Spin transport in dangling-bond wires on doped H-passivated Si(100)

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Abstract
New advances in single-atom manipulation are leading to the creation of atomic structures on H-passivated Si surfaces with functionalities important for the development of atomic and molecular based technologies. We perform total-energy and electron-transport calculations to reveal the properties and understand the features of atomic wires crafted by H removal from the surface. The presence of dopants radically change the wire properties. Our calculations show that dopants have a tendency to approach the dangling-bond wires, and in these conditions, transport is enhanced and spin selective. These results have important implications in the development of atomic-scale spintronics showing that boron, and to a lesser extent phosphorous, convert the wires in high-quality spin filters.

Keywords: spintronics, electronic transport, DFT, NEGF, dopant

1. Introduction

The integration of semiconductors and magnetic materials is of great importance for the creation of new technology in which digital data are encoded in the spin of electrons [1]. In this respect, the use of molecules that can become spin devices is a very interesting possibility [2]. Indeed, molecular devices are very small, adaptable and easy to create using chemical engineering. Their spin functionalities are also very interesting, and they have been deemed superior to more common spintronic strategies [3, 4]. As in molecular electronics [5, 6], the problem comes from creating efficient atomic-size interconnects to form complete circuits [6, 7].

Interconnects that can transport spin are thus desirable for spintronics application. Promising candidates for surface interconnects can be found in carbon nanotubes (CNTs) [8, 9], as they present both easy synthesis and complex physics. In particular, the low Z of carbon, assures very small spin-orbit coupling and hence long spin lifetimes. However, an important issue with CNTs is that their properties are extremely sensitive to the topological structure of the tube. Other serious candidates emerge from the variety of silicon nanowires (Si NWs) that can be grown and that happen to present easier control over their physical properties [10–21]. A new type of nanowire has been recently proposed with embedded phosphorous in a silicon crystal. The resulting one-dimensional (1-D) system exhibits a very low resistivity [22, 23]. An alternative path consists of using the scanning tunneling microscope to selectively remove hydrogen atoms from a H-passivated Si(100) surface along the Si dimer row leading to a dangling-bond (DB) wire [24–30]. At variance with isolated DBs, which introduce localized mid-gap states, these wires give rise to dispersive bands with a marked 1-D character. The stability and the transport properties of such wires have been extensively studied by tight-binding as well as ab initio methods [31–42] and several experimental proofs-of-concept have been reported [26, 27, 43]. Spin lifetimes in silicon are known to be long; however, DB wires present some problems for transport: (i) transport properties of simple 1-D wires are limited due to the appearance of an electronic
between the electrodes is established by applying an electric field along the transport direction. Mobile charges inside the electrodes screen the electric field, resulting in the usual electric potential profile (flat inside the electrodes, potential drop in the scattering region). Only electrodes that are three-dimensional metals guarantee this kind of screening. In this configuration, however, it becomes very difficult to disentangle the contributions to the resistance of the electrode-semiconductor interface from those of the sub-surface dopant scattering. We believe that our simplified model gives a better insight into the physics of electron transport through DB wires in the presence of dopant, because all the observed effects (stabilization of a magnetic solution, leakage, etc.) necessarily stem from the presence of the impurities. Our zero-bias calculations should be representative of long wires at low biases where the homogeneous bias drop along the wires leads to a negligible effect in the transport properties. Bias drops in shorter wires will surely change the results, but it is difficult to say in what direction. Including metallic electrodes for short wires is not realistic because of the very large spatial scale of the Schottky barrier formed between the electrode and the wire. Therefore, gating can be a realistic option [52]; however, unsolved issues are the profile of the potential in the interface between the gated electrode and the wire, which will very much depend on the method of gating. Hence, our results should be perfectly reliable to treat transport in wires longer than a few dangling-bonds. In all cases, an energy cutoff of 200 Ry for real-space mesh size has been used.

