Electronic structures of [1 1 1]-oriented free-standing InAs and InP nanowires

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Abstract
We report on a theoretical study of the electronic structures of the [1 1 1]-oriented, free-standing, zincblende InAs and InP nanowires with hexagonal cross sections by means of an atomistic $sp^3s^*$, spin–orbit interaction included, nearest-neighbor, tight-binding method. The band structures and the band state wave functions of these nanowires are calculated and the symmetry properties of the bands and band states are analyzed based on the $C_3$v double point group. It is shown that all bands of these nanowires are doubly degenerate at the $\Gamma$-point and some of these bands will split into non-degenerate bands when the wave vector $k$ moves away from the $\Gamma$-point as a manifestation of spin-splitting due to spin–orbit interaction. It is also shown that the lower conduction bands of these nanowires all show simple parabolic dispersion relations, while the top valence bands show complex dispersion relations and band crossings. The band state wave functions are presented by the spatial probability distributions and it is found that all the band states show $2\pi/3$-rotation symmetric probability distributions. The effects of quantum confinement on the band structures of the [1 1 1]-oriented InAs and InP nanowires are also examined and an empirical formula for the description of quantization energies of the lowest conduction band and the highest valence band is presented. The formula can simply be used to estimate the enhancement of the band gaps of the nanowires at different sizes as a result of quantum confinement.

Keywords: semiconductor nanowire, band structure, InAs, InP, spin–orbit interaction, tight-binding method

(Some figures may appear in colour only in the online journal)
these nanowires are in the range of a few nanometers to about one hundred nanometers.

Previously, the electronic structures have been studied for the InAs and InP nanowires oriented along a (100) crystallographic direction [39]. In this paper, we report on a theoretical study of the electronic structure of InAs and InP nanowires oriented along the [1 1 1] crystallographic directions. In comparison with an InAs or InP nanowire oriented along a (100) direction, unit cells in a nanowire of similar size oriented along the [1 1 1] direction are much larger and the computation for the electronic structure is much more demanding. An sp$^3s^*$ nearest-neighbor, spin–orbit interaction included, tight-binding formalism is employed in the calculation for the band structures and wave functions of the [1 1 1]-oriented InAs and InP nanowires. We show that although the lowest conduction bands of these nanowires display good parabolic dispersions, the top valence bands exhibit complex structures. Furthermore, all the band states at the $\Gamma$-point are doubly degenerate. Some of them will however split into non-degenerate bands when the wave vector $k$ moves away from the $\Gamma$-point. In addition, the wave functions of the band states of the InAs and InP nanowires show characteristic patterns with symmetries as described by the irreducible representations of the $C_{3v}$, double point group and could in general not be reproduced by the calculations based on simple one-band effective mass theory.

The rest of the paper is organized as follows. In section 2, a brief description for the calculation method is presented. Section 3 is devoted to the description and discussion of the calculated electronic structures of the [1 1 1]-oriented InAs and InP nanowires with hexagonal cross sections of different sizes. Finally, the paper is summarized in section 4.

2. Method of calculations

Theoretical methods, such as first-principles methods [27–30], the $k \cdot p$ method [31–33], pseudopotential methods [34] and tight-binding methods [35–43], have been employed for the study of semiconductor nanowires. Among them, tight-binding methods are empirical, atomistic approaches which take into account the lattice structures of materials and can accurately describe the band structures of the systems with only a minimal number of empirical parameters. Thus, in comparison with other methods, tight-binding methods formed in an sp$^3$, sp$^3s^*$, or sp$^3d^*$ basis [46–49] have been proved to be more powerful for the calculations of the electronic structures of semiconductor nanowires with diameters in the range of a few nanometers to more than 100 nanometers over the entire Brillouin zone.

