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Hole mobility in Ge/Si core/shell nanowires: What could be the optimum?

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Recent experimental works have shown that Ge/Si core/shell nanowires (NWs) are very attractive for nanoelectronics and for low-temperature quantum devices, thanks to the confinement of holes in the Ge core. Reported hole mobilities of the order of 200 cm^2/V/s are promising for high-performance field-effect transistors. However, we demonstrate that mobilities more than ten times higher, up to 8000 cm^2/V/s, could be reached in Ge/Si NWs. Atomistic calculations reveal the considerable influence of the strains induced by the Si shell on the hole transport, whatever the NW orientation. The enhancement of electron-phonon interactions by confinement, which usually degrades the mobility in NWs, is therefore outbalanced by the effect of strains. *© 2014 AIP Publishing LLC*.
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Semiconductor nanowires (NWs) have attracted considerable attention not only for fundamental studies on one-dimensional (1D) structures but also as building blocks for nano-devices.[1,2] Among them, Ge/Si core/shell NWs with a radial heterostructure are particularly attractive.[3–7] The valence band offset between the Ge core and the Si shell indeed confines the holes in the core, where they form a 1D gas.[3] Ge/Si NWs are serious candidates for high-performance field-effect transistors (FETs), since the Si shell reduces scattering of holes by the NW surface.[4–6,8,9] As a matter of fact, recent experimental studies confirm that the presence of a Si shell strongly enhances the mobility of holes in Ge NWs, by a factor up to ten.[6,9] The measured mobilities in Ge/Si NWs can be of the order of 700 cm^2/V/s,[4] and a recent comprehensive study reported a constant mobility of 200 cm^2/V/s in 15–30 nm diameter Ge cores with a 3 nm Si shell.[9] Even if the mobilities extracted from measurements on Ge/Si NW FETs are somehow scattered,[4–6,8–10] they are consistently within the same order of magnitude, i.e., hundreds of cm^2/V/s, which can be exploited in high-performance devices[4,11] and low-temperature quantum devices.[3,10]

In spite of these very promising results, the measured hole mobility remains much smaller in Ge/Si NWs than in bulk Ge (1900 cm^2/V/s).[12] It is not clear whether this important reduction is intrinsic (electron-phonon coupling) or extrinsic (e.g., interface roughness or impurity scattering). It is well known that the electron-phonon coupling in NWs is strongly enhanced by confinement, but this can be compensated by a decrease of the hole effective masses.[13–16] In addition, the presence of a Si shell induces radial compressive strains on the Ge core that shall increase the hole mobility in Ge NWs,[17,18] as already known in bulk Ge.[19] In order to assess the performances of present and future devices, it is therefore essential to understand how large the intrinsic mobility can be in perfect Ge/Si NWs.

In this context, we present atomistic calculations of the low-field phonon-limited mobility in Ge/Si core/shell NWs taking into account the effects of quantum confinement and strains on the electron and phonon band structures, and on the electron-phonon coupling. We show that the strains imposed by the Si shell considerably enhance the hole mobility in Ge/Si NWs with respect to pure Ge NWs and even bulk Ge, whatever the NW orientation. For NWs with 10 nm diameter cores and 1 nm thick shells, we predict mobilities ranging from 3 000 to 10 000 cm^2/V/s, and mean-free-paths above 100 nm at 300 K. Although the hole mobility decreases at high carrier density, it remains much larger than the reported experimental data, which suggests that extrinsic scattering processes still limit the mobility in spite of the hole confinement by the Si shell. In addition, we cannot exclude that the experimental protocols based on NW FETs underestimate the mobilities,[9] which would be consistent with the quasi-ballistic transport and the mean-free-paths above 100 nm reported at room temperature.[3,20]

