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Adsorption of gold on hydrogen terminated Si(0 0 1): Formation of chain structure

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Possible formation of stable Au atomic wire on the hydrogen terminated Si(0 0 1): 3 × 1 surface is investigated under the density functional formalism. The hydrogen terminated Si(0 0 1): 3 × 1 surface is patterned in two different ways by removing selective hydrogen atoms from the surface. The adsorption of Au on such surfaces is studied at different sub-monolayer coverages. At 4/9 monolayer (ML) coverage, zigzag continuous Au chains are found to be stable on the patterned hydrogen terminated Si(0 0 1): 3 × 1 surface. The reason for the stability of the wire structures at 4/9 ML coverage is explained. It is to be noted that beyond 4/9 ML coverage, the additional Au atoms may introduce clusters on the surface. The continuous atomic gold chains on the substrate may be useful for the fabrication of atomic scale devices.

1. Introduction

Research interest on the formation of wire structures on the semiconducting surfaces [1–5] is increasing due to its potential technological application as atomic scale devices or as interconnects in nano-devices [6]. Silicon substrate is one of the most widely used substrate for technological applications and particularly Si(0 0 1) is one of the surfaces of choice. Recently, the hydrogen terminated Si(0 0 1) surface is being used for growing nano-structures of desired shapes. Hydrogen terminated Si(0 0 1) surface reconstructs into 3 × 1, 2 × 1 and 1 × 1 pattern depending on the hydrogen coverage and the experimental environment [7–13]. However, with the use of STM tip a hydrogen terminated Si(0 0 1): 3 × 1 surface may be patterned according to our desire by removing selective hydrogen atoms from the Si(0 0 1):3 × 1 surface. The possible formation of Al, Ga and In wires on patterned hydrogen terminated Si(0 0 1): 1 × 1 surface has been studied earlier [14]. A variety of one-dimensional chain structures of gold on high index silicon surfaces have been observed experimentally [15–19]. However, our interest lies on the formation of gold wire structures on the stable Si(0 0 1) surface. A recent theoretical study revealed that a stable gold atomic wire may be obtained on the patterned hydrogen terminated Si(0 0 1): 1 × 1 surface [20]. Here, we explore the possible formation of stable wire structures on the hydrogen terminated Si(0 0 1): 3 × 1 surface. We therefore, pattern the hydrogen terminated Si(0 0 1):3 × 1 surface in various ways by removing the desired hydrogen atoms from the surface and perform systematic study of Au adsorption on the patterned hydrogen terminated Si(0 0 1): 3 × 1 surface and hence search for the possible formation of Au wire structures on such surface. This study eventually reveals that formation of stable gold atomic chain of zigzag nature on the patterned hydrogen terminated Si(0 0 1):3 × 1 surface is indeed possible.

2. Method

First principle total energy calculations are carried out within density functional theory at zero temperature using the VASP code [21–23]. The wave functions are expressed by plane waves with the cutoff energy $|k+G|^2 \leq 300$ eV. The Brillouin zone (BZ) integrations are performed by using the Monkhorst–Pack scheme with 4 × 4 × 1 k-point meshes for 3 × 3 primitive cells. The results for fully relaxed atomic structures are obtained using the PW91 generalized gradient approximation (GGA). The preconditioned conjugate gradient method is used for the wave function optimization and the conjugate gradient method for ionic relaxation. The convergence criteria for energy are taken to be 10^{-5} eV and the systems are relaxed until the forces are below 0.005 eV/Å. The convergence with respect to the energy cutoff and with respect to k-point meshes is achieved with the given parameters. The hydrogen terminated Si(0 0 1):3 × 1 surface is represented by a repeated slab geometry. Each slab contains five Si atomic planes with hydrogen atoms passivating both the top and bottom layers of Si atoms of the slab (see Fig. 1). The consecutive slabs are separated by a vacuum space of 10 Å [24–27]. The Si atoms of bottom layer and the hydrogen atoms passivating the