Here, we employ the sp$^3s^*$ nearest-neighbor, spin–orbit interaction included, tight-binding formalism in the calculations for the electronic structures of the [1 1 1]-oriented InAs and InP zincblende nanowires. In the tight-binding formalism, Bloch sums of the form [47, 51]

$$|\alpha, \nu, k\rangle = \frac{1}{\sqrt[3]{N}} \sum_R e^{ik \cdot R_e}|\alpha, R_e\rangle,$$

(1)

are used as a basis, where $|\alpha, R_e\rangle$ stands for an atomic orbital $\alpha$ at position $R_e$, $N$ is the number of lattice sites. In the sp$^3s^*$ nearest-neighbor, spin–orbit interaction included, tight-binding formalism, the atomic orbitals are chosen as 10 localized, spin-dependent orbitals. In the basis of the Bloch sums, the Hamiltonian $\mathbf{H}$ can be written in a matrix form with matrix elements given by

$$H_{\alpha\nu, R}(k) = \sum_{R'} e^{-ik \cdot R_{e'}}\langle \alpha, R_e | H | \beta, R_{e'} \rangle,$$

(2)

and the eigenfunctions in a form of

$$|n, k\rangle = \sum_{\alpha, \nu} c_{n, \alpha, \nu}|\alpha, \nu, k\rangle.$$

(3)

In the nanowire geometry, only the translational symmetry along the growth direction is preserved and an unit cell in a nanowire with a large lateral size (>10nm) consists of an extremely large number of atoms and the resulting Hamiltonian matrix becomes too large in size to be solved by a standard diagonalization procedure. For example, for a [1 1 1]-oriented nanowire with a lateral size of $d = 30$ nm, there are more than 30 000 atoms in a unit cell and the corresponding Hamiltonian matrix size is in the order of $300 000 \times 300 000$ or larger. In this work, the Lanczos algorithm [52] is employed to solve for the eigenvalues and eigenvectors of equation (2).

Figure 1 displays an atomistic model structure of the considered InAs and InP nanowire systems. These nanowires are zincblende crystals oriented along the [1 1 1] crystallographic direction and have a hexagonal cross section and {1 1 0} facets. The period of unit cells in a nanowire is $\sqrt[3]{3} a$ and the Brillouin zone is defined in $-\pi/(\sqrt[3]{3} a) \leq k \leq \pi/(\sqrt[3]{3} a)$, where $a$ is the lattice constant of the corresponding bulk material. The lateral size of these nanowires is defined as the distance $d$ between two most remote corners in the hexagonal cross section as shown in figure 1(a). In an atomistic model, $d$ takes
discrete values of \( d = \frac{2n\alpha}{\sqrt{3}} \), where \( n \) is a positive integer number. The dangling bonds at the surface of the nanowires are passivated using hydrogen atoms to eliminate the effects of these dangling bonds on the band states near the fundamental band gaps. In the calculations, the InAs and InP tight-binding parameters are taken from [50] and the parameters involving the passivation hydrogen atoms are determined by the procedure presented in [44] and [45]. For further details about the method of calculations, we refer to [38] and [40].

3. Results and discussion

In this section, we present the results of calculations for the band structures and wave functions of the [1 1 1]-oriented InAs and InP nanowires with hexagonal cross sections. These nanowires are symmetric under the operations of the \( C_{3v} \) point group (with its rotational axis along the nanowire axis). The corresponding double point group has one two-dimensional irreducible representation \( \Gamma_4 \) and two one-dimensional irreducible representations \( \Gamma_5 \) and \( \Gamma_6 \) [53–55]. However, at the \( \Gamma \) point, all the band states are doubly degenerate due to the Kramers’ degeneracy. When the wave vector \( k \) moves away form the \( \Gamma \) point, the band structure Hamiltonian does not possess time-reversal symmetry and the \( \Gamma_5 \) and \( \Gamma_6 \) bands would split into nondegenerate bands. However, the \( \Gamma_4 \) bands will remain doubly degenerate at all wave vector points.

3.1. Band structures

We first present the calculated band structures of the [1 1 1]-oriented InAs and InP nanowires. Figure 2 shows the calculated band structures of the [1 1 1]-oriented InAs nanowires with hexagonal cross sections of size \( d = 12.4 \) nm ((a) and (b)), \( d = 24.7 \) nm ((c) and (d)), and \( d = 37.1 \) nm ((e) and (f)). The bands are labeled according to the irreducible representations, \( \Gamma_4 \), \( \Gamma_5 \) and \( \Gamma_6 \) of the \( C_{3v} \) double point group. Here we note that all bands are doubly degenerate at \( k = 0 \) (the \( \Gamma \)-point). In the figure, labels \( \Gamma_5 \) and \( \Gamma_6 \) are ordered in such a way that the first one labels a band that initially has the lower energy after splitting as the wave vector moves away from the \( \Gamma \)-point.

