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Quantized conductance of Si atomic wires

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We have performed first-principles pseudopotential calculations of the quantum transport properties of a chain of Si atoms connected to the outside through long leads. By solving a three-dimensional quantum scattering problem we have computed the conductance for several atomic wires with up to eight Si atoms. The Si atomic wires are found to be metallic and we observed quantized conductance in units of $2e^2/h$. A conductance dip is found to develop near the onset of the second quantized plateau as the number of atoms increases, and this can be explained by the existence of a gap in the density of states when the atomic chain is infinitely long. [S0163-1829(97)52032-7]

In the last decade extensive research effort has been devoted to the development of Si based optoelectronic technology. A particularly exciting result is the production of porous Si microstructures which have visible light photoluminescence. More recently, Si based atomic wires with sizes as small as several nanometers across, have been fabricated by several laboratories. Quantized conductance with sizes as small as several nanometers across, have been fabricated by several laboratories.2–5 Quantized conductance with sizes as small as several nanometers across, have been fabricated by several laboratories.6

Using a scanning tunneling microscope (STM) one can measure the quantum conductance of a tip near a substrate, and quantized conductance has indeed been observed at room temperature7–11 for a number of tip-substrate systems. For Si based freestanding atomic wires, Ref. 2 reported observations of conductance quantization up to a temperature of 210 K, and Coulomb blockade effect up to 100 K. So far, theoretical analysis has largely focused on the important problem of quantum conductance through the tip-substrate arrangement.10,12–14 In particular, first-principles pseudopotential calculations for Si based nanowires have been carried out for optical properties to explain certain observed features of the porous silicon.15,16 Lang14 has advanced a first-principles quantum scattering theory to study quantum conductance through atomic scale tip-substrate systems and the theoretical predictions for the case of a few Xe atoms sandwiched in between two substrates are in quantitative agreement with STM measurements.11 The authors have made ab initio calculations of quantum transport through Al based freestanding atomic wires and predicted dc as well as ac conductances for these wires.17 Furthermore, Mehrrez et al. have explained observed features of electric conduction through an atomic junction based on the behavior of density of states,18 and Watanabe et al. investigated the electronic band structure of the dangling-bond Si wires.19

Clearly, due to the importance of the problem, there is a need to further investigate quantum conductance through various atomic wire systems. It is also important and useful to directly compute quantum conductance from first principles by solving the quantum scattering matrix. Results from this kind of approach are especially strong in their predictive power as shown by the impressive results of Ref. 11. The purpose of this work is to report our investigation on Si based freestanding wires using an ab initio method. Si wires are interesting and important, as they are the base semiconductor material of the electronics industry and Si atomic wires have been fabricated, as mentioned above. In particular, we shall consider the atomic wire model shown in the inset of Fig. 2, where a chain of several Si atoms is connected to the outside by three-dimensional (3D) leads. Electrons come in from the left lead, scatter off the Si atoms, and transmit to the right lead or reflect back. By solving the quantum scattering process using first principles, we compute the conductance for the whole system which can be viewed as a long 3D wire with an atomic chain in the middle. Our results will then be compared with those of metallic Al wires.17

To solve the quantum conduction problem including the atomic degrees of freedom, we have developed a two-step numerical procedure.20,17 In the first step, we solve the ground-state properties of the Si chain and the left and right leads by minimizing the Kohn-Sham total-energy functional, where the valence electrons are treated explicitly and the core is introduced through a pseudopotential. We have fixed the ionic positions in our ground-state calculation. The well-
known Kohn-Sham energy functional in standard density functional theory is the subject of many review articles, e.g., in Ref. 21, and to save space we refer interested readers to them. The equilibrium analysis produces the self-consistent Kohn-Sham electronic wave functions $\psi_i(\mathbf{r})$ with a self-consistent effective potential $V_{\text{eff}}(\mathbf{r}) = \delta U / \delta \rho(\mathbf{r})$ which is seen by all the electrons. Here $U[\rho]$ is the total self-consistent potential energy while $\rho$ the electron density obtained from $\{\psi_i\}$.\textsuperscript{21,22} We have used the parameterization of Ref. 23 for the exchange-correlation term, and a local pseudopotential\textsuperscript{24} for the core. The second step of our calculation involves the evaluation of the scattering matrix of an electron traversing the atomic wire defined by $V_{\text{eff}}$. For this purpose we have developed a transfer-matrix technique to solve the 3D quantum scattering problem based on a method reported in Ref. 25. From the scattering matrix we obtain conductance using the Landauer formula.\textsuperscript{26} As noted before,\textsuperscript{20,27} the crucial point of the two-step procedure is to include the long leads into the equilibrium analysis of the effective potential $V_{\text{eff}}$ which allows the eigenstates obtained from the ground-state density-functional calculation to be brought into the form of scattering states of the wire.