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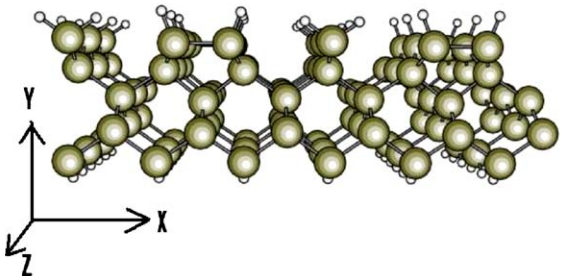

Fig. 1. Hydrogen terminated Si(0 0 1):3 × 1 surface within the 6 × 3 super-cell is shown here. The bigger and smaller circles represent the Si and hydrogen atoms respectively.

bottom silicon layer are kept fixed to simulate the bulk-like termination and the rest of the atoms are allowed to relax. It is clear from Fig. 1 that the hydrogen terminated Si(0 0 1): 3 × 1 surface has alternative monohydride Si-dimer rows and dihydride Si-monomer rows.

The hydrogen terminated Si(0 0 1):3 × 1 surface is patterned two different ways and they are named as hydrogen terminated Si(0 0 1): 3 × 1 surface with Pattern-1 and Pattern-2 respectively. The hydrogen terminated Si(0 0 1): 3 × 1 surface having Pattern-1 is schematically shown in Fig. 2(a) where six hydrogen atoms are removed from the surface within the 3 × 3 supercell (one hydrogen atom from each Si atom of the Si-monomer row and the Si atoms attached to the neighbor Si atoms of the Si-dimer row) and Pattern-2 surface is schematically shown in Fig. 2(b) where one hydrogen atom is removed from each Si atom of the Si-monomer row within the 3 × 3 supercell.

3. Results and discussion

Here we present the results and discussions of Au adsorption on the hydrogen terminated Si(0 0 1):3 × 1 surface having Pattern-1 and Pattern-2 respectively.

3.1. Hydrogen terminated Si(0 0 1):3 × 1 surface having Pattern-1

The hydrogen terminated Si(0 0 1): 3 × 1 surface having Pattern-1 has a row of dangling bonds extending along the [1 $\bar{1}$ 0] direction. The electronic structure and energetics for the adsorption of Au at different sub-monolayer coverages are discussed. Here one mono-layer (ML) is defined as one atom per surface Si atom.

Adsorption of one Au atom within the 3 × 3 super-cell of the Si(0 0 1): 3 × 1 surface having Pattern-1 corresponds to 1/9 ML