Figure 2. Band structures of the [1 1 1]-oriented InAs nanowires with hexagonal cross sections of lateral sizes \( d = 12.4 \) nm ((a) and (b)), \( d = 24.7 \) nm ((c) and (d)), and \( d = 37.1 \) nm ((e) and (f)). The bands are labeled according to the irreducible representations, \( \Gamma_4 \), \( \Gamma_5 \) and \( \Gamma_6 \) of the \( C_{3v} \) double point group. Here we note that all bands are doubly degenerate at \( k = 0 \) (the \( \Gamma \)-point). In the figure, labels \( \Gamma_5 \) and \( \Gamma_6 \) are ordered in such a way that the first one labels a band that initially has the lower energy after splitting as the wave vector moves away from the \( \Gamma \)-point.
In detail, it is seen in figures 2(a), (c) and (e) that the lowest and the second lowest conduction bands of a [111]-oriented InAs nanowire with a hexagonal cross section are all \( \Gamma \) symmetric and thus doubly degenerate, and the next two lowest conduction bands are \( \Gamma_5 \) and \( \Gamma_6 \) bands, which are in general non-degenerate bands except for at the \( \Gamma \)-point. However, it is seen that the second lowest conduction band and the \( \Gamma_5 \) and \( \Gamma_6 \) bands are very close in energy and they tend to the formation of a nearly four-fold degenerate band as the nanowire lateral size is increased. The next two lowest conduction bands are again \( \Gamma_5 \) and \( \Gamma_6 \) bands. These two bands are close in energy to the next lowest \( \Gamma \) band to form another nearly four-fold degenerate band. Figures 2(b), (d) and (f) show that the two highest valence bands of the [111]-oriented InAs nanowire with a hexagonal cross section are \( \Gamma_4 \) symmetric, doubly degenerate bands. The next two highest valence bands are a \( \Gamma_5 \) and a \( \Gamma_6 \) band whose states are, in general, non-degenerate, but very close in energy, except for at the \( \Gamma \) point at which the two band states are exactly degenerate due to the presence of time reversal symmetry in the Hamiltonian. The next two highest valence bands of the [111]-oriented nanowires are again the \( \Gamma_5 \) and \( \Gamma_6 \) bands with degenerate or nearly degenerate energies. At a large nanowire lateral size (see the cases for \( d = 24.7 \) and 37.1 nm), these two bands are very close to the next highest \( \Gamma_4 \) valence band in energy, leading to the formation of a nearly four-fold nearly degenerate valence band.

Figure 3 shows the band structures of the [111]-oriented InP nanowires with hexagonal cross sections of lateral size \( d = 12.0 \) nm ((a) and (b)), \( d = 24.0 \) nm ((c) and (d)), and \( d = 36.0 \) nm ((e) and (f)). The bands are labeled according to the irreducible representations, \( \Gamma_4 \), \( \Gamma_5 \) and \( \Gamma_6 \) of the \( C_3v \) double point group. Here we note that all bands are doubly degenerate at \( k = 0 \) (the \( \Gamma \)-point). In the figure, labels \( \Gamma_4 \) and \( \Gamma_5 \) are ordered in such a way that the first one labels a band that initially has the lower energy after splitting as the wave vector moves away from the \( \Gamma \) point.

![Figure 3](image)

Figure 3. Band structures of the [111]-oriented InP nanowires with hexagonal cross sections of lateral size \( d = 12.0 \) nm ((a) and (b)), \( d = 24.0 \) nm ((c) and (d)), and \( d = 36.0 \) nm ((e) and (f)). The bands are labeled according to the irreducible representations, \( \Gamma_4 \), \( \Gamma_5 \) and \( \Gamma_6 \) of the \( C_3v \) double point group. Here we note that all bands are doubly degenerate at \( k = 0 \) (the \( \Gamma \)-point). In the figure, labels \( \Gamma_4 \) and \( \Gamma_5 \) are ordered in such a way that the first one labels a band that initially has the lower energy after splitting as the wave vector moves away from the \( \Gamma \) point.

