Atomic-scale Reconstructions on Metal and Semiconductor Surfaces

Andrew T. S. Wee

Department of Physics, National University of Singapore,2 Science Drive 3, S117542, SINGAPORE

The combined use of STM (scanning tunneling microscopy), LEED (low energy electron diffraction) and synchrotron experiments, as well as computational studies using tensor LEED analysis and density functional theory (DFT) calculations on several metal and semiconductor single crystal surfaces is presented. We have studied multilayer relaxations of high index fcc transition metal surfaces by pseudopotential DFT calculations [1]. A general rule for the multilayer relaxation sequence of open high index metal surfaces is proposed [2]. In particular, the multilayer relaxation of Cu(210) has been elucidated by layer-doubling LEED analysis and pseudopotential density functional theory (DFT) calculations [3]. The formation of oxygen-induced reconstructions on Cu(210) has been observed using STM [4] and LEED, and its detailed structure calculated by tensor LEED [5]. Two-dimensional mesoscopic triangular checkerboard patterns are also formed after the etching of Cu(210) by bromine [6].

The SiC(0001) wide bandgap semiconductor surface displays a range of interesting surface reconstructions [7]. We have reported the formation of metastable (6x6)-Si nanoclusters on 6H-SiC(0001)-(3x3) [8],[9]. The occurrence of these regularly-sized "magic" clusters demonstrates the potential of nanostructure formation of Si on SiC. Monodispersed Co nanoclusters of 3 to 5 nm sizes have been deposited on the C-terminated 6H-SiC(0001) 6√3x6√3R30° template (Fig. 1) [10], which we have also studied in detail using synchrotron photoemission techniques. *In-situ* STM shows that the average cluster size remains constant for different Co coverage, and the cluster density is linearly dependent on the coverage. The monodispersion of the cluster size is suggested to be due to the physical confinement of the Co clusters by the porous honeycomb structure of the SiC reconstructed surface. For GaAs(001), we propose a new model for the Ga-rich c(8x2) reconstruction based on high resolution STM data [11]. We have also studied the transitional GaAs(001)-(n x 6) reconstructions [12], including the (6x6) and (4x6) reconstructions.

Figure 1: The C-terminated 6H-SiC(0001) 6√3x6√3R30° reconstruction imaged by STM.
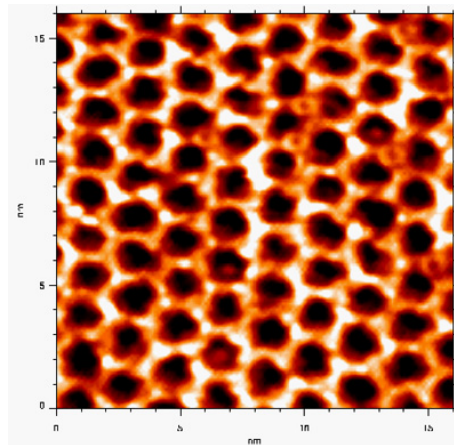
References
[1]   Y. Y. Sun, H. Xu, Y.P. Feng, A. C. H. Huan, A. T. S. Wee, *Surf. Sci.* **548**, 309 (2004).
[2]   Y. Y. Sun, H. Xu, Y.P. Feng, A. C. H. Huan, A. T. S. Wee, *Phys. Rev. Lett.*, **93** (2004) 136102.
[3]   Y. Y. Sun, H. Xu, J. C. Zheng, J. Y. Zhou, Y. P. Feng, A. C. H. Huan, A. T. S. Wee, *Phys. Rev. B* **68**, 115420 (2003).
[4]   A. T. S. Wee, J. S. Foord, R. G. Egdell, J. B. Pethica, *Phys. Rev. B* **58**, R7548 (1998).
[5]   Y. P. Guo, K. C. Tan, H.Q. Wang, C. H. A. Huan, A. T. S. Wee, *Phys. Rev. B* **66**, 165410 (2002).
[6]   A. T. S. Wee, T. W. Fishlock, R. A. Dixon, J. S. Foord, R. G.Egdell, J. B. Pethica, *Chem. Phys. Lett.* **298**, 146 (1998).
[7]   X. N. Nie, H. Q. Wang, A. T. S. Wee, K. P. Loh, *Surf. Sci.* **478**, 57 (2001).
[8]   W. J. Ong, E. S. Tok, H. Xu, A. T. S. Wee, *Appl. Phys. Lett.* **80**, 3406 (2002).
[9]   E. S. Tok, W. J. Ong, A. T. S. Wee, *Surf. Sci.* **558**, 145 (2004).
[10] W. Chen, K. P. Loh, H. Xu, A. T. S. Wee, *Appl. Phys. Lett.* **84**, 281 (2004).
[11] H. Xu, Y. Y. Sun, Y. G. Li, Y. P. Feng, A. T. S. Wee, A. C. H. Huan, *Phys. Rev. B* **70**, 081313 (2004).
[12] H. Xu, Y. G. Li, A. T. S. Wee, C. H. A. Huan, E. S. Tok, *Surf. Sci.* **513** (2002) 249.