Transactions of the Materials Research Society of Japan 24 [2] 213-216 (1999)

Electronic Structures of Atomic Wires on a H-Terminated Si(100) Surface

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We theoretically predict the atomic and electronic structures of Ga, Al, and As atomic wires, which are chemically bound to a dangling-bond wire on a H-terminated Si(100) surface, via first-principles calculations within the local-density-functional approach. We show the chemical trend and carrier-doping effect in the conducting properties of the atomic wires, sensitively depending on the different species and concentration of adsorbed atoms. As an intriguing byproduct, we found that the As-wire has an unusually *flat* (dispersionless) energy band, where the flat band can be half-filled by electron-doping. According to so-called "flat-band ferromagnetism" theory, we show a novel possibility to create ferromagnetic nanowires, which are made up only of nonmagnetic atoms.

Recent progress in nano-fabrication technology using scanning tunneling microscope has opened up a new way to artificially design nanostructures on solid surfaces[1, 2, 3, 4, 5, 6, 7]. It is unequivocally crucial from viewpoints of potential industrial application to nano-scale electronic devices, as well as exploration of interesting physical phenomena. The confined electrons in nanostructures, such as quantum dots and nanowires, play a vital role in quantum interference and electron-correlation effects.

Among other things, Hashizume *et al.*[6] fabricated a Ga atomic wire bound to a H-terminated Si(100)2 × 1 surface and attempted to obtain the electronic structure via scanning tunneling spectroscopy. Also, Shen *et al.*[7] constructed Al atomic wires on a H-terminated Si(100) surface in a similar way and examined the nucleation mechanism of Al atoms in detail. However, information as to what functions these fabricated nanowires hold is not ample at present, because of some difficulties in measuring the lateral properties of single atomic-scale wires, *e.g.*, via macroscopic electrodes. Therefore, in addition to these experimental studies, a theoretical investigation by means of first-principles calculations is indispensable for exploring the electronic properties of such atomic wires. For instance, Haye *et al.*[8] have investigated Na-doped dangling-bond wires on a H-terminated Si(100) surface and found that the dangling-bond wires have a one-dimensional metallic character with a large conduction-band width, for low coverage of Na atoms. In this paper, we present a systematic first-principles study of Ga, Al (group III), and As (group V) wires on a H-terminated Si(100) surface, to clarify that atomic wires exhibit a rich variety of electronic properties, depending on the atomic species and the concentration of adsorbed atoms (adatoms).

A slab model with five silicon layers is used for the present calculations. For periodic boundary conditions, a 4×2 surface unit-cell with 4×2 Si atoms at the surface layer is chosen. Adatoms are put on a single dangling-bond wire which lies along the Si-dimer row. The electronic structures are obtained using the local-density-approximation approach, specifically utilizing plane-wave-based ultrasoft pseudopotentials[9, 10]. Here, the energy cutoff is taken as 9 Rydberg (Ry). We also perform structural optimization for each atomic geometry, by setting a convergence criterion that all of the forces acting on each atom are reduced to within 1×10^{-3} Hartree/a.u.

We first present the calculated results for the Ga wires [11, 12]. When the number of adsorbed Ga atoms coincides with the number of dangling bonds (two Ga atoms for two dangling bonds, per unit cell), the most stable structure is given in Fig. 1(a). This structure is mainly characterized by an asymmetric arrangement (dimer) of the Ga atoms due to Jahn-Teller distortion, resulting in a semiconductive electronic state as shown in Fig. 1(b). When the three Ga atoms are adsorbed for two dangling bonds, two Ga atoms take similar positions to those shown in Fig. 1(a) and the third Ga atom intervenes between the two Si-dimers as shown in Fig. 2(a). From Fig. 2(b), we can see that this system becomes conductive, thereby implying that the increase in the number of Ga adatoms results in carrier doping.

