding properties of adsorbates.

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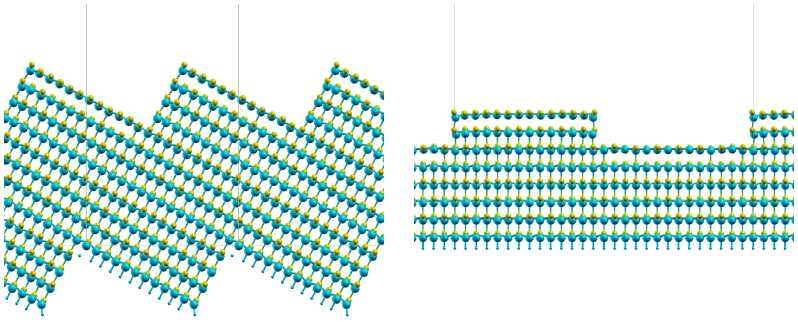

(a) (b)

Figure 1: Supercells used to model steps along $\langle 11\bar{2}0\rangle$ direction on 4H-SiC-{0001} surfaces. Vertical lines represent supercell borders. (a) *Saw model*: describes steps with one cell height. (b) *Stripe model*: describes steps with a half cell height.