The electron band structure of the NWs is computed with the $sp^3d^5s^*$ tight-binding model of Ref. 21, which reproduces all effective masses and deformation potentials of bulk Si and Ge. Spin-orbit coupling is taken into account. We calculate the phonon-limited mobility within a fully atomistic framework.[13,16] For that purpose, we compute the phonon band structures using a Valence Force Field model.[22] The electron-phonon interactions are obtained from the derivatives of the tight-binding Hamiltonian with respect to the atomic positions. All scattering processes fulfilling energy and momentum conservation are considered. Boltzmann's transport equation is solved exactly for the low-field mobility. Details on the methodology are given in Refs. 13 and 16. Unless specified, the mobility is calculated at low carrier density ($E_f - E_v \gg kT$, where E_f is the Fermi energy and E_v is the top of the valence band). Using exactly the same methodology, the hole mobility in bulk Ge is 2280 cm^2/V/s, 20% larger than the experimental value (1900 cm^2/V/s)[12] usually

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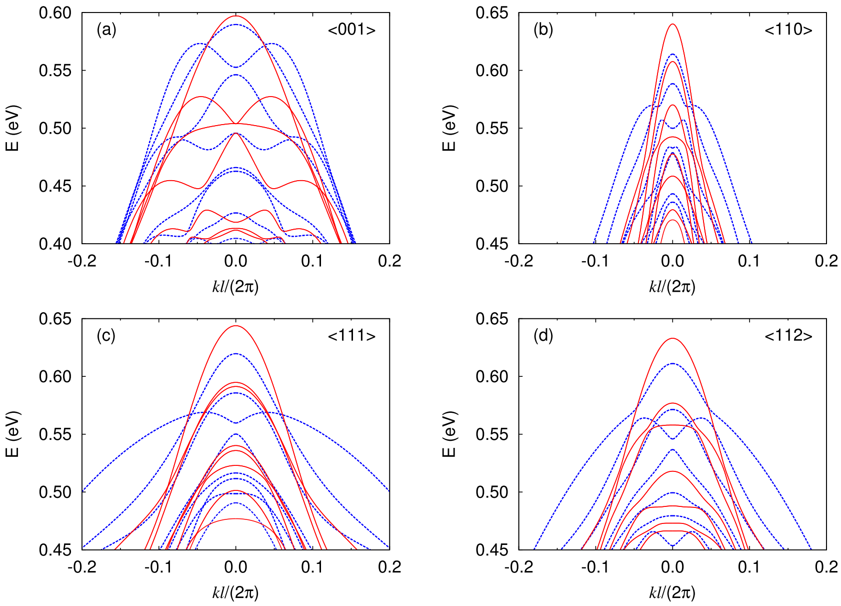

FIG. 1. Valence band structures of NWs with ⟨001⟩ (a), ⟨110⟩ (b), ⟨111⟩ (c), and ⟨112⟩ (d) orientations. Blue dashed lines: pure Ge NWs (diameter = 6 nm); red solid lines: Ge/Si core/shell NWs (core diameter = 6 nm, shell thickness = 1 nm). l is the length of the NW unit cell.

taken as reference (higher values were reported, such as $2060\,cm^2/V/s$ in Ref. 23).

Hereafter, the NWs will be characterized by their core diameter d and their shell thickness t. In order to account for the 4.2% lattice mismatch between Ge and Si, the atomic structure of the NWs is relaxed with the same Valence Force Field model as for phonons. The elastic energy is expanded in power series of variables $\tilde{h}_{ii} = u_i^2 - 3$ and $\tilde{h}_{ij} = \mathbf{u_i} \cdot \mathbf{u_j} + u_i^2/6 + u_j^2/6$.[13,22,24] Here, i labels the bonds of vector $\mathbf{x_i}$ joining two neighbor atoms, $\mathbf{u_i}$ being equal to $4\mathbf{x_i}/a_i$, where a_i is the lattice parameter. $\tilde{h}_{ii}$ and $\tilde{h}_{ij}$ measure bond stretching and bond-angle bending, respectively, (i and j share a same atom).[24] Only second order terms are considered in the power expansion as it was already demonstrated that higher-order terms have a negligible effect on structural and transport properties of Si NWs under strains up to several percent.[25] The coefficients of expansion are taken from Ref. 22 for Si and Ge, and average coefficients are used for Si-Ge bonds, following an approximation that works remarkably for Si_xGe_{1-x} alloys.[21] In agreement with linear elasticity theory,[26] we have found that the resulting strains parallel ($\varepsilon_\parallel$) and perpendicular ($\varepsilon_\perp$) to the NWs are fairly homogeneous in the Ge core. For example, $\varepsilon_\parallel \approx -1.22\%$ and $\varepsilon_\perp \approx -0.2\%$ for a ⟨001⟩ NW with $d = 10$ nm and $t = 1$ nm.

