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Quantum conductance oscillation in linear monatomic silicon chains

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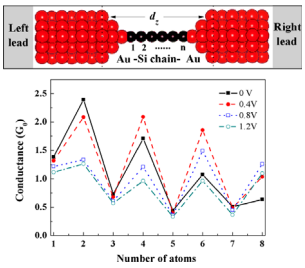
HIGHLIGHTS

- The conductance oscillates with a period of two atoms as the number of atoms in the silicon atomic chain is varied.
- The transport channel is mainly contributed by p_x and p_y orbital electrons of silicon atoms.
- The even–odd oscillation is robust under external voltage up to 1.2 V.

GRAPHICAL ABSTRACT

Linear silicon atomic chains with $n=1$–8 atoms sandwiched between Au electrodes. The conductance oscillates with a period of two atoms as the number of atoms in the chain is varied. The even–odd oscillation is robust under external voltage up to 1.2 V.



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ABSTRACT

The conductance of linear silicon atomic chains with $n=1$–8 atoms sandwiched between Au electrodes is investigated by using the density functional theory combined with non-equilibrium Green's function. The results show that the conductance oscillates with a period of two atoms as the number of atoms in the chain is varied. We optimize the geometric structure of nanoscale junctions in different distances, and obtain that the average bond-length of silicon atoms in each chain at equilibrium positions is 2.15 ± 0.03 Å. The oscillation of average Si–Si bond-length can explain the conductance oscillation from the geometric structure of atomic chains. We calculate the transmission spectrum of the chains in the equilibrium positions, and explain the conductance oscillation from the electronic structure. The transport channel is mainly contributed by p_x and p_y orbital electrons of silicon atoms. The even–odd oscillation is robust under external voltage up to 1.2 V.

1. Introduction

With the progress in micro-fabrications and self-assembly techniques, it is possible to synthesize and manipulate the ultimately thin wires made of single atomic chains [1]. Low dimensional form of materials can have properties quite different from those of their bulk structures [2]. Monatomic chain, being the simplest object to be connected into a circuit, can be considered as the ultimate limit in the miniaturization of electronics. Thus, the investigation of atomic chains in experiments and theories become one of the center topics in nano-materials science [3].

Quantized conductance has been observed at room temperature for a number of tip-substrate systems by a scanning tunneling microscope [4]. Transport properties of atomic contacts have been investigated in experiments and theoretical calculations for many years [5]. Lang first studied the dependence of the conductance on the number of Na atoms in the wire, and found that the conductance of a chain of Na atoms between electrodes oscillates with a period of two atoms as the length of the chain is varied [6]. This oscillation effect was also found in Au, Pt, Ir, and Al atomic

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chains [7–11]. Apart from chains of metal atoms, the chains of semiconductor or insulator atoms have also been investigated. The conductance of monatomic chains of C, Si, S, Ge, and Sn elements, and of binary compounds such as InP, GaAs, AlSb, BN, SiC, GaN, and AlN have been reported [12–14].

Silicon is of paramount importance in the microelectronics industry. Small silicon clusters have been a subject of intensive studies. Roland et al. investigated the transport behavior of small Si_n (n=1–10, 13, 20) nano-clusters between atomistic Al and Au leads, and found that all of the clusters display metallic I–V characteristics [15]. Landman et al. studied the conductance of silicon nanowires connected to aluminum electrodes, and found that the short wires are fully metalized [16]. Senger et al. also studied the structural, electronic, and transport properties of atomic chains of silicon. Their calculations revealed that the monatomic chains of silicon are stable and metallic [17]. Although it is possible to measure conductance of atomic chains in mechanically controlled break junction experiments, the detailed structure of chains remain unknown in the measurements. So it is very valuable to simulate the transport properties from first-principles calculations. In this paper, in order to systematically understand the transport properties of silicon atomic chains, based on our previous research [18], we have interest in examining the conductance of silicon chains attached to Au leads using the density functional theory combined with the non-equilibrium Green's function method.

2. Theoretical mode and calculation details

Fig. 1 depicts the physics model which is comprised of silicon chains with different number atoms coupling with two semi-infinite Au (1 0 0) metal electrodes. The device system is divided into three regions: left and right electrodes, and a central extended molecule (scattering region), which includes some electrode atomic layers respectively at each side of the junction to screen the perturbation effect. The left and the right electrodes are considered perfect crystals. The unit cell of the extended molecule comprises 127 Au atoms of 13 (1 0 0)-oriented Au atomic lays in a (3×3) super cell and n (from 1 to 8) silicon atoms in the short chains. The potential is well approximated by that of a perfect bulk electrode. The transport properties have been calculated with the ab initio transport code SMEAGOL [19,20], which calculates the density matrix and the transmission coefficients of a two-probe device using the non-equilibrium Green's function formalism. The scattering potential is calculated self-consistently by using the SIESTA implementation of the density functional theory [21].

