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Carrier mobility in strained Ge nanowires

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We present fully atomistic calculations of the electron and hole mobilities in Ge nanowires with diameter up to 10 nm. We show that the phonon-limited mobility is strongly dependent on the diameter and on the orientation of the nanowire, and is also very responsive to uniaxial strains. The similarities and differences with the case of Si nanowires are highlighted. In strained Ge nanowires, the mobility can reach $>3000 \text{ cm}^2/\text{V/s}$ for electrons and $12\,000 \text{ cm}^2/\text{V/s}$ for holes. Ge nanowires are therefore promising nanostructures for ultimate electronic devices. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4759346>]

Ge nanowires (NWs) receive growing attention because their integration in electronic devices could present several advantages.^{1–9} NWs in general are promising channels for ultimate transistors, thanks to excellent gate control and reduced short channel effects.¹⁰ They are also attractive building blocks for flexible electronics.¹¹ In this context, Ge is considered as a worthwhile alternative to Si in low-power logic applications because of its small bandgap and its *p*-type mobility which is the highest among all known semiconductor materials.^{12–14} Theoretical works have actually predicted that Ge NWs could have a high potential for microelectronics.^{15–18} But accurate calculations of the carrier mobilities are still missing in the assessment of the electrical performances of Ge NW devices. Recently, we have shown that fully atomistic calculations of the phonon-limited mobility could be achieved in Si NWs with diameters up to 10 nm.^{19–21} In agreement with other works,^{22,23} we have found that the transport properties of Si NWs are strongly dependent on their orientation and diameter.^{19–21} The mobility is also very sensitive to strains,²¹ which provides real opportunities to engineer the transport properties of Si NW devices.²⁴

In this paper, we apply the same atomistic methods to the mobility in free-standing and strained Ge NWs. We present a detailed study of the mobility of electrons and holes versus size, orientation, and strain. Compared to Si, the conduction band of Ge displays several minima very close in energy, which makes the interplay between confinement and strains much more complex and interesting in this system. We predict that electron and hole mobilities over $3000 \text{ cm}^2/\text{V/s}$ can be reached in strained Ge NWs, which is not possible in Si NWs.^{19–21} This points out the importance of strain engineering in Ge NW devices.

We compute the phonon-limited mobility within a fully atomistic framework. We apply a longitudinal strain ϵ_{\parallel} along the NW axis, then relax the atomic position using the valence force field (VFF) model of Ref. 25. We next compute the phonon band structure of the strained Ge NW with the same VFF model. The electron band structure of the Ge NW is computed with the $sp^3d^5s^*$ tight-binding (TB) model of Ref. 26, which

reproduces all effective masses and deformation potentials of bulk Ge. Spin-orbit coupling is taken into account in the valence bands. The electron-phonon couplings are then computed from the derivatives of the TB hamiltonian with respect to the atomic positions. The band structures are searched for all electrons and phonons fulfilling the energy and momentum conservation rules. Finally, Boltzmann's transport equation is solved exactly for the low-field mobility at low carrier concentration ($T = 300 \text{ K}$). Details can be found in Refs. 19 and 20.

The electron mobility in free-standing Ge NWs is plotted as a function of the diameter in Fig. 1(a). It is considerably lower in sub-10-nm NWs than in bulk Ge, whatever the orientation, due to the enhancement of the electron-phonon interaction in NWs.^{19,20,22,23} The electron mobility is also remarkably anisotropic like in Si NWs.^{19,20} But, in contrast to Si, the $\langle 001 \rangle$ Ge NWs show the poorest mobilities while the $\langle 110 \rangle$ Ge NWs show the best mobilities in the whole investigated range of sizes.

This hierarchy can be understood from the conduction band structure of Ge NWs (Fig. 2). In bulk Ge, there are four equivalent conduction-band minima at the L points ($\langle 111 \rangle$ directions), one at Γ and six equivalent ones along ΓX ($\langle 001 \rangle$ directions). The valleys at Γ and along ΓX are, respectively, 170 meV and 230 meV above the L valleys. The effective masses at the L minima are very anisotropic (longitudinal mass $m_l^* = 1.59 m_0$, transverse mass $m_t^* = 0.08 m_0$). In $[111]$ Ge NWs (Fig. 2), the four L minima fold at $k = \pm\pi/l$ (l is the length of the unit cell), with the $[\bar{1}11]$, $[1\bar{1}1]$, and $[11\bar{1}]$ valleys at lower energy than the $[111]$ valleys due to quantum confinement. The former three valleys also display a much smaller longitudinal transport mass ($\approx 0.25 m_0$) than the latter ($\approx m_l^*$). The conduction-band minimum folds at $k = \pm\pi/l$ in $\langle 001 \rangle$ NWs and at $k = 0$ in $\langle 110 \rangle$ NWs, with a clear bulk L character in both cases.²⁷ The transport mass is $\approx 0.55 m_0$ in $\langle 001 \rangle$ NWs and $\approx m_t^*$ in $\langle 110 \rangle$ NWs. Therefore, the $\langle 110 \rangle$ Ge NWs, which exhibit the smallest masses, are the best electron conductors, while the $\langle 001 \rangle$ Ge NWs are the worst ones for the opposite reason.

