Materials Science and Engineering B 177 (2012) 705–711

Contents lists available at SciVerse ScienceDirect

Materials Science and Engineering B

journal homepage: www.elsevier.com/locate/mseb

Short communication

Band structure analysis in SiGe nanowires

Michele Amato[a,b], Maurizia Palummo[c,d], Stefano Ossicini[a,b,c,e,*]

[a] "Centro S3", CNR-Istituto Nanoscienze, via Campi 213/A, 41100 Modena, Italy
[b] Dipartimento di Scienze e Metodi dell'Ingegneria, Università di Modena e Reggio Emilia, via Amendola 2 Pad. Morselli, I-42100 Reggio Emilia, Italy
[c] European Theoretical Spectroscopy Facility (ETSF)
[d] CNR-INFM-SMC, Dipartimento di Fisica, Università di Roma, 'Tor Vergata', via della Ricerca Scientifica 1, 00133 Roma, Italy
[e] Centro Interdipartimentale "En&Tech", Università di Modena e Reggio Emilia, via Amendola 2 Pad. Morselli, I-42100 Reggio Emilia, Italy

ARTICLE INFO

Article history:
Received 9 June 2011
Received in revised form
20 September 2011
Accepted 31 October 2011
Available online 12 November 2011

Keywords:
Silicon-germanium nanowires
Band structure
Band offset
Composition
DFT
Diameter

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

* Corresponding author at: Dipartimento di Scienze e Metodi dell'Ingegneria, Università di Modena e Reggio Emilia, via Amendola 2 Pad. Morselli, I-42100 Reggio Emilia, Italy. Tel.: +39 0522 522211; fax: +39 0522 522609.
E-mail address: stefano.ossicini@unimore.it (S. Ossicini).

0921-5107/$ – see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.mseb.2011.10.008

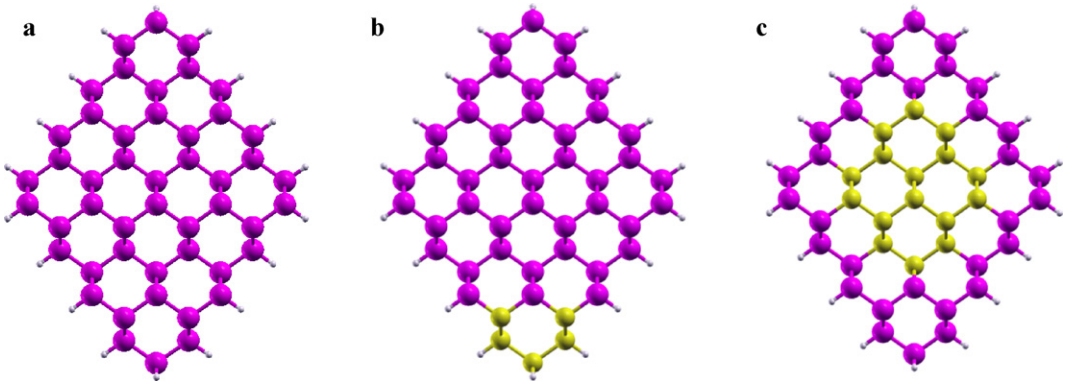

Fig. 1. Transverse cross section of a pure Ge NW (left), an abrupt NW with $x_{Ge} = 0.895$ (central) and a core-shell NW with $x_{Ge} = 0.333$ (right). All the wires have a diameter $d = 1.6$ nm. Yellow spheres represent Si atoms, magenta spheres Ge atoms, while the small white spheres are H atoms used 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