In our calculations, we use the Perdew–Zunger [22] version of the local density approximation to the exchange-correlation functional. Valence electron configuration is $5d^{10}6s^1$ for Au atoms and $3s^23p^2$ for Si atoms, and they are expanded in single-zeta basis sets for Au atoms and double-zeta basis sets for Si atoms. Troullier–Martins [23] pseudo-potential in nonlocal form is generated. A periodic boundary condition is applied in the basal plane (orthogonal to the transport direction) with four irreducible k-points in the two-dimensional Brillouin zone. A k-grid sampling of $2\times2\times100$ for the gold electrodes is employed. The cut-off energy and iterated convergence criterion for total energy are set to 200 Rydberg and 10^{-4}, respectively. Furthermore, the charge density is integrated over 50 energy points along the semi-circle, 20 energy points along the line in the complex plane and 20 poles are used for the Fermi distribution.

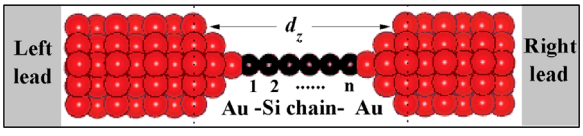

Fig. 1. Model used for the calculation of the different silicon chains connecting (1 0 0) oriented fcc Au leads.

The conductance (G) associated to the two-probe device can be calculated by using the Fisher–Lee's relation $G=(2e^2/h)\,Tr[\Gamma_L G_M^{R+}\Gamma_R G_M^R]$ [24], where the $\Gamma_{L/R}$ is the anti-hermitian parts of the self energy, e is the electron charge and h is the Planck constant. G_M^R, which contains all the information about the electronic structure of the extended molecule, is the retarded Green's function of the scattering region. Then the two-terminal current can be calculated through the formula: $I=(2e/h)\int dETr[\Gamma_L G_M^{R+}\Gamma_R G_M^R][f(E-\mu_L)-f(E-\mu_R)]$ [25], where f is the electron distribution function of the two electrodes, and $\mu_{L/R}$ is the chemical potential for the left/right electrode. More calculation details on how this procedure is performed in SMEAGOL can be found in the literature [19,20].

3. Results and discussion

The parameters of Au electrodes and slicon atomic chain structures are taken from the experimental data. Due to the interactions between electrodes with atomic chains, the junctions structure will be changed. We perform geometry relaxation by keeping all atoms in the bulk of Au electrodes fixed and relaxing the apexes of the point contact until the force on each atom is small than 0.1 eV/Å in the optimization [26]. The distance between the outer slices (not relaxation) was defined as d_z. In order to calculate the most stable structure for each chain attached to leads in different distances, we calculate the cohesion energy as a function of d_z during the simulation process. The cohesion energy is defined as follows: $E=E$ (Au electrodes+silicon chain)$-E$ (silicon chain)$-E$ (Au electrodes). The calculated results are shown in Fig. 2 (marked in solid squares and right-hand side axis). It is found that there is a parabola in the curve of the total energy as a function of d_z for each chain. The minimum energy in every curve is located at the equilibrium distances.

The distances $d_{z,eq}$ corresponding to those energy minima describe the equilibrium position, where the system will naturally form if the electrodes are free to relax. For more details, when the number of atoms in silicon chains increase from 1 to 8, the equilibrium distances is $d_{z,eq}$=12.16 Å, 14.01 Å, 15.84 Å, 18.10 Å, 20.74 Å, 22.19 Å, 24.84 Å, and 26.68 Å, respectively. We investigate the Si–Si bond-length in the silicon atomic chains and Si–Au bond-length in point contact at the equilibrium position. Each specific bond-length of silicon chains at equilibrium position is listed in Table 1. When the junctions are in the equilibrium positions, the Si–Si bond-length, r_{Si-Si}, is 2.15 ± 0.03 Å, the Si–Au bond-length r_{Si-Au}, in the junction contact is 2.29 ± 0.02 Å for each chain. We find that the average Si–Si bond-length oscillates as the number of atoms in the chain is increases. When the number of atoms is even, the average bond length is smaller than that of odd.

We calculate the conductance as a function of distance d_z after geometry relaxation, i.e. we simulate a slow junction breaking process. The details of conductance that varied with the distance for all chains are shown in Fig. 2. The conductance marked in open squares and left-hand side axis. It is easy to see that the change of conductance with distance is different for each silicon atomic chain, and the conductance is not necessarily the biggest at most stable stations. In general, the distance is an important factor to the conductance, the small change of the distance will lead to a big change of conductance for all chains. So, the conductance is sensitive to the distances as the junction is stretched. Furthermore, all silicon atomic chains have shown good conductance in their