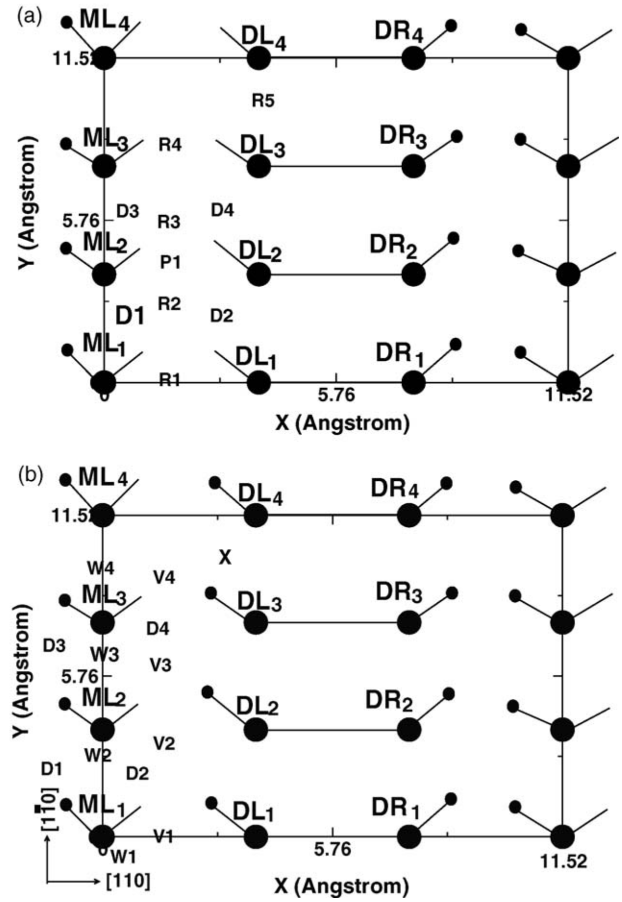

Fig. 2. Schematic diagram of the top layer of different patterned hydrogen terminated Si(0 0 1): 3 × 1 surface within 3 × 3 super-cell. The 3 × 3 super-cell closed by thick borders is shown here. The bigger circles correspond to the surface Si atoms and they are denoted by ML_1, ML_2, ML_3, DL_1, DL_2, DL_3, DR_1, DR_2 and DR_3 respectively while surface hydrogen atoms are represented by the smaller circles. The dangling bond wires extending along the [1 $\bar{1}$ 0] direction is visible. (a) The possible sites on Pattern-1 surface for Au adsorption are denoted as R1, P1, D1, D2 respectively. The chain configuration is denoted as R1R2R3R4 and the configurations deviated from chain are denoted as R1R2R3R5 and D1D2D3D4. (b) The chain configurations on Pattern-2 surface is denoted as W1W2W3W4 and the configurations deviated from chain are denoted as V1V2V3V4 and V1V2V3X respectively.

coverage. Various possible adsorption sites are denoted as R1, D1 and D2 and they are shown in Fig. 2(a). The R1, P1, D1 and D2 sites are in the middle of the line joining the Si atoms denoted by ML_1 and DL_1, ML_2 and DL_2, ML_1 and ML_2, and DL_1 and

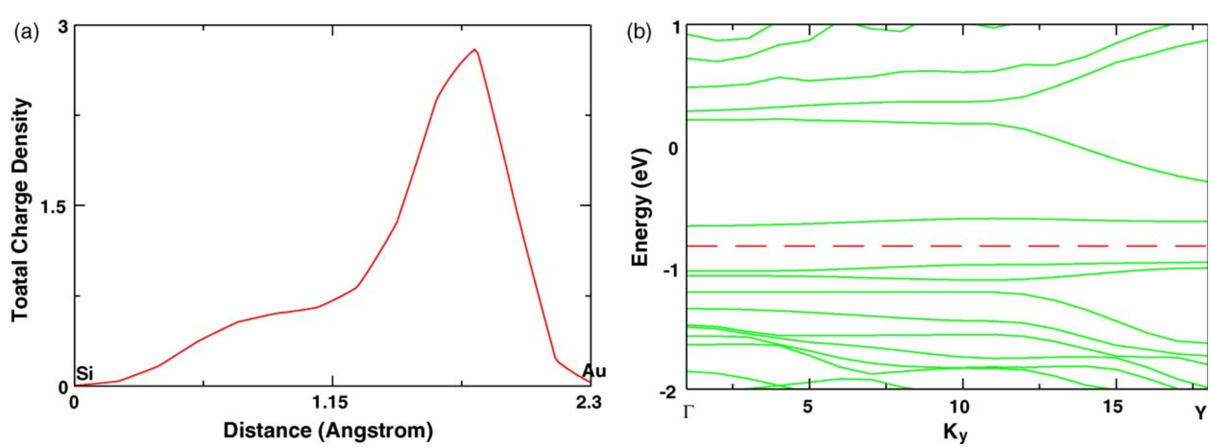

Fig. 3. Left panel: The total charge density is plotted along the line of Au–Si bond. Right panel: This shows the band structure plot along [1 $\bar{1}$ 0] direction when 4/9 ML is adsorbed on the patterned hydrogen terminated Si(0 0 1): 3 × 1 surface having Pattern-1. Fermi level is indicated by dashed line.