Short communication

Band structure analysis in SiGe nanowires

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ABSTRACT

One of the main challenges for Silicon-Germanium nanowires (SiGe NWs) electronics is the possibility to modulate and engine their electronic properties in an easy way, in order to obtain a material with the desired electronic features. Diameter and composition constitute two crucial ways for the modification of the band gap and of the band structure of SiGe NWs. Within the framework of density functional theory we present results of ab initio calculations regarding the band structure dependence of SiGe NWs on diameter and composition. We point out the main differences with respect to the case of pure Si and Ge wires and we discuss the particular features of SiGe NWs that are useful for future technological applications.

1. Introduction

Scaling down of semiconductor structures to nanometer sizes poses strict requirements on electronic material properties that cannot be satisfied by traditional bulk semiconductors [1,2]. In this context semiconductor's manipulation through size reduction and through alloying represent one of the most used route to develop and create materials which present the desired properties and, at the same time, that can be easily integrated into existent Si microelectronics [3–6]. A striking example of this class of material is represented by SiGe nanostructures (SiGe NSs) [7–10]. In these nanomaterials the electronic, transport and optical properties are strictly related not only to the size of the system (like the corresponding pure Si and Ge nanostructures [11–13]) but also to their relative composition in Si and Ge atoms, and to the particular geometry of the Si/Ge interface [14–17]. The role that SiGe NSs can play in various technological fields has been clearly demonstrated, for example regarding the possibility to use these nanostructures to realize electronic [18,19], photovoltaic [20], optoelectronic [21] and thermoelectric [22] devices. During the last decade an

increasing attention, both from the experimental [18,23–31] and theoretical point of view [14,15,32–46], has been dedicated to SiGe nanowires (SiGe NWs), that are one-dimensional nanoalloys that can be synthesized using top-down [24,25] or bottom-up [5,26,27] approaches and for which it is possible to reach a precise control of the size, the morphology and the electronic properties. Several types of SiGe NWs have been grown: core-shell NWs [5], which are radial heterostructures, synthesized firstly by the Lieber's group in 2002; axial heterojunctions [31], that present a sharp interface between Si and Ge along the axial direction of the wire; random NWs [16], where the relative configuration of Si and Ge atoms is completely random; triangular shaped NWs [23], produced in different ways and, very recently, object of theoretical investigation [46]. In our previous works we have analyzed an innovative geometry for the SiGe NWs [14,15,42,44], characterized by the presence of a sharp interface in the transverse cross-section of the wire (in the following, we will call this geometry abrupt NWs). We have demonstrated how this type of geometry (in particular through the presence of a sharp interface) can originate very interesting electronic and optical properties. In fact the study of the dependence of the electronic band gap on the wire's diameter shows the occurrence of a strong reduced quantum confinement effect (RQCE) with respect to the corresponding pure nanowires [14] (i.e. for the same diameter reduction the band gap increase due to confinement is less pronounced). This effect is also present if both composition and diameter of the wire are modulated. Moreover since these NWs

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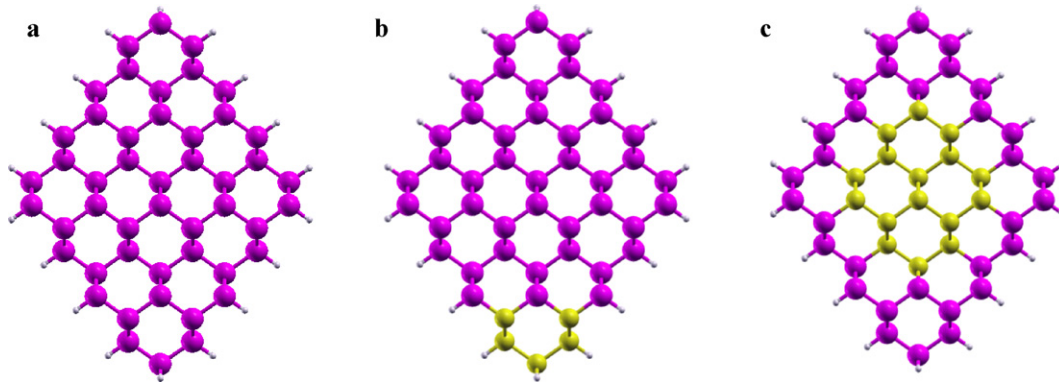
Fig. 1. Transverse cross section of a pure Ge NW (left), an abrupt NW with $x_{Ge} = 0.895$ (central) and a core-shell NW with $x_{Ge} = 0.333$ (right). All the wires have a diameter $d = 1.6$ nm. Yellow spheres represent Si atoms, magenta spheres Ge atoms, while the small white spheres are H atoms used to saturate the dangling bonds. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

show a perfect parabolic dependence of the electronic band gap on the composition [15], they offer in principle a very easy way to predict and engine the band gap.