The details of the model and system parameters are as follows.\textsuperscript{28} The leads are modeled by the jellium model where the positive charges are uniformly distributed. A jellium lead has a cross section area of $7.25 \times 7.25$ (a.u.)\textsuperscript{2}, length $L = 30.78$ a.u., and its charge is specified\textsuperscript{29} by $r_s = 2.0$ a.u., mimicking metallic leads. This results in a total of 96 electrons in the jellium leads. The chain of Si atoms is sandwiched in between two leads. The atom-atom distance is fixed by the Si dimer bond length of 4.25 a.u. For the atom-jellium distance, we used the value 2.3 a.u. which is the equilibrium bond length of a Si adatom on top of a jellium plane as determined in Ref. 29. The whole system (see inset of Fig. 2), atomic chain plus the leads, is put into a supercell of size $21.77 \times 21.77 \times (2L + d)$ (a.u.)\textsuperscript{3}, which we checked to be large enough, for the standard plane-wave based \textit{ab initio} calculations\textsuperscript{21} using a preconditioned conjugate gradient minimization scheme. Here $d$ is the length of the atomic chain including the atom-jellium distances. We have investigated atomic wires which contain up to eight Si atoms and used an upper energy cutoff of eight Ry.

Figure 1 shows the effective potential of a wire with six Si atoms. $V_{\text{eff}}$ in the 3D leads is affected by the atoms near the atom-lead junctions, but this effect is quickly screened out away from the junctions, indicating that the length of the leads is approaching the desired asymptotic limit. In the jellium leads, $V_{\text{eff}}$ is a potential well with a depth $\sim -0.5$ a.u. below the Fermi level in the cross section plane $(x,y)$ plane for the six-atom wire. Similar values are obtained for other wires. In the atomic chain of the wire, Fig. 1 shows clear covalent bonding between the Si atoms. In addition, $V_{\text{eff}}$ has rather high peaks due to the ionic core of the atoms. Surrounding the cores there is the usual attractive part of atomic potential. Finally, the bonding between the Si atom and the jellium leads are also clearly obtained in Fig. 1, and it is quite similar to that of a Si adatom on top of a jellium plane.\textsuperscript{29}

Figures 2 and 3 show the conductance $G(E)$ as a function of the incoming electron energy $E$ for several wires with one to eight Si atoms in the chain. Several observations are in order. First, all wires show some degree of conductance quantization with clear conductance plateaus.\textsuperscript{30} However, the plateaus are not at perfect integer values of $2e^2/h$ due to scattering at the atom-jellium junction which leads to finite reflection coefficients. This is similar to that of the experimental situation where parasitic series resistance in the leads reduces the total conductance.\textsuperscript{7} For Si wires the atom-jellium junction scattering is more severe as compared with that of Al wires which we studied previously.\textsuperscript{17} This may be understood since the Si atom closest to the leads makes a covalent bond with the next Si atom down the chain, while the covalent bond\textsuperscript{29} with a lead is certainly much weaker. Hence the charge density and $V_{\text{eff}}$ is not symmetric on the two sides of this atom. Such an asymmetry in $V_{\text{eff}}$ leads to scattering of the incoming electron wave which produces a nonzero reflection.
The consistency between the general transport characteristics of Si atomic wires is certainly long Si chain has a band gap below the Fermi energy. The conductance dip observed here reflects the fact that an infinitely long Si structure shows a gap below the Fermi energy with a relative energy difference at 4.09 a.u., as shown in the inset of Fig. 3. Indeed, the band structure of an infinitely long Si chain with bond length 4.09 a.u. shows a gap below the Fermi level.