The behavior of the hole mobility versus NW diameter and orientation is basically the same in Ge [Fig. 1(b)] and in Si,²⁰ as expected from their qualitatively similar valence bands. The mobility is, however, much larger in Ge than in

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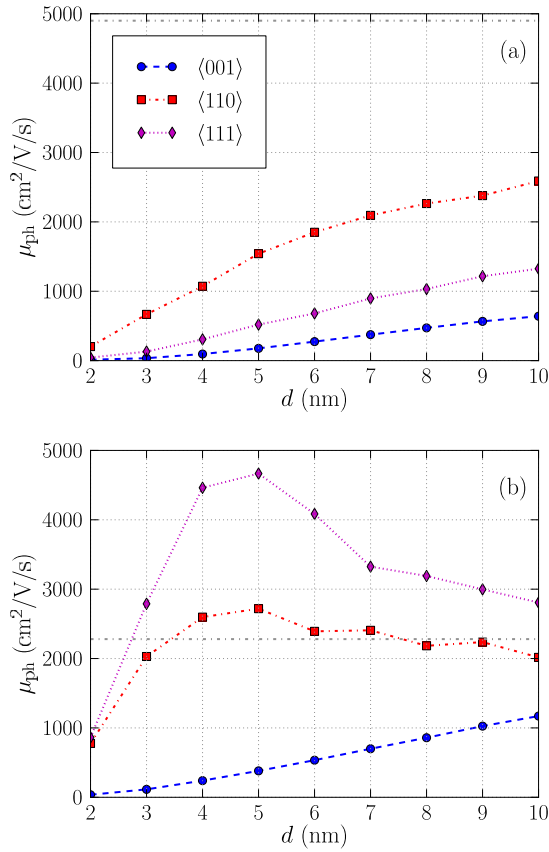


FIG. 1. Electron (a) and hole (b) mobility as function of diameter d in unstrained Ge NWs, for three different orientations. The horizontal dashed line is the calculated bulk mobility ($4900 \text{ cm}^2/\text{V/s}$ for electrons, $2280 \text{ cm}^2/\text{V/s}$ for holes).

Si NWs, due to the lower hole masses. The remarkable peak ($\approx 4700 \text{ cm}^2/\text{V/s}$) of the mobility in $\langle 111 \rangle$ Ge NWs around $d = 5 \text{ nm}$ is due to the fact that the highest hole subbands acquire a marked light-hole character ($m^* < 0.1 m_0$) and are

well separated one from each other (Fig. 3). The trend is similar although less favorable in $\langle 110 \rangle$ Ge NWs where the hole mobility remains close to the bulk value for $3 \leq d \leq 10 \text{ nm}$. On the contrary, the topmost valence bands are much heavier in $\langle 001 \rangle$ NWs (Fig. 3), which explains the comparatively low mobility in this orientation.

Strain engineering is widely used in advanced logic devices.²⁴ It is also known that the band structure of Ge NWs can be modulated by strains.^{6,17} We have therefore investigated the transport properties of uniaxially strained Ge NWs. After relaxation of the atoms, the strain ε_{\perp} perpendicular to the NW is fairly homogeneous and proportional to the applied longitudinal strain ε_{\parallel} (but opposite in sign), in agreement with elasticity theory. In the following, we discuss the mobility versus the uniaxial component of the strain, $\varepsilon_{\text{uni}} = \varepsilon_{\parallel} - \varepsilon_{\perp}$ because we have shown in the case of Si NWs that the mobility mostly depends on ε_{uni} rather than on ε_{\parallel} and ε_{\perp} separately²¹ (in Ge, $\varepsilon_{\text{uni}} = 1.26 \varepsilon_{\parallel}$ for $\langle 001 \rangle$ NWs, $\varepsilon_{\text{uni}} = 1.18 \varepsilon_{\parallel}$ for $\langle 110 \rangle$ NWs, and $\varepsilon_{\text{uni}} = 1.14 \varepsilon_{\parallel}$ for $\langle 111 \rangle$ NWs).