The origin of these particular properties has been ascribed to the presence of a type II band offset that comes out at the planar interface between silicon and germanium [47,48]. The presence of a type II band offset is a direct consequence of two facts: (i) the quantum confinement effect (QCE) is stronger in Ge than in Si [49–52] and (ii) for these SiGe NWs, holes (valence states) are always located on Ge region, while electrons (conduction states) are located on Si region [14].

Finally the optical properties of abrupt NWs present an enhanced absorption peak in the near infrared region [44], suggesting intriguing applications in the field of optical fiber communications. Moreover, regarding the exciton formation, a spatial separation of electron and hole is present, that is a basic requirement for photovoltaic applications. A confirmation of the importance of the presence of abrupt interfaces for photovoltaics has been demonstrated in the case of the doped core-shell SiGe nanowires [53].

In this paper we go deeper in our analysis, presenting a detailed discussion of the results of ab initio calculations regarding the band structure behaviour of abrupt NWs. We depict how composition and diameter represent two crucial tools in order to modulate and engine the electronic features of these materials, paving the way to exciting technological perspectives. In particular we show how their electronic band structure can be easily modulated changing the diameter, thus presenting very different features with respect to the case of pure wires. Regarding the effect of composition an interesting comparison between abrupt NWs and core-shell NWs is presented, pointing out the main differences between these two geometries. The paper is organized as follows: Section 2 describes the theoretical method used; Section 3 contains the results of calculations concerning the band structure dependence on diameter and composition, while Section 4 is devoted to the conclusions.

2. Method

The atomistic models we use to describe NWs are the same depicted in Refs. [14,15,42,44,53]. In particular we study [1 1 0] free-standing NWs, whose surface atoms have been saturated by H atoms in order to cancel their metallic character due the presence of dangling bonds [54]. All details of the geometrical construction of NWs can be found in Ref. [15]. In this paper we analyze pure Si, pure Ge, core-shell and abrupt SiGe NWs. As mentioned before this last geometry is characterized by the presence of a planar sharp interface along the shortest dimension of the

transverse cross-section of the wire. While core-shell NWs are radial heterostructures made by coaxial cylinders of different materials. For all the considered wires the diameter's length varies from 0.8 to 1.6 nm (the definition of the diameter of our wires is the same of Ref. [15]). The variation of composition in the abrupt SiGe NWs is obtained by adding or deleting some rows of one type of atom in the transverse section of the wire (along the shortest dimension), thus preserving a sharp interface between Si and Ge regions, as clearly shown in Ref. [15]. For core-shell NWs, instead, the compositional change is obtained by progressively increasing the core region [15]. The composition x for core-shell and abrupt NWs is defined as the relative amount of one type of atom with respect to the total number of atoms in the unit cell, thus ranging from 0 to 1. As examples we report in Fig. 1 images of the transverse cross-section of a pure Ge NW (left), an abrupt NW with $x_{Ge} = 0.895$ (central) and a core-shell NW with $x_{Ge} = 0.333$ (right). All our calculations have been carried out in the framework of density functional theory (DFT) in the local density approximation (LDA) as implemented in the PWSCF code [55]; where norm-conserving pseudo-potential have been used. In the unit cells the vacuum space between NWs replicas in the supercell has been set to more than 10 Å. The cutoff energy for the plane wave expansion is fixed to 30 Ry. A $16 \times 1 \times 1$ Monkhorst and Pack grid has been chosen for the sampling of the Brillouin Zone. For all the wires a full geometry optimization through the Broyden–Fletcher–Goldfarb–Shanno technique has been performed. In order to calculate the band structure of the wires, after relaxations a non-self consistent calculation has been performed, sampling the Brillouin Zone with 51 k-points from Γ to X. A whole overview on the computational details of our calculations can be found in Refs. [14,15].