3. Results and discussion

The impact of dopants on the current carried by DB wires depends critically on their distribution with respect to the surface. Hence, our first goal was studying the surface segregation of these defects. Broadly speaking, impurities prefer to be closer to the surface where the strain can be more easily released or, generally, closer to any interface. Indeed, phosphorus and boron impurities have been shown experimentally to segregate at the interface, under the appropriate annealing conditions. This is a well-known behaviour in systems, like unpassivated Si surfaces [53, 54] and in Si NWs [13, 55, 56]. In oxidized Si NWs [16, 57], both classes of impurities are found to move close to the semiconductor-oxide interface, with the P atoms favoring substitution at the Si side of the interface, and B atoms preferring the oxide side of the interface. These results have been corroborated by theoretical calculations [57, 58] and similar conclusions have been recently reported for Si nanodots [59]. While some cases exist where impurities prefer to sit in the innermost part of the wire (see the case of Mn in Si NWs [60]), the general rule is that, whenever given the opportunity, i.e. when sufficient energy is supplied, for instance by thermal annealing, they prefer to move close to the interface/surface. Our calculations show the same trend in the H-passivated Si(100) surface. For both B and P, nearly 150 meV are gained in the most stable surface position (see figure 1(b) and table 1). As the dopant gets...
closer to the surface, the formation energy becomes much more site-specific. It appears that positions can be paired as follows (A, D), (B, E), and (C, F). Each pair is made of similar positions lying either shifted with respect to the surface dimers or below them (see figure 1(a)). Close to the surface, the couple (B, E) is energetically favored, whereas (A, D) and (C, F) lie higher in energy. These differences vanish quickly moving away from the surface and are within the numerical accuracy of the calculation at 15 Å from the surface. In the following, we limit our discussion to the case of substitutions at sites D, E, and F which are either more stable or almost degenerate with substitutions at A, B, and C sites.

The site selectivity observed in figure 1(b) depends on several intertwined factors (e.g. strain relaxation, electronic states of the neighbouring DBs), but can be roughly tracked back to the amount of charge transfer by the dopant depending on the site substituted. We find that the most stable site corresponds to the largest charge transfer, i.e. to the strongest bond formed between the dopant and its Si neighbours (see figure 1(c)).

Starting from the previous structures, DB wires are drawn on the surface by removing a row of Hydrogens along the [110] direction. In the absence of dopants, such wires are known to be unstable and relax following either a non-magnetic (NM) Peierls distortion or a spin-polarized solution that leads to antiferromagnetic (AFM) ordering [31, 32, 34–38, 40, 41]. The two solutions are very close in energy with the NM configuration more stable than the AFM one by 5 meV/DB [41]. Our results show that surface segregation is enhanced by the presence of such DB wires. Indeed, whatever the site of substitution for B or P is, the formation energy is smaller than in the bulk position (see table 1). This is in agreement with previous results on Si NWs [55, 61], where dopants are found to form electrically inactive complexes with isolated DBs. Also here, the tendency to surface segregation is more pronounced with P, as observed in the case of Si NWs and unpassivated Si(100) surface [55, 61].

More interestingly, we have found that both B and P stabilize the magnetic solution with respect to the NM distorted one, regardless of the site of substitution (see table 2). The destabilization of the NM wire is due to the increased distortion caused by the dopant. The shortening going from Si-Si to Si-B or Si-P bonds is conflicting with the buckling imposed by the NM Peierls-like structure. As an example, the buckling in the non-doped NM structure gives differences of \( \Delta z \approx 0.69 \text{ Å} \) in the vertical direction between neighbouring DBs. In a B-doped (P-doped) system, this height difference becomes as high as \( \Delta z \approx 1.34 \text{ Å} \) (\( \Delta z \approx 1.52 \text{ Å} \)) close to the dopant. In the undistorted AFM wire the deformation introduced by the dopant is much less: \( \Delta z \approx 0.16 \text{ Å} \) and 0.24 Å for B and P, respectively. The geometry of the magnetic solution is preserved. Thus, in the presence of dopants the AFM

Table 1. Formation energies (in meV, see text) for sites D, E, and F with and without DB wires. The notations X@H-passivated, X@NM and X@AFM stand for a system with the dopant X (X = B, P) below a H-passivated surface, a NM and AFM wire, respectively.

|       | D   | E   | F   |
|-------|-----|-----|-----|
| B@H-passivated | 29  | −148| 214 |
| B@NM   | −14 | −415| −12 |
| B@AFM  | −10 | −110| −123|
| P@H-passivated | −61 | −145| 105 |
| P@NM   | −237| −488| −57 |
| P@AFM  | −329| −539| −180|

Table 2. Energy differences (in meV/DB) between NM and AFM configurations for top sites D, E, and F. In the absence of dopant this difference is \( \approx 5 \text{ meV/DB} \) [41].

|       | B@D | B@E | B@F | P@D | P@E | P@F |
|-------|-----|-----|-----|-----|-----|-----|
|       | 10  | 22  | 16  | 20  | 15  | 21  |
solution becomes the ground state, yielding a magnetic ordering that can be exploited for spin transport related applications.