Figure 1 shows the hole band structures calculated for Ge/Si NWs. Results for pure Ge NWs are also presented for comparison. The additional shell of Si ($t = 1$ nm) in Ge/Si NWs has a strong influence on the bands. The heavy-hole bands are clearly pushed to lower energy with respect to the valence-band edge. Remarkably, this effect prevails in ⟨001⟩, ⟨110⟩, ⟨111⟩, and ⟨112⟩ orientations.

In the situations shown in Fig. 1, holes in Ge/Si NWs mainly occupy light-hole bands, at least when the carrier concentration is not too high. As a consequence, the influence of the Si shell is considerable on the hole mobility (Fig. 2). Whatever the NW orientation, the mobility is much larger in Ge/Si NWs than in Ge NWs without Si shell. Even in ⟨001⟩ NWs, where low mobilities are predicted in pure Ge NWs,[18] the effect of the shell is such that the mobilities become larger than in bulk Ge for $d > 6$ nm. Remarkably, in the 2–10 nm range where we are able to perform the calculations, the mobilities continuously increase with diameter, with almost no sign of saturation. Previous works on Si NWs[13–16] have shown that the mobility is influenced in a subtle manner by many scattering processes between different bands, explaining why its variation with size may not be perfectly monotonous, as shown, for example, in Fig. 2 by the small dip at $d = 8$ nm for the ⟨110⟩ orientation. This sensitivity is even larger here since the mobility is high and therefore scattering rates are small.

It was found in Refs. 18 and 25 that the mobility of stretched Si or Ge NWs basically depends on a single parameter, $\varepsilon_\parallel - \varepsilon_\perp$. As shown in Fig. 2, Ge/Si NWs indeed show similar mobilities as Ge NWs stretched to the same $\varepsilon_\parallel - \varepsilon_\perp$. We therefore conclude that the large enhancement of the mobility in Ge/Si NWs is entirely due to the strains induced by the shell.

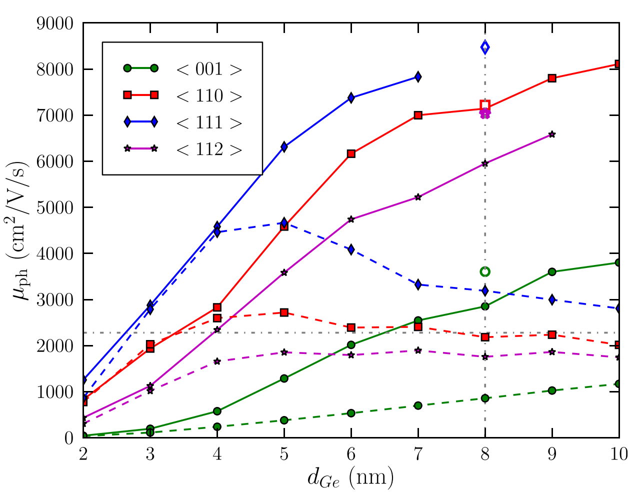

FIG. 2. Mobilities in unstrained pure Ge NWs (dashed lines) and Ge/Si core/shell NWs (solid lines) with ⟨001⟩, ⟨110⟩, ⟨111⟩, and ⟨112⟩ orientations at $T = 300$ K. The hollow markers at $d = 8$ nm represent the mobilities in pure Ge NWs under the same strain ($\varepsilon_\parallel - \varepsilon_\perp$) as in Ge/Si core/shell NWs.

