Physica E 90 (2017) 24–27

Contents lists available at ScienceDirect

Physica E

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

Indirect to direct gap transition in low-dimensional nanostructures of Silicon and Germanium

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ARTICLE INFO

Keywords:
Direct band gap
First principles calculation
Low-dimensional nanostructure

ABSTRACT

The electronic band structures of Si and Ge low-dimensional nanostructure such as nanofilms and nanowires have been calculated using first principles based on density functional theory (DFT) with the generalized gradient approximation (GGA). The calculation results show that a direct band gap can be obtained from Si orientation [100] or in Ge orientation [111] confined low dimensional nanostructure. However, an indirect band gap is still kept in the Si orientation [111] or in the Ge orientation [110] confined low dimensional nanostructure. The calculation results are interesting and the transition mechanism from indirect to direct band gap in low dimensional nanostructures is given in the physical structures model.

1. Introduction

Modern microelectronic devices are mainly based on Silicon (Si) and germanium (Ge) material. However, luminous efficiency lowly due to indirect band structure their applications in the fields of optoelectronics are still limited. The possible way to resolve the problem might be to prepare the low dimensional nanostructures based on the effect of quantum confinement. In recent decades, the valuable research of experimental and theoretical work has done on Si and Ge low dimensional nanostructures [1–5]. The optical properties of both Si and Ge low-dimensional structures have been experimentally studied [5–8], such as Justin et al. shown that different luminescence properties have been observed for SiNWs grown along different crystal orientations. At the same time, the band structures of Si and Ge low-dimensional structures have widely studied from a theory angle [9–24]. The results of theoretical study shown that the band gaps of both nanofilms and NWs could be either indirect or direct, depending on the crystal constrained orientation. However, the transition mechanism from indirect to direct-gap in low dimensional nanostructures of Si and Ge has not yet been given.

In this work, we present transition mechanism from indirect to direct-gap in low dimensional nanostructures of Si and Ge based on first-principles calculations of the electronic band structures for Si (or Ge) nanofilms and NWs, and the energy band structures of NWs are explained based on the analysis of the energy band structures of the nanofilms.

2. Model and calculation method

Electronic structure calculations have been performed for Si (Ge) nanofilms in (100), (110), (111) and (112) surfaces as well as Si (Ge) NWs along [100,110] and [111] crystallographic directions. Periodic boundary condition is employed and a vacuum layer of 2 nm is taken in every model to avoid interaction between subsequent low dimensional structures. All dangling bonds on the surfaces of nanofilms and NWs are saturated by hydrogen atoms for obtaining the stable minimum energies. The lattice structure and atomic spacing of Si and Ge low-dimensional structure is taken to be equal to that of bulk Si and Ge material,[9] and the Si-H and Ge-H bond length are equal to those determined in SiH_4 and GeH_4 molecules, respectively.[10] The thickness of film is defined as the distance between the upper surface and the lower surface of the hydrogen passivation film, as shown in Fig. 1.

The structure optimization and energy band structure calculations of Si and Ge low dimensional structures are performed using density functional theory (DFT) under the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) function as the exchange and correlation potential [25–27]. For the calculation, the plane-wave energy cutoff is set at 380 eV, the SCF convergence tolerance of electronic energy is 1.0×10−5 eV/atom, the maximum stress is 0.05 GPa, the maximum ionic displacement is 0.001 Å, and the

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http://dx.doi.org/10.1016/j.physe.2017.03.004
Received 5 January 2017; Received in revised form 9 March 2017; Accepted 11 March 2017
Available online 12 March 2017

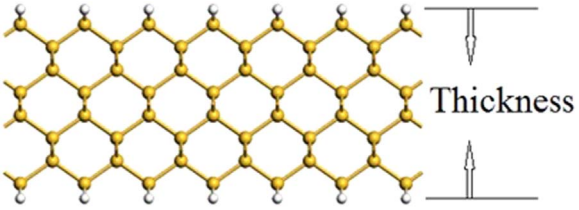

Fig. 1. The definition of thickness of Si nanofilm. The Si and H atoms are represented by yellow and gray balls.

ultrasoft pseudopotential is used.

3. Results and discussions

After geometry optimizations, the lattice constants, atomic bond lengths and band gaps of Si (111) single atomic layer and Ge(111) single atomic layer are 3.905 Å, 2.361 Å, 2.17 eV and 4.06 Å ,2.46 Å 1.29 eV, respectively, which are in accord with the previous results [11–13]. With increasing the thickness of films, the band gaps of Si (100), (110), (111) and (112) nanofilms are changed as shown in Fig. 2. In the diagram, the blue lines and red lines describe the change of energy level of nanofilms in the valleys of $\Gamma(E_{\Gamma\text{-}\Gamma})$ and conduction band minimum (E_{gap}), respectively, in which a direct band gap will occur when the two are overlap. It is clear that Si (100) nanofilm with thickness range of calculation ($d < 7.64$ nm) is a direct band gap semiconductor, Si (110) and (112) nanofilms are direct band gap semiconductor with a thickness of less than 1.96 nm and 0.83 nm and transform into indirect-gap structure with the thickness greater than that thickness, respectively, and Si (111) nanofilm no matter how thin is an indirect band gap semiconductor. The result is consistent with the previous theoretical result that the Si (111) nanofilm exhibit indirect band gap structure, but they are different from that Si(100) and (110) nanofilms are direct band gap semiconductor when the thickness of nanofilms are less than 1.05 nm and 1.14 nm, respectively. [14].