Figure 4(a) shows that the electron mobility can be either enhanced or reduced by the strains. The variations of the mobility however differ from those obtained in Si NWs,²¹ but can be easily understood with band-structure arguments (Fig. 2).¹⁷ Basically, the mobility is enhanced when the valleys with the smallest effective mass are lowered with respect to the others, increasing the proportion of fast electrons and limiting intervalleys scattering. This is particularly striking at positive (tensile) strain in $\langle 110 \rangle$ NWs, even if the mobility never reaches the bulk value. Compressive strains tend to reduce the electron mobility whatever the NW orientation.

The effects of strains on the hole mobility are almost the same as in Si NWs [Fig. 4(b)].²¹ Compressive strains strengthen the light-hole character of the highest valence subbands whatever the NW orientation (Fig. 3).^{17,28} In this

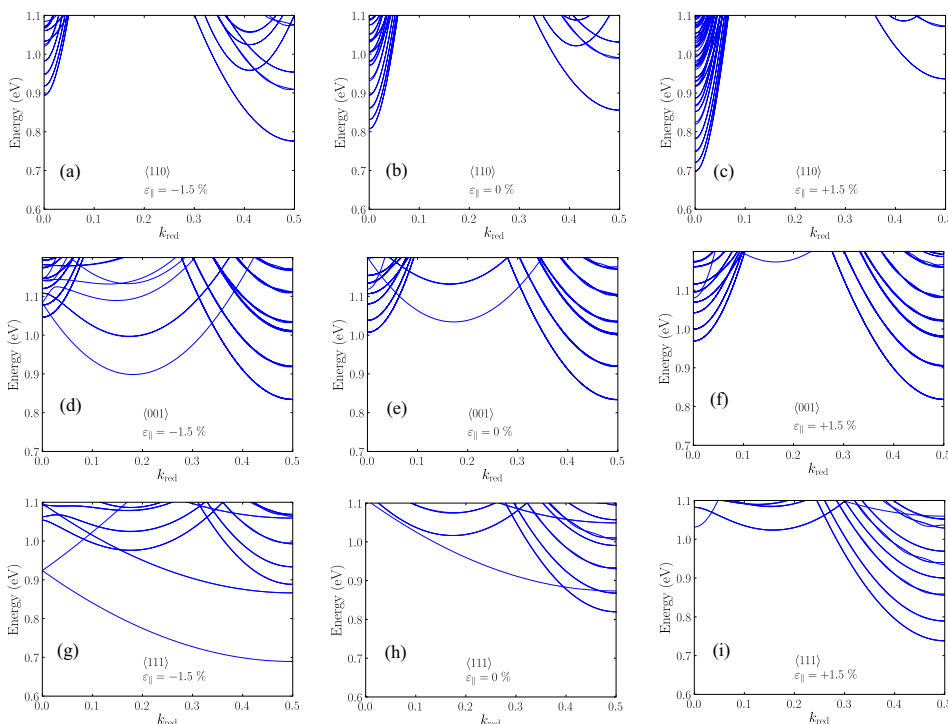


FIG. 2. Conduction-band structure of $\langle 110 \rangle$ (top), $\langle 001 \rangle$ (middle), and $\langle 111 \rangle$ (bottom) oriented Ge NWs with diameter $d = 8 \text{ nm}$ for three values of the longitudinal strain ε_{\parallel} (-1.5%, 0%, +1.5%). k_{red} is equal to $k/(2\pi/l)$ where l is the length of the NW unit cell ($l = a$ in $\langle 001 \rangle$ NWs, $l = a/\sqrt{2}$ in $\langle 110 \rangle$ NWs, $l = a/\sqrt{3}$ in $\langle 111 \rangle$ NWs, a being the lattice parameter).

