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Quantum conductance of In nanowires on Si(1 1 1) from *first principles* calculations

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Abstract

The quantum conductance of the paradigmatic quasi-one-dimensional In/Si(1 1 1) surface system is calculated for 4×1, 4×2 and 8×2 surface reconstructions. In agreement with experiment, we find the recently suggested formation of hexagons within the In nanowires [C. Gonzalez, F. Flores, J. Ortega, Phys. Rev. Lett. 96 (2006) 136101] to drastically modify the electron transport along the In chains. In contrast, the formation of trimers barely changes the quantum conductance.

Keywords: In nanowires; Silicon surface; Density functional calculations; Electron transport

Fueled by the expectation to observe fascinating phenomena such as charge-density waves (CDW), spin-density waves, triplet superconductivity, and Luttinger-liquid behavior, one-dimensional (1D) electronic systems are currently intensively investigated. (Quasi)-1D systems, however, are not only interesting from a fundamental point of view. Due to the rapid miniaturization of electronic devices, they may soon be utilized as atomic-scale interconnects. For these reasons, there is presently an intense ongoing search for real quasi-1D systems with internal atomic structures that allow to study the properties of such systems in detail.

In this context, the adsorption of indium on Si(1 1 1) is a popular model system because it is easily accessible from both experimental and computational points of view. The room temperature (RT) monolayer adsorption leads to self-assembled In "nanowires" along the $[\bar{1}10]$ direction separated by about 3.8 Å, resulting in a 4×1 translational symmetry of the adsystem. Based on X-ray diffraction data [1] and total-energy calculations [2], a structural model was developed that explains largely the observed electronic properties, optical response and scanning tunneling microscopy (STM) images [3–10]. Each nanowire consists of two zigzag chains of In atoms, with the edge In atoms adsorbed in H_3 and T_4 sites (at an "up" position), and the inner In atoms at bridge sites (at a "down" position). The nanowires are separated by zigzag Si chains resembling the π-bonded chains of the clean Si(1 1 1)2×1 surface.

The low-temperature (LT) structure of this system and its properties are controversial; below about 125 K a reversible temperature-induced phase transition leads to a 8×2 surface periodicity clearly seen in STM [11–16]. However, the precise nature of the phase transition and its driving forces are unclear. It has been suggested that the transition is driven by charge-density waves, by a single-band [11] or triple-band [13] Peierls instability or by a simple energy lowering due to a periodic lattice distortion [17,2,9,8,7]. While the RT 4×1 phase is a quasi-1D metal [18] that gives rise to electron transport attributed to In

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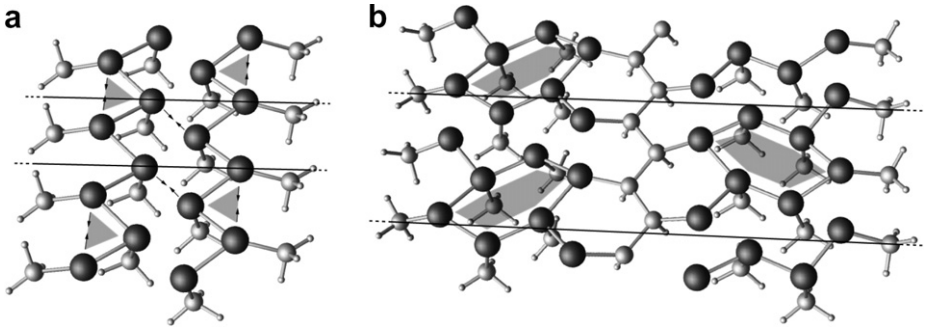

Fig. 1. Geometries of the model systems (see text) used for the unreconstructed In/Si(1 1 1)4 × 1 surface (a) and the hexagon formation within 8 × 2 translational symmetry (b). The dimerization and shear movements as well as trimer and hexagon orientation are indicated by arrows and polygons, respectively. Large, medium and small symbols indicate In, Si and H atoms.

related surface states [19,12,18], many experimental studies conclude that the phase transition leads to a fundamental energy gap of 0.1–0.3 eV [11–14]. Others only state a reduced density of states at the Fermi energy (E_F) [17,20,15] or remain inconclusive [21]. In any event, the electron conduction through the nanowires ceases for the LT phase [19,12] and the Drude tail in high-resolution electron-energy loss spectra is drastically reduced [22].

Most *ab initio* calculations [2,5,7–10], however, find no gap opening upon phase transition. They predict the pairing of the outermost atoms in the zigzag subchains and the formation of trimers. These structural changes open pseudogaps in the triple-band structure, but one surface band still crosses the Fermi level. In contrast to that, recent calculations by the Flores group [23] obtained a different surface ground state: shear distortions in neighbouring In chains – indicated in Fig. 1 – allow for the formation of In hexagons in a 4 × 2 surface periodicity. This structure was found to be insulating. The metallic 4 × 1 surface observed at RT was explained by dynamic fluctuations between degenerate ground states [24].

