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Modelling the Si(110) surface VERONIKA BRAZDOVA, University College London, UK, MARTIN SETVIN, Charles University Prague, Czech Republic, KAZUSHI MIKI, National Institute for Materials Science, Tsukuba, Japan, CYRUS F. HIRJIBEHEDIN, DAVID R. BOWLER, University College London, UK
— The Si(110) surface has been less intensively studied than Si(001) and Si(111). However, it also shows interesting scientific and technological properties, including a complex stepped (16x2) surface reconstruction. We will present results of comprehensive density functional theory studies on the diffusion of Si and H adatoms on Si(110)-(1x1), as well as of the driving mechanisms behind the surface reconstruction. The diffusion studies are a necessary starting point for understanding the growth of features with (110) sidewalls; the Si adatom diffusion will also feed into the studies of Si(110)-(16x2), as the formation of this reconstruction seems to involve significant amounts of mass transport. Barriers and structures resulting from diffusion will be presented, and their implications for growth and reconstruction will be discussed. We will discuss the implication of Si atom adsorption and surface defect formation on the reconstruction of the surface. [1] T Mizuno et al, IEEE Trans Electron Devices 2005, 52, 367. [2] Y Suda et al, Appl Surf Sci 2003, 216, 424.

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