3. Band structure analysis

As clearly demonstrated in several theoretical and experimental works [15,16,29,32–36,38,40,41,57–58], the electronic structure of a SiGe NW with a particular geometry can be strongly modified varying intrinsic (relative composition between Si and Ge atoms) and extrinsic (diameter of the wire) parameters. Following this idea we perform here an analysis of our calculated band structure looking at the influence of diameter' changes and composition's variations. Thus this section contains two paragraphs: in the first one, results of calculations on the dependence of the band structure on the wire's diameter are presented, in particular pointing out main differences with respect to the behaviour of pure Si and Ge NWs; whereas, in the second paragraph, we show how the band structure of abrupt NWs with diameter equal to 1.6 nm, changes
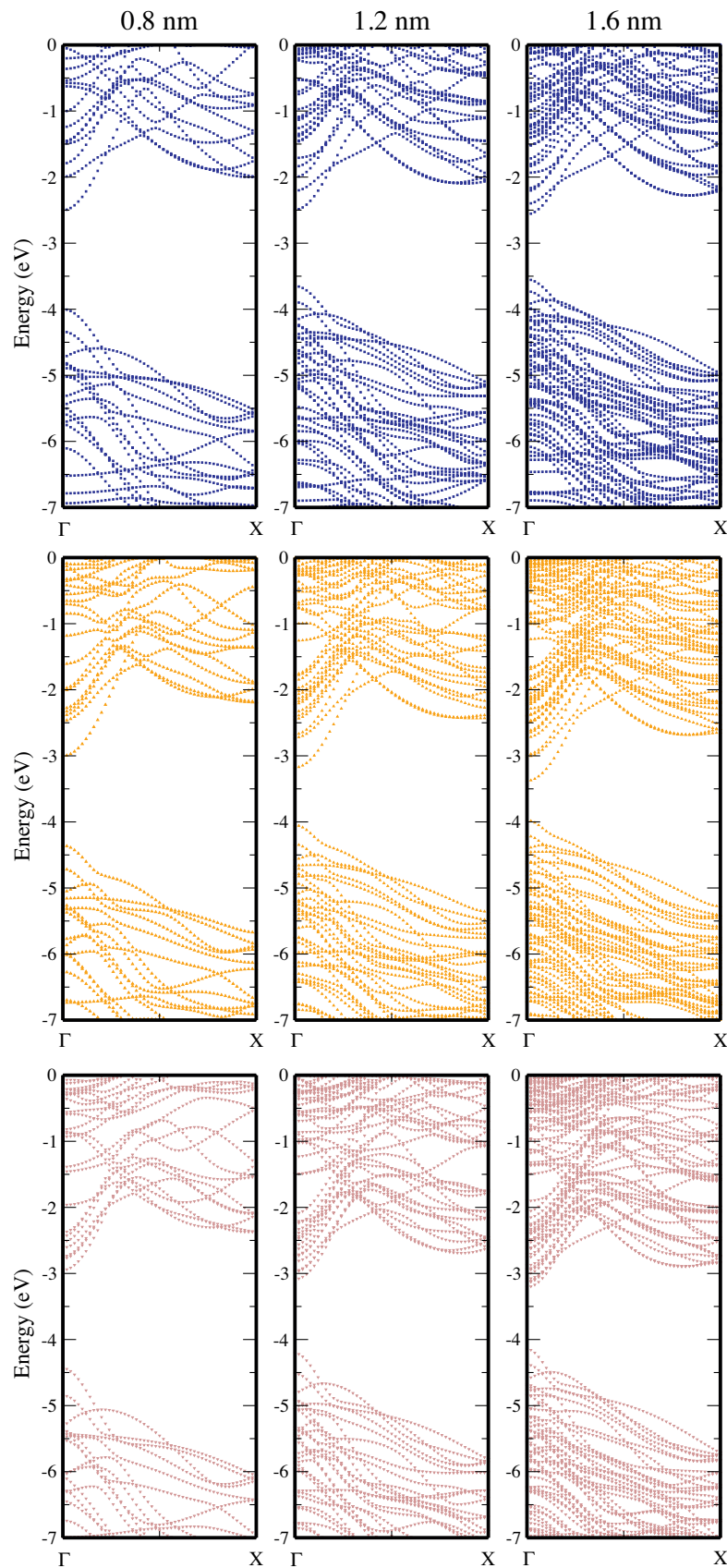