The horizontal line is the calculated Fermi energy of the infinite structure of an infinitely long Si chain with bond length 4.09 a.u. The vertical line indicates the position of the calculated Fermi level, $E_F$. Notice the development of the conductance dip below $E_F$ as the length of the atomic section increases. Inset: calculated 1D band structure of an infinitely long Si chain with bond length 4.09 a.u. The conductance dip comes from, we have computed the 1D band structure of a system at its Fermi energy, and we have predicted the quantum conductance of the wires ranging from the smallest $\sim 4.54$ kΩ for the one atom case, to $\sim 7.28$ kΩ for the wire with a wider lead.

To compare the results of Si system with those of Al system, while the main features of conductance quantization and the formation of quantum wires are similar, there exists several important differences. As discussed above, the Si atom-jellium junction provides scattering to the incoming electron which in turn produces nonzero reflection coefficients. This was due to a difference in the bonding between a Si atom to the leads and to its neighboring atom. For Al wires, the effective potential between an atom to the leads and to its neighboring atom is more spherical, thus the atom-junction scattering is not as severe, thereby producing more perfect conductance plateaus. Another difference is the conductance dip observed in Si wires; such a feature was not observed for Al wires consisting of up to four Al atoms in the atomic chain although such a conductance dip may still develop in Al wires with a longer atomic chain. Finally, the equilibrium Fermi energy for Al wires examined in Ref. 17 is located at the transition region between the first and second conductance plateau where $G(E)$ changes rapidly, leading to different resistances at the Fermi level for different wires. For Si wires studied here, the Fermi energy of the wires locates on the second conductance plateau, thus for all the wires examined the resistances at the Fermi energy have values within a smaller range.

To summarize, we have investigated the quantum transport properties of a model atomic wire made of a chain of Si atoms connected to two external long leads. Our prediction is based on a self-consistent ab initio total-energy calculation of the effective ground-state potential of the wire, and a solution of a full 3D quantum scattering problem. Our results show that the Si atomic wire is metallic at its Fermi energy, and we have predicted the quantum conductance of the wires as a function of the incoming electron energy within the model. For all the wires studied some degree of conductance quantization is observed. A very interesting feature is the development of a conductance dip below the Fermi energy of the atomic wire as the length of the atomic section is increased. This behavior can be explained by the existence of a gap in the infinitely long 1D Si chain band structure. Finally, we comment that the curves of $G = G(E)$ are useful for giving a first estimate of the electrical current as a function of a voltage across the wire: one obtains the current in the usual fashion by integrating $G(E)$ over energy convoluted with a Fermi function. As mentioned in the Introduction, Si based freestanding atomic wires with sizes in the nanometer range have been fabricated using several experimental techniques. On the other hand our model studied here is for ideal chains of Si atoms connected to external leads. Such chains may be produced using the atomic manipulation ability of a STM on top of a substrate. Clearly, a transport measurement of such a system will be extremely useful and interesting.

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28 We present results in atomic units throughout this work.


30 Notice that the plateau at 2 - 2\(\frac{e^2}{h}\) is missing, which is a result for 3D wires. For a perfect 3D wire with a square cross section, the transverse quantization gives conductance steps of 1, 3, 4, 6, ... in units of \(2\frac{e^2}{h}\).

31 We have used the ab initio method of Sankey and Niklewski to compute the 1D band structure. See O. F. Sankey and D. J. Niklewski, Phys. Rev. B 40, 3979 (1989).

32 The band structure of an infinitely long 1D Si chain has been computed before using a tight-binding theory. See, for example, Toshishige Yamada and Yoshihisa Yamamoto, Phys. Rev. B 54, 1902 (1996). Our results, shown in the inset of Fig. 3, are consistent with theirs.