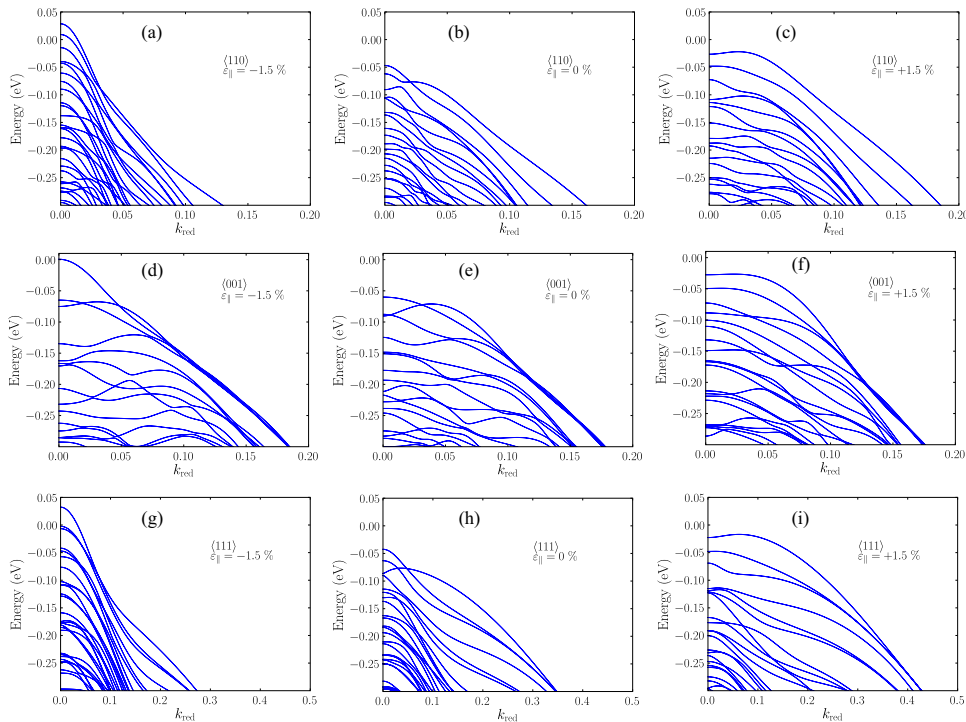


FIG. 3. Same as Fig. 2 but for valence bands.

condition, the mobility can reach huge values, for example $12000 \text{ cm}^2/\text{V/s}$ in $\langle 001 \rangle$ NWs for $\varepsilon_{\text{uni}} = -3\%$ ($d = 8 \text{ nm}$), more than five times the bulk value. These predictions confirm that compressive strains can be an important booster of

the hole mobility in semiconductor nanowires. Large compressive strains can, in particular, be achieved in Ge NWs surrounded with a $\text{Si}_x\text{Ge}_{1-x}$ shell.⁶ For example, we calculate a strain $\varepsilon_{\text{uni}} \approx -2.5\%$ in 8 nm Si NWs surrounded by an infinite shell of Si.

In conclusion, we have computed the phonon-limited carrier mobility in Ge NWs with diameters up to 10 nm . The highest electron mobility is found in $\langle 110 \rangle$ NWs and can be further enhanced by tensile uniaxial strains, even if it remains below the bulk value. The hole mobility in $\langle 111 \rangle$ NWs can be larger than in bulk Ge due to the strong quantum confinement. Under compressive uniaxial strains, the hole mobility increases up to $\approx 12000 \text{ cm}^2/\text{V/s}$. Electrons and holes mobilities above $3000 \text{ cm}^2/\text{V/s}$ can be achieved in Ge NWs with a diameter of 8 nm , showing that Ge NWs are promising candidates for efficient nanoelectronic devices.

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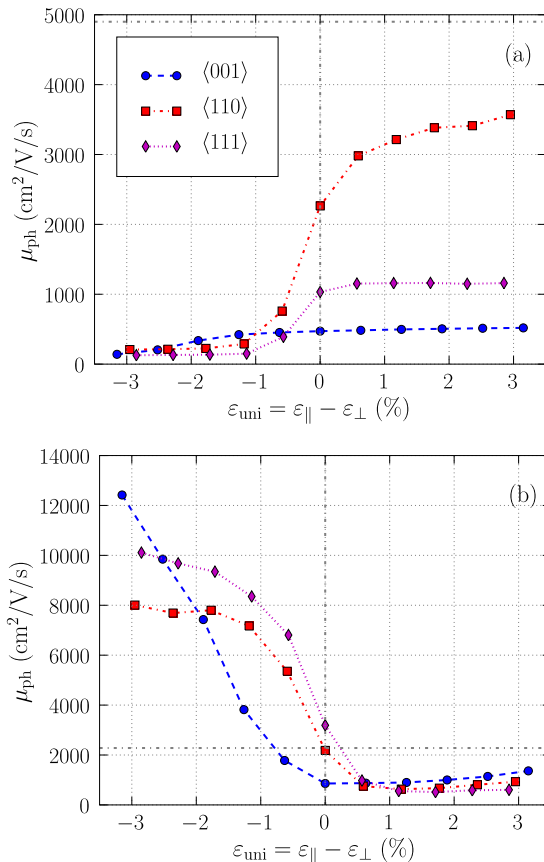


FIG. 4. Phonon-limited mobility of electrons (a) and holes (b) as a function of the strain $\varepsilon_{\text{uni}} = \varepsilon_{\parallel} - \varepsilon_{\perp}$ in stretched Ge NWs with $\langle 001 \rangle$, $\langle 110 \rangle$, and $\langle 111 \rangle$ orientations (diameter $d = 8 \text{ nm}$).

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