Fig. 2. Energy band structure calculations as a function of diameter d for pure Si NWs (top row), abrupt SiGe NWs (middle row) with $x_{Ge} = 0.5$ and pure Ge NWs (bottom row). The diameter varies from 0.8 to 1.6 nm. The vacuum level of the wire is taken as the zero of energy and it has been calculated from the cylindrical averaged local potential in the vacuum region, where it becomes a constant in the supercell.
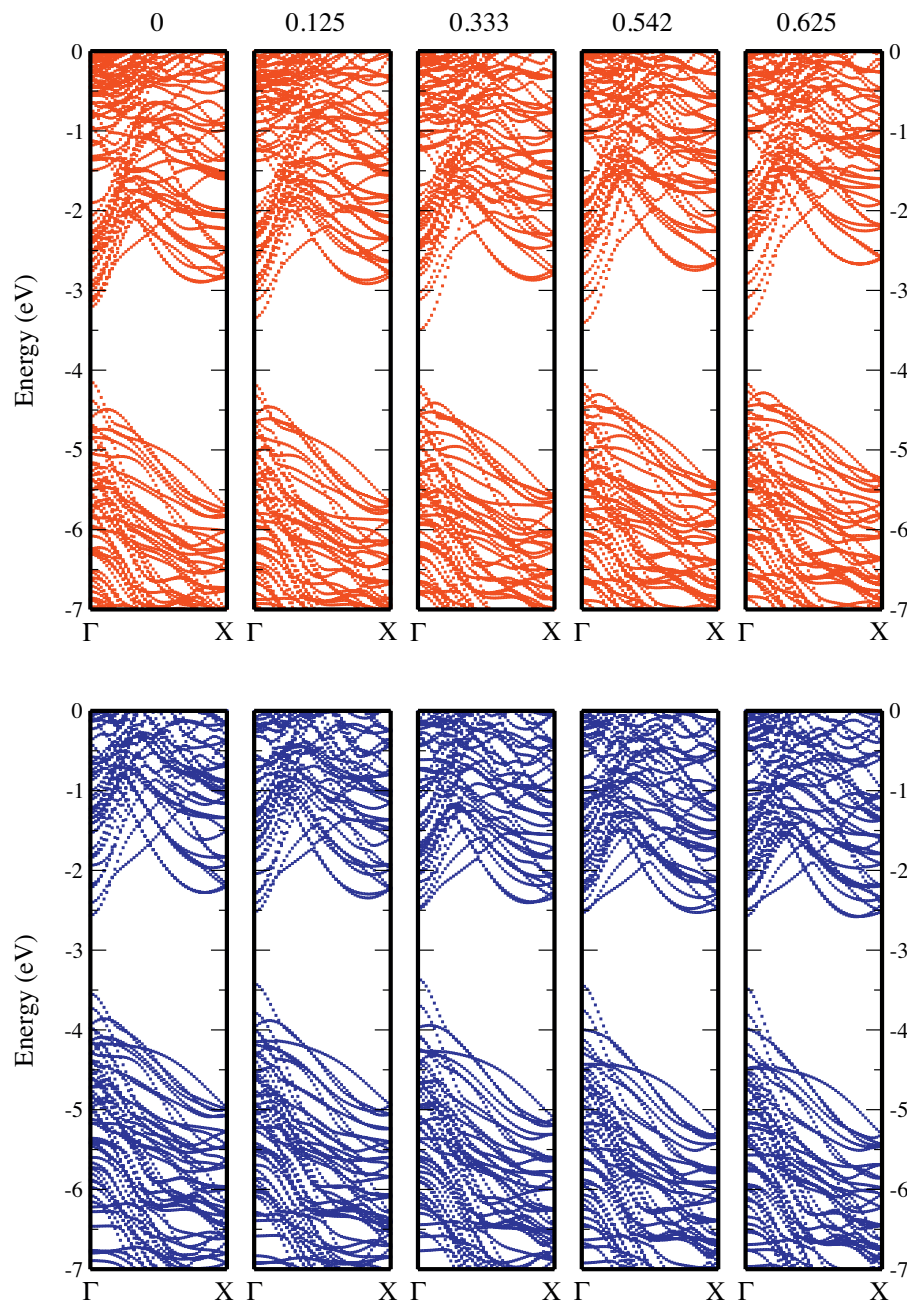
Fig. 3. Energy band structure calculations for core-shell NWs as a function of composition x. Top row (bottom row) contains band calculations for Si_{core}/Ge_{shell} (Ge_{core}/Si_{shell}) NWs as a function of x_{Si} (x_{Ge}). The composition x varies from 0 (pure Si or Ge NWs, depending on the type of core-shell) to 0.625. The vacuum level of the wire is taken as the zero of energy and it has been calculated from the cylindrical averaged local potential in the vacuum region, where it becomes a constant in the supercell.

