Electron transport in SiGe alloy nanowires in the ballistic regime from first-principles

M. Amato, [1] S. Ossicini,[2] R. Rurali [3]
[1] Laboratoire des Solides Irradiés, École Polytechnique, 91128 Palaiseau, France andUniversité Paris Sud, Laboratoire de Physiques des Solides, 91405 Orsay, France
[2] Dipartimento di Scienze e Metodi dell'Ingegneria and Centro Interdepartmentale En&Tech, Università di Modena e Reggio Emilia, Via Amendola 2 Pad. Morselli, I-42100 Reggie Emilia, Italy
[3] Institut de Ciència de Materials de Barcelona (CSIC), Campus de la UAB, 08193 Bellaterra, Spain
e-mail: rrurali@icmab.es

The possibility of achieving large thermoelectric efficiencies in one-dimensional conductors was first predicted in 1993 [1] Recent reports of a figure of merit *ZT* approaching 1 in Si nanowires (NWs) [2] boosted a resurgent interest in this field [3,4]. Since these works, many theoretical studies attempted to propose novel approaches to further increase those efficiencies. All these theoretical proposals, however, focused on the decrease of the thermal conductivity, mostly neglecting the effects on the electrical conductivity. Such an approach is rigorous only in the idealized case of isotope blends, where different isotopes are mixed on purpose. In these systems the ballistic electrical conductance is not affected because the electronic structure does not change, while phonon transmission can suffer additional scattering, leading to a drop in the thermal conductivity. The use of different isotopes is not practical, however, and similar schemes have been explored in SiGe systems, where a significant difference in the mass offers the possibility of engineering phonon scattering, while the similar electronic structure allows expecting a limited degradation of the electrical conductivity.

Here we study from first-principles the electrical conductance of $Si_{1-x}Ge_x$ alloy nanowires in the ballistic regime [5]. On the basis of single-impurity scattering (see Figure 1) the assumption that Ge alloying does not affect significantly the conductance seems sound: (i) only interstitial defects act as efficient scattering centers, but their concentration is expected to be negligible; (ii) substitutional defects are easily incorporated in the Si lattice and the transport channels of the pristine wire are only marginally affected.

Yet, in SiGe alloy NWs Ge concentrations of up to 70% can be reached, thus we addressed explicitely the study of $Si_{1-x}Ge_x$, with x ranging from 0.1 to 0.7. The calculated conductances show that in all the cases the concentration turns out to be sufficiently high so that the alloy NW behaves in practice as an abrupt Ge NW inclusion, with scattering concentrated at the interface. This is an important result, because abrupt junctions are difficult to obtain, while (random) concentration gradients can be obtained in an easier way. Peculiarly, distributing the impurities along a longer wire section yields a larger scattering, thus lower concentrations can result in lower conductances. This happens because in the limit of low Ge concentration the conductance results from a series of individual scattering events, while in heavily alloyed wires scattering only occurs at the interface and the scattering is reduced.

REFERENCES

[1] L. D. Hicks, and M. S. Dresselhaus, *Thermoelectric figure of merit of a one-dimensional conductor*, Physical Review B **47**, 16631 (1993).
[1] R. Rurali, *Structural, electronic, and transport properties of silicon nanowires*, Reviews of Modern Physics **82**, 427 (2010).
[3] A. I. Boukai *et al.*, *Silicon nanowires as efficient thermoelectric materials*, Nature **451**, 168 (2008).
[4] A. I. Hochbaum *et al.*, *Enhanced thermoelectric performance of rough silicon nanowires*, Nature **451**, 163 (2008).
[5] M. Amato, S. Ossicini, and R. Rurali, *submitted.*

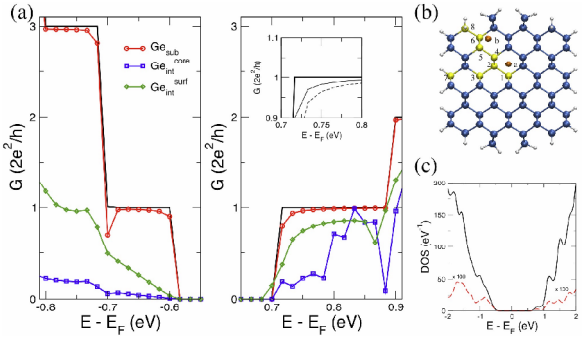

Fig. 1. (a) Conductance of a Si NW with a single Ge impurity substituting at a Si lattice site (red circles), at an interstitial site in the core of the wire (blue squares) and at an interstitial site close to the surface (green diamond). All the substitutional defects considered give a very similar conductance, thus one single curve is plotted [defect 1, see panel (b)]. To resolve the difference between the lowest and highest case among the eight substitutional configurations, a magnified view is shown in the inset. The conductance of the pristine Si NW is shown by the continuous black line. (b) Cross-section view of the Si NWwhere the substitutional and interstitial Ge defects considered are shown in yellow and light orange spheres (blue and white spheres representing Si and H atoms, respectively). (c) Total density of states (continuous black line) and projected density of states of a Ge substitutional in position 1 (dashed red line).

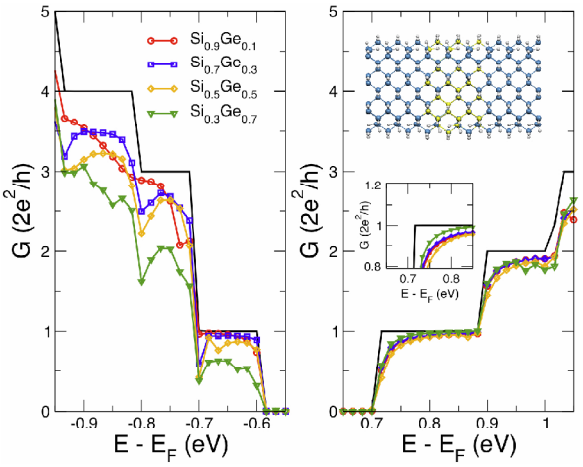

Fig. 2. Conductance of a Si / Si1−xGex / Si NW with x = 0.1, 0.3, 0.5 and 0.7. The conductance of the pristine Si NW is shown by the continuous black line. A side view of the NW in the case of a Si0.5Ge0.5 scattering region is also shown. The inset shows a magnified view of the first transmission channel of the conduction band