The low mobilities predicted in the thinnest NWs (Fig. 2) are due to the strong enhancement of the electron-phonon coupling by the confinement.[13–16] However, with increasing diameter of the NWs, this is outbalanced by the effects of strains induced by the Si shell.

Our calculations show that mobilities up to 8000 $cm^2/V/s$, and probably above for larger diameters, could be reached in Ge/Si NWs. As a result, very long mean free paths above 100 nm are predicted at 300 K (Fig. 3). Experimentally, room-temperature ballistic transport has been reported in Ge/Si FETs with a 170 nm long channel ($d = 10$ nm).[3]

As expected, the phonon-limited mobility of holes in Ge/Si NWs strongly depends on the temperature (Fig. 4). It varies like $T^{-2.4}$ at high T ($T > 200$ K) when holes are scattered by both acoustic and optical phonons, and approximately like T^{-1} at lower T when only acoustic phonons are involved. A similar temperature behavior is found in bulk Ge.[27] In average, the mobility increases by factor ∼14 when T is reduced from 300 K to 100 K. For comparison, the mobility measured in $Ge/Si_{0.7}Ge_{0.3}$ NW FETs varies only by a factor ∼2 in the same range of temperature,[6] while in bulk Ge it varies by a factor ∼13.[27]

In order to study the influence of the carrier density on the mobility, we have also performed self-consistent Schrödinger-Poisson calculations. We have considered a gate-all-around geometry with a 1-nm-thick HfO_2 gate oxide. Self-consistency can have significant effects on the charge distribution and band structure, with a continuous transition from bulk toward interface accumulation at large concentration. For $d = 6$ nm and $t = 1$ nm, the hole mobilities significantly decrease for carrier densities above $1 \times 10^6\,cm^{-1}$ (or $3 \times 10^{18}\,cm^{-3}$) (Fig. 5). Indeed, the average carrier velocity goes down as the lower-lying heavy-hole bands get populated, and scattering is strengthened since there are many more allowed transitions.[16]

Even if experiments are usually performed on somehow thicker NWs ($d > 10$ nm),[4–6,8–10] the large gap between measured and calculated mobilities (more than a factor 10) suggests that extrinsic scattering mechanisms limit the hole transport in Ge/Si core/shell NWs, even at room temperature. The experimental dependence of the mobility on temperature,[6] which is much weaker than our predictions and than in bulk, also supports this conclusion. Since the NWs are not intentionally doped, the most probable extrinsic mechanisms are growth impurities and defects, remote Coulomb, and interface roughness scattering. This last mechanism is usually dominant at high carrier density—yet it was recently ruled out because the mobility measured on Si/Ge FETs was found independent on the diameter in the 15–30 nm range.[9] However, such a diameter-independent mobility likely results from the localization of holes at the Si/Ge interface in the strong inversion regime, which makes the hole gas more "2D" than "1D"-like at high densities in this range of diameters. Therefore, the observed independence of the mobility on the diameter does not necessarily mean that interface roughness scattering is not present.

It is interesting to compare the situation in Ge/Si NWs with the well-known case of GaAs/AlGaAs heterostructures.[28,29] After many years of efforts, it has been possible to grow remotely doped high quality layers characterized by a high

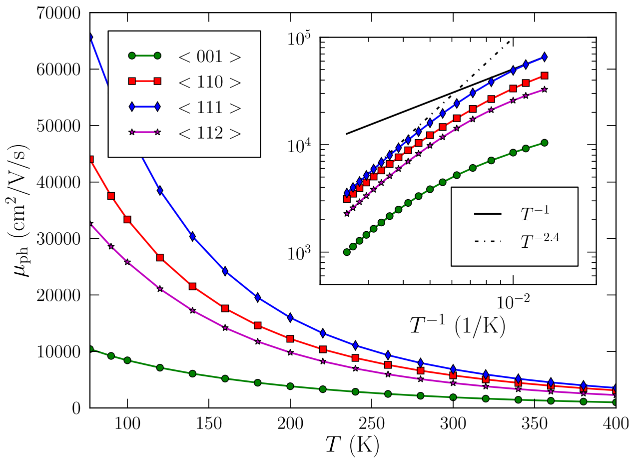

FIG. 4. Temperature dependence of the low field mobility in Ge/Si core/shell NWs (core diameter = 6 nm, shell thickness = 1 nm).