varying the atomic composition; here the main differences with respect to core-shell NWs are then pointed out.

3.1. Effect of diameter

In Fig. 2 the band structures for pure Si NWs (top row), pure Ge NWs (bottom row) and abrupt SiGe NWs with $x_{Ge} = 0.5$ (middle row) are reported as a function of diameter.

The results regarding pure NWs are in good agreement with other theoretical studies [11,59,60]. For these types of wires the reduction of the size leads to an increase of the band gap and to a strong discretization, energy separation, of the electronic states as a consequence of the QCE [11–13,59,61,62]. This effect can be qualitatively described by a particle in a box model [63]. Moreover due

to the folding of electronic states in the [1 1 0] 1-D first Brillouin Zone, the semiconductor indirect bulk band gap becomes direct at Γ point: the Valence Band Maximum (VBM) and the Conduction Band Minimum (CBM) occur at the same point in the k-point space [64]. Looking at Fig. 2 one can conclude that the increase of the diameter of the NWs preserves the existence of a direct gap at Γ and no direct to indirect band gap transitions are observed for the considered diameters. On the other hand it is worth to note that the first indirect band gap located near to the X point is only few tens of meV higher than the CBM at Γ point. Observing the first and third rows of Fig. 2 it is possible to deduce a different behaviour for the QCE in pure Si and Ge NWs: Ge NWs present a stronger QCE than Si ones and, while for Si NWs the confinement acts mainly for the valence states, the effect of QCE for Ge NWs is similar for

$x_{Ge}=0$ 0.104 0.312 0.5 0.687 0.895
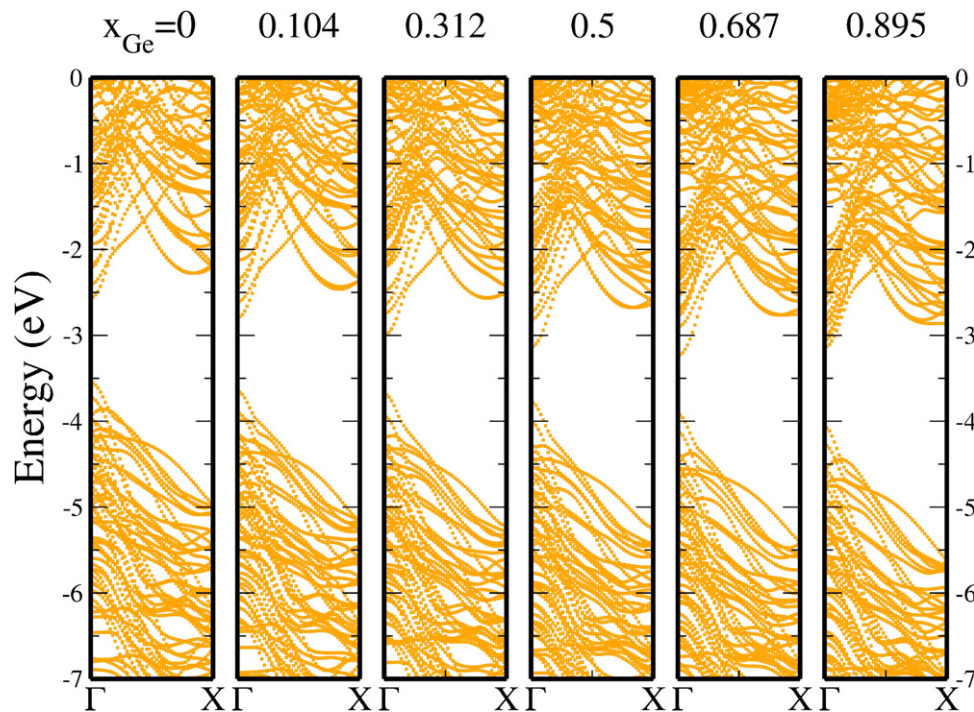
Fig. 4. Energy band structure calculations as a function of Ge composition x_{Ge} for abrupt NWs with $d = 1.6$ nm. The composition x varies from 0 (pure SiNW) to 0.895. The vacuum level of the wire is taken as the zero of energy and it has been calculated from the cylindrical averaged local potential in the vacuum region, where it becomes a constant in the supercell.