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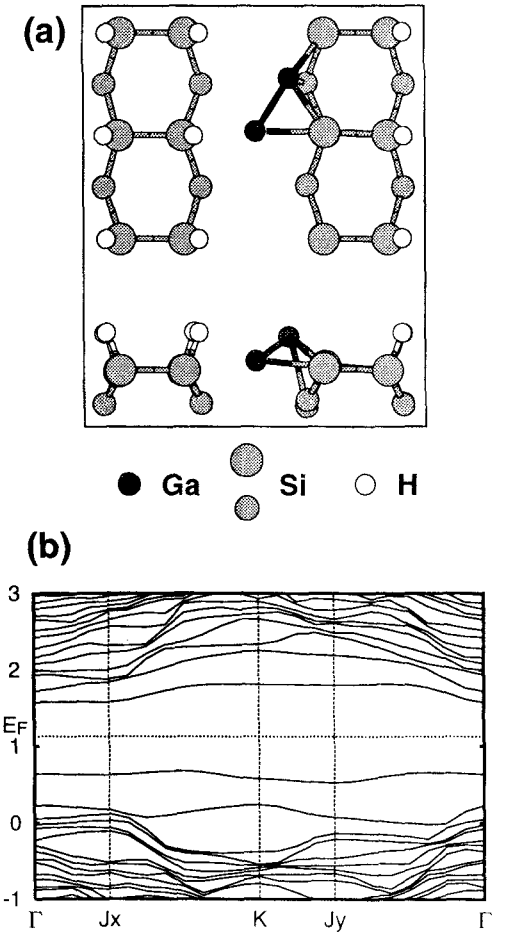

Figure 1: (a) The stable atomic structure with two Ga atoms adsorbed per 4×2 unit cell (top: surface view, bottom: side view), and (b) its energy band structure.

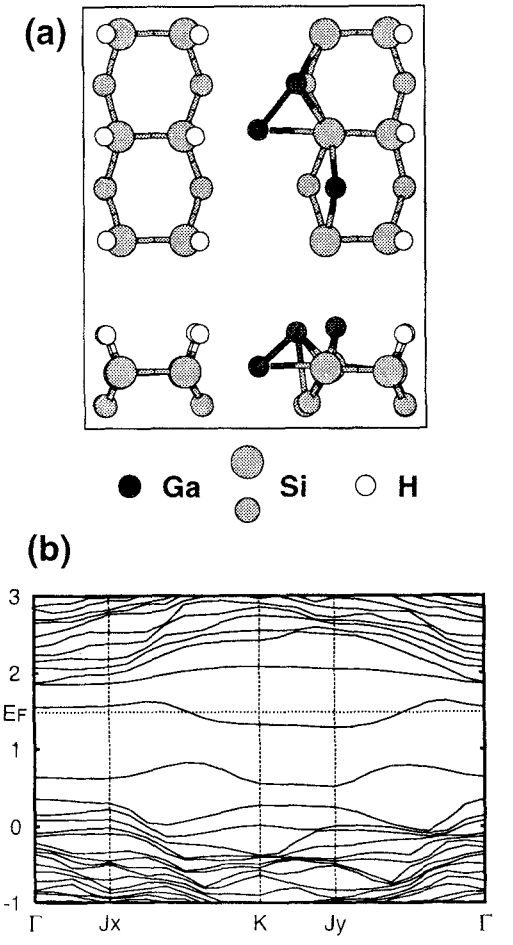

Figure 2: (a) The stable atomic structure with three Ga atoms, and (b) its energy band structure.

For the above reasons, it seems possible to control the electronic feature of atomic wires by changing the concentration of adsorbed atoms.

Next, we show the results for the Al wires.[13] When two Al atoms are adsorbed on the two dangling bonds, they are arranged in a direction parallel to the Si-dimer rows, as shown in Fig. 3(a). In spite of the good symmetry of the stable structure, the energy-band structure (see Fig. 3(b)) shows that this system is semiconductive. A distinct difference of the Al-wire from Ga-wire consists in its stable structure, i.e., each Al atom takes its position equally distant from two Si-dimers while the two Ga atoms form a dimer (see Fig. 1(a)). Although the obtained structure of the Al-wire is not conductive, Al atom has a much weaker tendency to dimerize than Ga atom. This is a desirable feature for constructing conductive wires, because dimer structures usually have an energy gap at the Fermi level.

Finally, we discuss the results of the As wires.[14] When the number of As atoms is equal to the number of dangling bonds, two As atoms are arranged parallel to the Si-dimer rows as shown in Fig. 4. The energy-band structure (see Fig. 4(b)) shows that this system is semiconductive. A remarkable feature of this energy-band structure is that the lowest unoccupied band is almost perfectly flat.