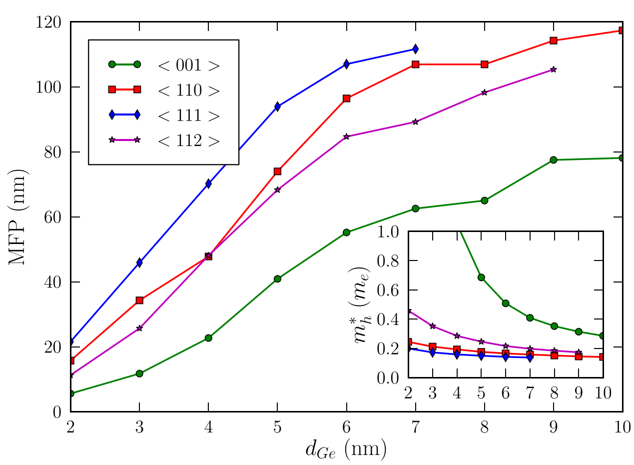

FIG. 3. Mean free paths corresponding to the phonon limited mobilities in Ge/Si core/shell NWs at 300 K. The mean free path is defined as $\frac{\mu_{ph}}{e}\sqrt{k_B T m_h^*}$, where m_h^* is the carrier effective mass at the top of valance band and is shown in the inset.

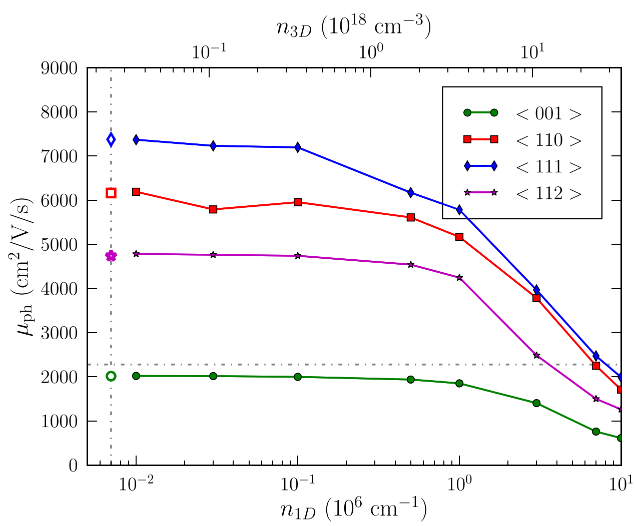

FIG. 5. Mobility versus carrier density in Ge/Si core/shell NWs (core diameter = 6 nm, shell thickness = 1 nm) at 300 K. The leftmost hollow markers are the low field (non self-consistent) mobilities.

mobility (~7000 cm^2/V/s at 300 K and >10^6 cm^2/V/s below 10 K). These figures are close to the inherent limits, i.e., the phonon-limited mobilities.[28,29] Therefore, we believe that there is considerable room for improvement in Ge/Si NWs. Obviously there are difficulties underlying the large lattice mismatch in the Ge/Si system. It is indeed hard to grow thick (>3 nm) epitaxial Si shells, especially on a cylindrical NW surface; the lattice mismatch may also favor Ge/Si interface and Si surface roughness,[30] which should in turn induce fluctuations of strains in the Ge core.

In summary, we have demonstrated that a Si shell on a Ge NW not only confines the holes in the Ge core but also induces strains that considerably improve the hole mobility, whatever the NW orientation. Very high mobilities, up to 8000 cm^2/V/s, can be reached if interface-roughness, impurity and remote Coulomb scattering can be reduced. These results should strongly motivate research on the growth of Ge/Si core/shell NWs with better surface and interface quality.

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