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Structure and electronic properties of silicon nanowires grown along the [110] direction: role of surface reconstruction T. AKIYAMA, K. NAKAMURA, T. ITO, Dept. of Phys. Eng., Mie Univ., Japan — Silicon single-crystal nanowires (SiNWs) are attracting great interest for future nanoscale devises in recent years. So far, the [110] grown SiNWs with diameters below 4 nm have been successfully fabricated by various methods[1]. Although the size dependence in electronic and optical properties for the [110] grown SiNWs terminated by H-atoms have been intensively studied[2], effects of surface reconstructions on the electronic structure have been rarely examined. Here, we investigate the atomic and electronic structures of SiNWs along the [110] direction with {001} and {111} facets using first-principles pseudopotential method. The calculations for SiNWs whose diameters are $\sim$4 nm demonstrate that the reconstructions on these facets are strongly dependent on H-chemical potential $\mu_{\rm H}$: The SiNW consisting of monohydride {001} and H-terminated {111} facets is stabilized for high $\mu_{\rm H}(\geq$-0.75 eV) while the pristine SiNW stabilized for low $\mu_{\rm H}(\leq$-0.82 eV). The reconstructions with partially hydrogenated facets appear for -0.82$<\mu_{\rm H}<$-0.75 eV. Peculiar features in the electronic structure are also found in partially hydrogenated SiNWs.

[1]Ma *et al.*, Science **299**, 1874(2003); Wu *et al.*, Nano Lett. **4**, 433(2004).
[2]Zhao *et al.*, Phys. Rev. Lett. **92**, 236805(2004).

Toru Akiyama
Department of Physics Engineering, Mie Univ.

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