Because we are interested in the magnetism caused by this flat band, as will be discussed later, we attempted to dope the carriers in this flat band by adsorbing one K atom for two As atoms per unit cell. Figure 5(a) shows the calculated stable structure of the K-doped As-wire. The obtained energy-band structure (see Fig. 5(b)) shows that electrons are successfully doped into the flat band and the band becomes half-filled. As shown in Fig. 6, the charge distribution of this conducting band is mainly confined around the As atoms on the surface. Therefore, we can say that this half-filled flat band indeed originates from the As-wire on the surface. It should be noted that the K atom acts as the electron donor as we expected, since no

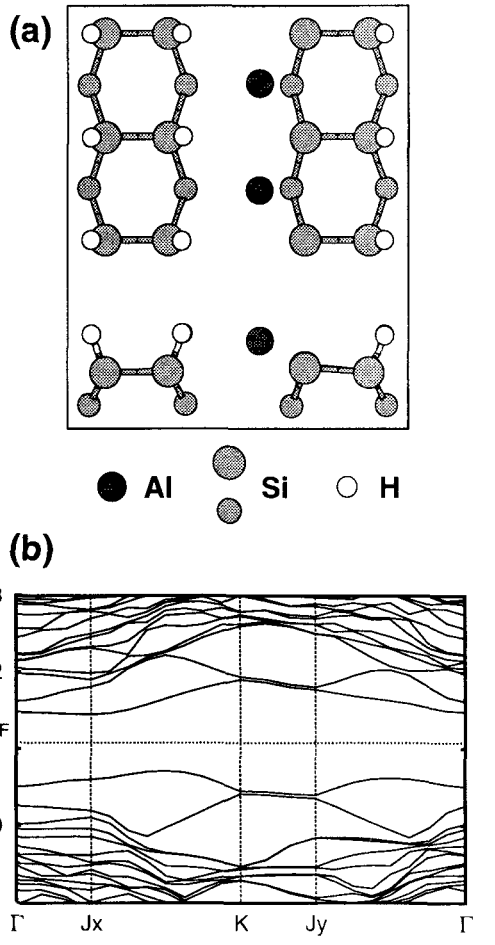

Figure 3: (a) The stable atomic structure with two Al atoms, and (b) its energy band structure.

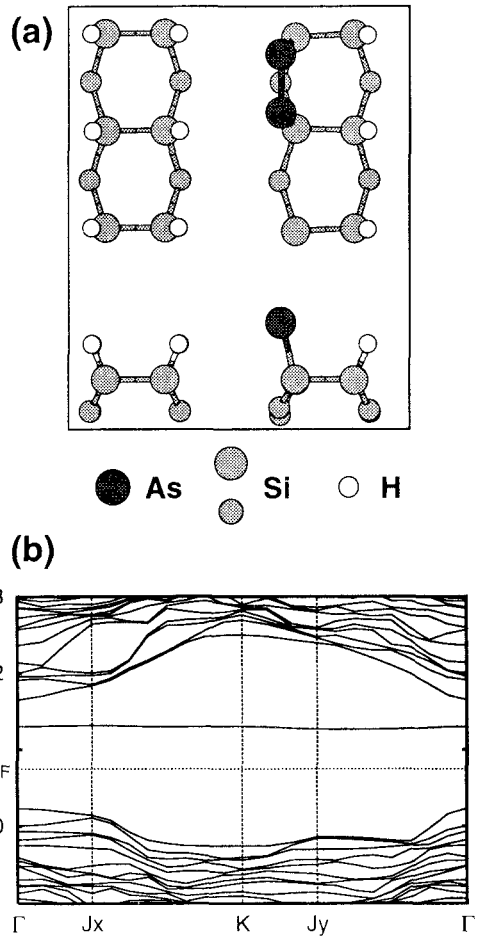

Figure 4: (a) The stable atomic structure with two As atoms and (b) its energy band structure.

charges remain around the K atom.