Dopants lead to an injection of holes or electrons. In the presence of DBs on H-passivated Si(100), the extra charges are trapped by these surface defects, leading to a decrease in the conductance. Here, however, where conduction is supposed to take place along the DB wires, this effect turns out to be positive by closing the electronic gap of the AFM wire and leading to a spin-specific quasi-metallicity.

Figure 2 shows the band structure of (a) an undoped AFM wire, (b) an AFM wire with a substitutional B atom in its most stable configuration (F site) and (c) an AFM wire with a substitutional P atom in its most stable configuration (E site). One can see the expected shifting of the Fermi energy (dashed line) controlled by the amount of extra charge/hole injected in the system through the dopant. The undoped AFM wire, figure 2 (a), shows two surface states leaving a surface-band gap of 0.56 eV. For each surface state, the bands corresponding to each spin overlap due to the AFM ordering. The B-doped system, figure 2 (b), displays a splitting of bands according to spin (red and blue for majority and minority spins). The splitting of bands is due to the introduction of an extra spin in an otherwise perfect AFM wire, leading to an unbalanced number of spins. The increase of the DB charge, also caused by the dopant, produces the reduction of the surface-band gap to 0.05 eV. In the case of P doping, the extra spin also produces the spin polarization of bands and a 0.09 eV gap. Therefore, the presence of dopants brings the initial insulating system to a spin-polarized quasi-metallic state.

Figure 3 shows the computed I-V curves for B- and P-doped AFM wires. In both cases, the bias required to obtain a current response is below 0.1 V in agreement with the above electronic gaps. In the case of P doping, the current contains a bulk contribution to the current. This leads to leakage current, i.e. a loss of surface current into the Si bulk. A previous study showed that this loss could represent as much as 30% of the total current for low biases (less than 0.5 V) [44]. Figure 3 displays the current along the DB wire that does not contain the fraction of the current lost into the bulk. This explains why the current is largely spin polarized despite having a larger number of bulk bands, because the wire current is mainly due to the first band below the Fermi energy, which is a surface band and hence spin polarized.

However, current leakage is negligible for B doping because there is no bulk band in the energy windows for low biases. Indeed, for biases between 0.05 V and 0.18 V the current remains on the surface and the current leakage is strictly zero. The spin-polarization for both dopings is the same, i.e. adding or subtracting one electron by the dopant will change the spin balance on the DB, but the majority spin will be the same spin. However, the surface current shows different spin-polarizations (see figure 3). This is due to the actual ordering of the DB bands, which changes under the dopant potential.

By defining the spin polarization as \( P = (I_\uparrow - I_\downarrow)/(I_\uparrow + I_\downarrow) \), we obtain that B-doped systems present a 100% polarization for biases below 0.17 V (see figure 4). Beyond this bias the presence of bulk bands contributes to current leakage and to the loss of spin polarization. In the case of the P-doped system, the bulk bands’ contribution starts as early as 0.09 eV, leading to a lower spin polarization. Therefore, for biases lower than 0.17 V, the B-doped DB wire drawn on H-passivated Si(100) system is a perfect spin-filtering surface interconnect thanks to the absence of current leakage and to the perfect spin polarization.

4. Conclusion

In summary, we have shown that boron and phosphorous dopants segregate to the H-passivated Si(100) surface. This
phenomenon is enhanced by the presence of DB wires. The first effect of dopants is to stabilize the magnetic form of DB wires over the NM Peierls distorted one. As observed in other doped Si systems, the extra charge brought by the dopant is captured by the DB wire. One consequence is the closing of the electronic gap leading to quasi-metallicity of AFM DB wires. Moreover, the presence of dopants induce a total magnetic moment on the electronic bands close to the Fermi energy, leading to spin-specific electron transport. In the case of B-doped AFM DB wire, the current is not only free of leakage from the wire but also spin-specific. Therefore, B-doped DB wires are perfect spin-filtering surface interconnects.

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