the valence and the conduction bands in agreement with previous results [14,15]. Nevertheless an analogous k-dispersion of the valence states can be recognized for Si and Ge NWs, due to the similarities between valence bands of the two bulk materials. It is important also to point out the absence, in the band structures, of intra-gap surface states that have been swept out by the presence of H passivation of the semiconductor surface atoms. For abrupt SiGe NWs the band structure analysis is more complicated, since, due to this particular geometry, it is not so straightforward to make a comparison with the electronic state dispersion of a particular reference bulk material. Moreover also the comparison with other studies on SiGe NWs is not easy, since this particular geometry has been introduced for the first time in our previous works [14,15,42,44] and up to know no other groups have investigated theoretically or experimentally abrupt SiGe NWs. Nevertheless very recently Pekoz et al. [46] by means of ab initio calculations, have investigated triangular shaped SiGe NWs with an abrupt Si/Ge interface in the transverse cross section of the wire. Even if they have a different cross-section, these particular wires can be qualitatively compared with our abrupt wires, because they present a sharp Si/Ge interface. Looking at the middle row of Fig. 2 one can note that the dependence of the band dispersion on the diameter does not change too much with respect to the pure Si and pure Ge NWs: in particular, for the valence states, this dispersion is not so different from that of pure Si and pure Ge NWs (they have similar dispersions), while for the conduction states it has a clear silicon character, according to the presence of a type II band offset. It is worth to note that for the abrupt SiGe NWs the band gap reduction, due to the increase of the diameter, is stronger than in the case of pure NWs, still as a consequence of the type II band offset that comes out at the sharp Si/Ge interface, which strongly localizes the onset of valence states on the Ge region and the onset of conduction states on the Si region [15,38]. Pekoz et al. [46] have demonstrated that the same preferential localization of valence and conduction states (electrons on Si and holes on Ge) occurs in abrupt triangular shaped NWs. The band gap of the abrupt SiGe NWs (see the middle row of Fig. 2) is still

direct at the Γ point for all the considered diameter, but the difference between the direct gap at Γ and the indirect band gap near the X point strongly increases, becoming nearly 0.8 eV when the length of the diameter d is only 0.8 nm. This finding, together with our previous results which demonstrated that the optical properties of abrupt SiGe NWs show an intense peak in the near-infrared region, envisage possible technological applications for these NWs, in particular in the field of photovoltaics [20].

3.2. Effect of composition

Several theoretical studies have deeply analyzed the effect of composition on the band structure of core-shell SiGe NWs, showing how increasing the thickness of the Si or Ge core or shell regions can strongly modify the band gap and the electronic states dispersion of the wire [32–36]. For instance Pekoz and Raty [32] have shown that, at fixed composition, Si_{core}/Ge_{shell} NWs have smaller band gaps than Ge_{core}/Si_{shell} ones. The same physical evidence was also demonstrated by Peng and Logan [36]. Our results for core-shell NWs with $d = 1.6$ nm are in agreement with these studies and are reported in Fig. 3. From the figure it is clear that in both the types of wire (Si_{core}/Ge_{shell} and Ge_{core}/Si_{shell}) there is a reduction of the energy band gap when the core of the wire is increased with respect to pure Si and Ge NWs of the same diameter. This is a consequence of the presence of a type II band offset between Si and Ge and of a RQCE. Looking at the figure, it possible to recognize that the RQCE is more pronounced for the Si_{core}/Ge_{shell} NWs (top row) than in the case of the Ge_{core}/Si_{shell} (bottom row) ones. The origin of this discrepancy has been ascribed to different QCE for Si and Ge for small diameters (less than 2 nm) and to the effect of strain and mismatch for larger diameters [15,32–36]. We underline that these results are in very good agreement with works of Pekoz and Raty [32] and Peng and Logan [36]. For both the Si_{core}/Ge_{shell} and the Ge_{core}/Si_{shell} NWs the energy band gap remains direct at the Γ point and no direct to indirect gap transition is observed for the considered compositional variations. Nevertheless the difference

