Bi-nanoline formation on Si(001) and H/Si(001) surfaces

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Self-organized atomic arrangements on semiconductor surfaces have been the subject of intense experimental and theoretical investigation. Bi nanolines, in particular, have been studied on Si(001) surfaces because it has been found that they can be grown defect free. The structural quality of the lines leads directly to exciting new opportunities for templating either with single Bi lines or with arrays of lines. The lines/line arrays could be used to guide or constrain the self-assembly of other lines with tailored electrical, optical and magnetic properties for nano-scale devices or sensors. Numerous investigations of the nanoline equilibrium atomic geometry have been reported and several different structural models have been proposed. However, no model is in full agreement with all experimental findings. Furthermore, in some templating scenarios it is important to passivate the topmost Si dimer plane with H, since the clean Si (001) surface is more reactive than the Bi--nanoline. Consequently, the electronic structure, energetic stability, and the equilibrium atomic geometry of the Bi--nanolines on the hydrogenated Si (001) substrate are important issues to be investigated.

In this work, we present a combined theoretical and experimental investigation of the Bi--nanolines on clean Si (001) and hydrogenated H/Si (001) surfaces. We have considered the two most plausible structural models, M and H (presented in Fig. 1) for the Bi--nanolines. The energetic stability of the H model for the nanolines on Si (001) has been confirmed. Similarly, our total energy results indicate that the H model is also the energetically most stable for the Bi--nanolines on the H/Si (001) substrate. The equilibrium geometry for both models have been detailed and compared with the experimental findings. Finally the electronic structure of the nanolines has been investigated by means of STM simulations and electronic structure calculations. The experimental investigations have been carried out for several positive and negative biases. The experimental and theoretical results have been analyzed carefully to present a coherent picture of the electronic features of the nanowire.