

Experimental evidence of orbital-rehybridization on the Si(113)3×1 surface

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Orbital-rehybridization on the Si(113)3×1 surface was investigated by using low energy electron diffraction and synchrotron radiation photoemission spectroscopy. We observed that annealings of the silicon-deposited surface at room temperature resulted in 1×2, 3×1 and 3×2 phases with increasing temperature. Two shoulders of Si 2p core level spectrum appeared obviously at higher and lower binding energy side of the bulk component with the structural transformation from the 1×2 to the 3×1. From the fitting of the Si 2p core level spectrum for the Si(113)3×1 surface, three surface components were resolved at binding energies of about 0.745, -0.554 and 0.34 eV, respectively. In comparison with theoretical calculations for a Ranke's 3x1 model, it seems that about 0.2 electronic charges per atom are transferred from the rests of tetramer to the dimer in the 3×1 unit cell and then, orbital is rehybridized toward s^2p^3 and sp^2 -like configuration on the Si(113) surface.