in energy between direct and indirect band gap near the X point strongly depends on the material that occupies the core: in particular we observe that, increasing the Si core region in a previous pure Ge NW, the difference between direct gap at Γ and indirect one at X, becomes very large (nearly 0.9 eV when $x_{Si} = 0.625$). On the other hand when then Ge core region increases in a previous pure Si NW this difference decreases and becomes very small when $x_{Ge} = 0.625$.

Concerning the effect of composition on the dispersion of the electronic states we can say that, in the case of Si_{core}/Ge_{shell} NWs, the discretization of the electronic states due to the QCE in the conduction band is more significant that the one for valence states, in agreement with other theoretical studies [32–36]; while for Ge_{core}/Si_{shell} NWs the separation in energy of the electronic states in the valence band is more significant than in the conduction band.

The effect of the compositional variation on the band structure of abrupt NWs (diameter $d = 1.6$ nm) is illustrated in Fig. 4. As mentioned before, for these types of wires the modification of the composition is obtained by progressively adding or deleting rows of one type of material (Si or Ge) in the transverse cross section. In Fig. 4 the effect of composition on the band structure is depicted starting from a pure Si NW (with $x_{Ge} = 0$). First of all we note that a change of the composition has a stronger effect on the energy band gap reduction with respect to the core-shell case. Moreover the variation of the composition has only a negligible effect on the valence bands dispersion; probably the origin of this result can be again ascribed due to the similarity of Si and Ge bulk band structure for the valence band states. As the number of Ge layers that substitute Si layers into the cross section of a pure Si wire increases, the direct band gap at Γ point strongly decreases as a consequence of the type II band offset between Si and Ge. The band gap energy reaches its minimum value for $x_{Ge} = 0.5$ and then increases reaching the value related to the up to pure Ge NW.[1] An analysis of the wave function localization shows that, at any composition, the electronic states near the valence band maximum are completely located on the Ge region of the wire, while the conduction band edge is completed dominated by Si related states, according to the presence of a type II band offset [15]. Indeed Fig. 4 shows that the atomic composition has no influence on the character of the energy band gap, that remains direct at the Γ point for any value of composition x_{Ge}. Moreover increasing the value of x_{Ge} the difference between direct and indirect band gap increases until $x_{Ge} = 0.7$ where it becomes again small assuming a clear Ge related character.

4. Conclusions

We have performed a first principles analysis in the framework of DFT of the dependence of the electronic band structure on diameter and composition for different SiGe NWs. By comparison with the state of art of theoretical studies on SiGe NWs, the study has demonstrated how diameter and composition represent two crucial tools in order to modulate the electronic band structure and therefore the optical and transport properties of SiGe NWs. In particular abrupt SiGe NWs offer the possibility to modulate the energy band gap in a very wide range as a consequence of a strongly reduced quantum confinement effect. Moreover this wide modulation of band gap together with the peculiar optical properties of these NWs (direct gap, enlarged difference between direct and indirect band gap, absorption peak in the near infrared region) offer the possibility to engine materials with different absorption prop-

erties, that envisages interesting applications in the optoelectronic and the photovoltaic fields.

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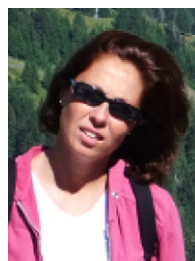[42] M. Amato, M. Palummo, S. Ossicini, Phys. Status Solidi B 247 (2010) 2096.

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[1] In Ref. [15] we have demonstrated that the band gap dependence on the composition for abrupt NWs with $d = 1.6$ nm is perfect parabolic and has the following analytical expression: $E_g(x_{Ge}) = 0.98292 - 1.3508 \cdot x_{Ge} + 1.3478 \cdot x_{Ge}^2$.

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