The band gaps of Ge (100), (110), (111) and (112) nanofilms are changed with increasing the thickness of the films as shown in Fig. 3. We can see that the Ge (111) nanofilm is a direct-gap semiconductor in the calculation thickness range ($d < 7.25$ nm), Ge (100) nanofilm is a direct-gap semiconductor with the thickness less than about 1.17 nm and transforms into indirect-gap structure with the thickness greater than that thickness, and Ge (110) and (112) nanofilms are indirect-gap semiconductor independent on the films thickness. The results are consistent with the previous theoretical results that the Ge (111) nanofilm exhibits a direct band gap structure and Ge (110) nanofilm exhibits an indirect band gap structure, but different from that Ge (100) nanofilm is a direct band gap semiconductor [9].

From the results of our calculations, we found that the direct band gap structure of Si (100) and Ge (111) films have the common characteristics that the symmetry points in the directions of Si [100] and Ge [111] in k-space both correspond to the lowest energy valley in bulk materials, respectively, as shown in Fig. 4. The relationship among energy valleys in the conduction band of Si and Ge are $E_X < E_K < E_L < E_\Gamma$ and $E_L < E_\Gamma < E_X < E_K$, respectively. When electrons are restricted in a direction, according to the Heisenberg uncertainty principle, the momentum error obtained in this direction becomes larger, which make it becoming easy that the momentum of any point in this direction and the momentum of Γ point are the same. In addition, the lattice periodicity of this direction is destroyed because the direction is limited, in other words, the period tends to infinity. Therefore, k ($k=n\pi/a$) tends to zero and same coordinates with Γ point, which means $E(\Gamma)=E(k)$. When electrons are restricted in the direction of Si [100] or Ge [111], Γ point energy level is pulled low relatively and same with the energy levels of any points in the direction of Si [100] or Ge [111], in which the relationship of these energy valleys turn into $E_\Gamma=E_X < E_K$ and $E_\Gamma=E_X < E_L$ in Si or $E_\Gamma=E_L < E_X$ and $E_\Gamma=E_L < E_K$ in Ge. Therefore, Si (100) and Ge (111) nanofilms are the direct energy band structure semiconductors. Likewise, when electrons are restricted in the direction of Si [111] or Ge [110], the energy level of Γ point equals the energy valley of Si [111] or Ge [110] in k-space, namely $E_X < E_\Gamma=E_L$ and $E_K < E_\Gamma=E_L$ in Si or $E_L < E_\Gamma=E_K$ and $E_X < E_\Gamma=E_K$ in Ge, so Si (111) and Ge (110) nanofilms are still the indirect band structure semiconductors. However, Si (110) and Ge (100) films are in between the two cases, therefore, they are shown as direct band gaps when the films thickness are thin, and shown as indirect band gaps when the films thickness are thicker and less affected by quantum confined (QC) effect.

According to the previous analysis of one-dimensional confined energy gap, it is still useful that the energy level of Γ point and the energy levels of the limited directions are equal for a two-dimensional confined NW, which is consistent with our calculation result, as shown in Fig. 5. We can see from Fig. 5(a) that symmetry points in the Brillouin zone of the orthorhombic lattice are shown, in which b_3 represents the direction of [111] SiNW, however, b1 and b2 represent the limited directions of [110] and [112]. The band structure of the [111] SiNW is shown in Fig. 5(b), in which the energy level of Γ point and the energy levels of the limited directions are equal.

The sectional view of [100,110] and [111] SiNW with two-dimensional confined as shown in Fig. 6. The directions of [100] and [110] are confined in the plane perpendicular to the axis of [100] SiNW as shown in Fig. 6(a), therefore, the energy level of Γ point and the energy levels of the limited directions of [100] and [110] are equal. The orientation of [100]SiNW is a direct band structure semiconductor due to the two-dimensional structure of [100] direction confined can form direct band gap for Si, as shown in Fig. 7(a), which is consistent with the previous theoretical results [15,16]. However, For Ge, the two-dimensional structure of [100] direction limited is an indirect band gap semiconductor, while the two-dimensional structure of [110] direction limited can form a direct band gap structure in a thinner thickness, so that [100]GeNW shows a direct band structure with a smaller diameter, and shows a indirect band structure with a large diameter, which is consistent with the previous theoretical result too [17].

As shown in Fig. 6(b), there are three crystal orientations of [100,110] and [111] in the confinement plane perpendicular to the NW extending along [110], so that [110] SiNW and [110] GeNW both are direct band gap structure semiconductors, due to that silicon can

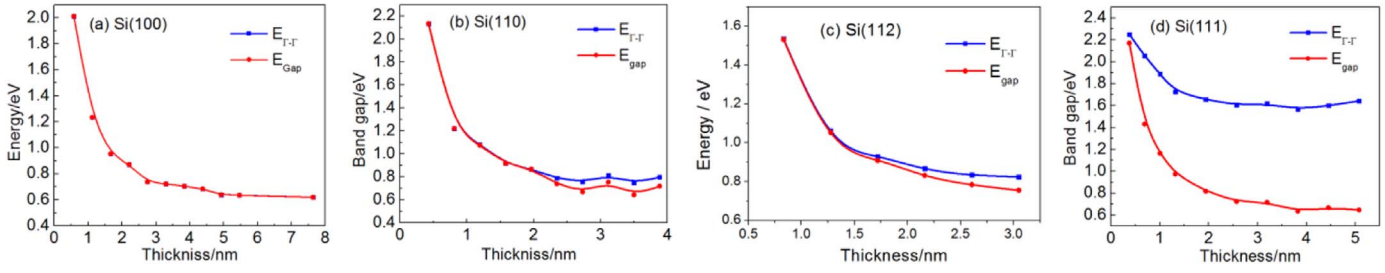

Fig. 2. The energy level of Γ point ($E_{\Gamma\text{-}\Gamma}$) in conduction band and CBM (E_{gap}) of (a) Si (100), (b) Si (110), (c) Si (112) and (d) Si (111) nanofilms changing with the increasing thickness of films.