According to the mechanism of "flat-band ferromagnetism"[15], the ground state of the half-filled perfectly flat band becomes ferromagnetic. Even though the flatness of the band is not perfect, the ground state can be still ferromagnetic, if the electron-electron repulsion energy, or the Hubbard U, is larger than a certain threshold value[16] depending on the degradation of the flatness. In order to study the magnetic property of the K-doped As wire, we constructed a four-site model with two sites corresponding to the Si backbone and the other two corresponding to the As adsorbates. Quite recently, Arita *et al.*[17] studied this model on the basis of the Hubbard Hamiltonian, and confirmed that the ground state of the model becomes ferromagnetic in a certain range of the on-site Coulomb repulsion energy, whose values are appropriate for the As wire.

To sum up, we numerically demonstrated that nanowires of Ga, Al, and As adatoms bound to a H-terminated Si surface have a variety of conductive/semiconductive properties, including the novel possibility of flat-band ferromagnetism, based on the first-principles study. The calculated results could be useful as a guiding principle to artificially design nanowires with desired functions in future atomic-scale electronics.

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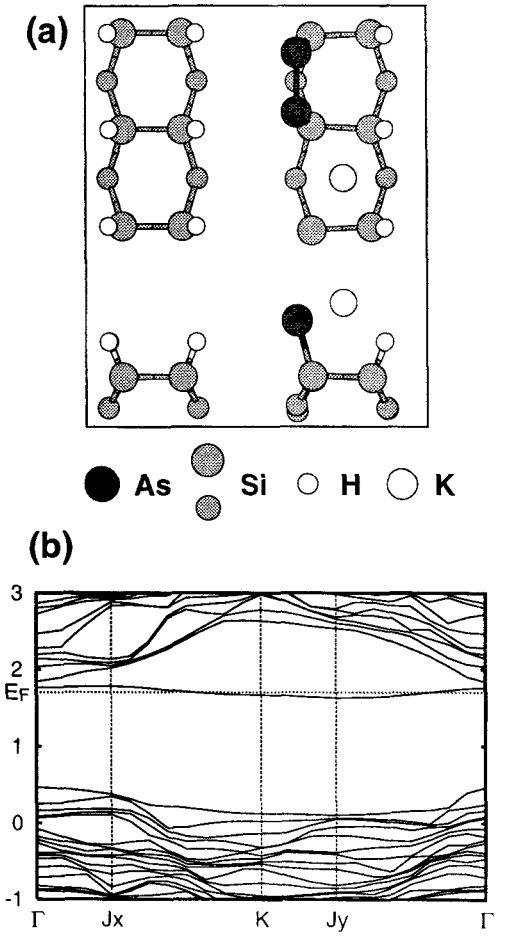

Figure 5: (a) The stable atomic structure with two As atoms and one K atom, and (b) its energy band structure.

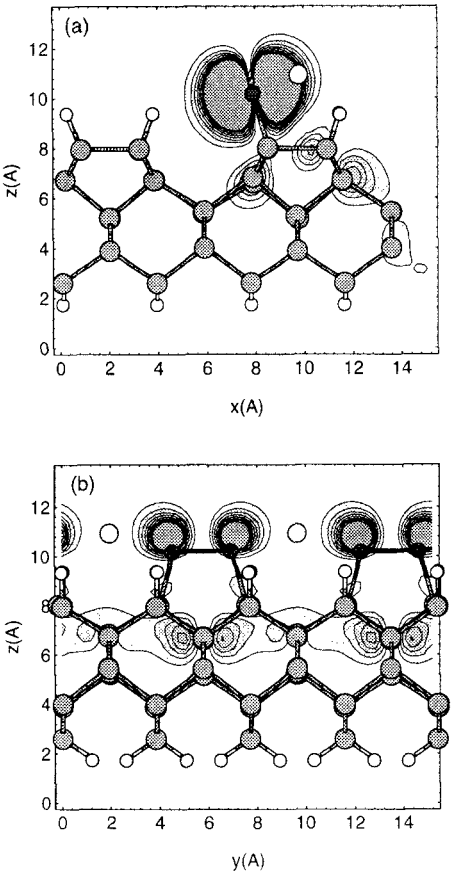

Figure 6: Contour plots of the spatial charge distribution of the conducting electrons in the cross section; (a) perpendicular, and (b) parallel to the As-wire.

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(Received December 11, 1998; accepted February 28, 1999)