The potential energy surface of this system is very flat and extremely sensitive with respect to the details of the calculations [25]. Therefore, total-energy calculations are inconclusive regarding the ground-state geometry. For this reason we compare the quantum conductance of the newly proposed hexagon model with trimer formation on the basis of *first principles* calculations.

Our results are obtained using density functional theory (DFT) within the local density approximation (LDA) [26] for exchange and correlation (XC) as implemented in PWscf [27]. Following the calculation of the electronic structure, the coherent electron transport is computed by the WanT approach [28,29], which uses a Green function formalism on top of the DFT *first principles* calculations based on "maximally localized Wannier functions" as a minimal basis set. To make these calculations numerically feasible, we exploit the fact that the In-related surface states close to E_F depend very little on the substrate [30] and study model systems that contain only the In and nearest neighbour Si atoms (cf. Fig. 1). The remaining Si dangling bonds are terminated with hydrogen.

In order to confirm the validity of this approach test calculations were performed where the Si substrate was modelled more realistically by one and two bilayers. As shown in Fig. 2, the transmittance for energies around (±0.5 eV) the Fermi level remains practically unchanged for different amounts of substrate.

In Fig. 3, we show the quantum conductance for five infinite nanowires that model different In/Si(1 1 1) systems. The atomic coordinates were taken from the relaxed surface structures calculated in Ref. [25]. For a meaningful comparison, all calculations were performed for isolated wires with a lateral 8 × 2 periodicity, irrespective of the actual translational symmetry. The non-negligible impact of the translational symmetry perpendicular to the wires can be seen by comparing the calculated conductance for the

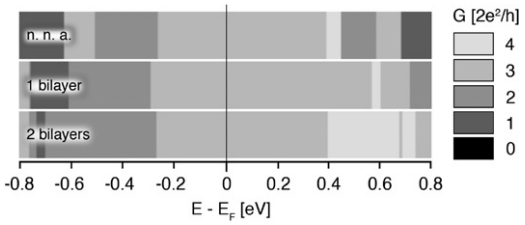

Fig. 2. Quantum conductance spectrum for electron transport along the chain direction calculated for In/Si(1 1 1)4 × 1 model structures calculated for In model wires containing only the nearest Si neighbour atoms or 1 and 2 substrate bilayers, respectively.

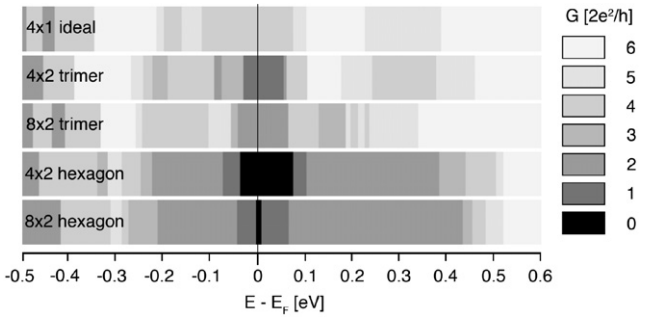

Fig. 3. Quantum conductance spectrum for electron transport along the chain direction calculated for In/Si(1 1 1) model structures, see text.

4×1 reconstructed wires in Figs. 2 and 3. In the latter case, the wire is effectively doubled, modeling an array of nanowires. Obviously the energy-dependent transmittance is very sensitive with respect to the wire geometry. Due to the free electrons in the metallic In wires of the In/Si(1 1 1)4×1 surface, its transmittance is nearly constant over the entire energy range of the Si bandgap. The value obtained in this calculation overestimates – by roughly a factor of two – the experimentally determined surface state conductances in the RT regime [19,12,18]. This we attribute to the effect of the metallic contacts and their scattering as well as to the thermal dissipative scattering due to phonons at finite temperature. The formation of In trimers with 4×2 or 8×2 symmetry does not quench the conductance, but leads to a reduction for energies very close to E_F, i.e., within about 10^{-1} eV. For energies farther below or above E_F, the transmittance resembles those of the ideal chains. Only some conduction channels slightly shift in energy or are somewhat reduced in magnitude. The conductance changes upon hexagon formation are significantly more pronounced. In both the 4×2 and the 8×2 symmetry, it strongly reduces the transmittance through surface states over an energy range of nearly 1 eV. For energies of 10^{-2} eV and 10^{-1} eV around E_F, there is zero conductance for hexagons arranged in 8×2 and 4×2 symmetry, respectively. These findings may well account for the vanishing surface-state conductance measured for the LT phase [19,12] of the In nanowires.

In conclusion, the calculated transport properties give strong evidence for hexagon formation. The quantum conductance of infinite In nanowires that model the surface chain structures explains the change of the measured wire resistance for variations between the RT and LT phases of the In/Si(1 1 1) system, provided hexagons form. Trimer formation, however, does not open a fundamental energy gap. Our results demonstrate the distinct influence of small changes of the nanowire geometry on its conductance.

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