In particular, all the low-energy conduction bands show simple parabolic dispersion structures and the top valence bands show complex dispersive, band-crossing characteristics. It is also seen that the symmetry ordering of the bands at the \( \Gamma \)-point remain the same as in the [111]-oriented InAs nanowires. However, some differences can be identified. In particular, as can be seen in figure 3, the second lowest conduction band (\( \Gamma_4 \) band) and the third and fourth lowest conduction bands (\( \Gamma_5 \) and \( \Gamma_6 \) bands) of the [111]-oriented InP nanowires become hardly distinguishable, forming a nearly four-fold degenerate conduction band, even at a small lateral size. For example, the energy separation between these bands at the \( \Gamma \)-point is about 0.3 meV in the InP nanowire with size \( d = 12 \) nm and is only about 0.01 meV in the InP nanowire with size \( d = 36 \) nm. The next lowest \( \Gamma_4 \), \( \Gamma_5 \) and \( \Gamma_6 \) conduction bands are also hardly distinguishable in energy and form a nearly four-fold degenerate conduction band already at a small nanowire lateral size. Overall, we see in figure 3 that all the \( \Gamma_4 \) and \( \Gamma_5 \) bands in the [111]-oriented InP nanowires are paired up to form nearly doubly degenerate bands.

As we mentioned above, the conduction bands and the valence bands move apart in energy as the cross section sizes of the [111]-oriented InAs and InP nanowires are decreased as a result of quantum confinement. It is found that the calculated edge energies of the lowest conduction bands and the topmost valence bands, \( E_c(d) \) and \( E_v(d) \), of the [111]-oriented InAs and InP nanowires with different lateral sizes \( d \) can be fitted to the following expression,
\[ \Delta E_{\alpha}(d) = E_{\alpha}(d) - E_{\alpha}(\infty) = \frac{1}{p_1d^2 + p_2d + p_3}, \]  

where \( \alpha = c \) or \( v \), \( E_{\alpha}(\infty) \) and \( E_{\alpha}(\infty) \) are the energies at the bottom of the conduction band and the top of valence band of the bulk materials, \( \Delta E_c \) and \( \Delta E_v \) stand for the energy shifts in the bottom conduction band and the top valence band due to quantum confinement, and \( p_1, p_2 \) and \( p_3 \) are fitting parameters. The results of fitting are shown in figure 4 with the obtained fitting parameters listed in table 1. It is seen that the effect of quantum confinement on the conduction band of the InAs nanowires is stronger than that of InP nanowires, consistent with the fact of InAs has a smaller electron effective mass. For example, the quantum confinement energy of electrons at the conduction band edge of the [1 1 1]-oriented InAs nanowire with a hexagonal cross section of size \( d \sim 22 \) nm is \( \sim 60 \) meV and the corresponding quantum confinement energy in the [1 1 1]-oriented InP nanowire of the same lateral size is \( \sim 24 \) meV. When the InAs nanowire has a lateral size of \( d \sim 38 \) nm, the electron quantization energy at the conduction band edge can still be \( \sim 24 \) meV. In comparison, for the InP nanowire with size \( d \sim 38 \) nm, the electron quantization energy at the conduction band edge is only \( \sim 8 \) meV. The quantum confinement energies of holes in the valence bands are, in general, very small when compared with the corresponding quantum confinement energies of electrons at the conduction bands of the nanowires. For example, the quantum confinement energies are only \( \sim 8 \) meV and \( \sim 6 \) meV at the valence bands of the InAs and InP nanowires with a lateral size \( d \sim 22 \) nm, respectively. As the lateral size \( d \) is increased to \( \sim 38 \) nm, the quantum confinement energies of holes in

![Figure 4](image-url)
spin-degenerate states, since the other one has an identical spatial probability distribution.

Figures 5 and 6 show the calculated wave functions for the five lowest conduction band states and the five highest valence band states at the \( \Gamma \)-point of a [1 1 1]-oriented InAs nanowire with a hexagonal cross section of size \( d = 12.4 \) nm. The wave functions are presented by the probability distributions on a (1 1 1)-plane of In atoms whose value at each atomic site is calculated by summing up the squared amplitudes of all the atomic orbital components on the atomic site and is normalized within each panel by the highest value found in the panel. Panels (a)–(e) show the wave functions of the five lowest conduction band states at the \( \Gamma \)-point, while panels (f)–(j) show the wave functions of the five highest valence band states at the \( \Gamma \)-point.

Figure 5. Wave functions of the five lowest conduction band states and the five highest valence band states at the \( \Gamma \)-point of the [1 1 1]-oriented InAs nanowire with a hexagonal cross section of size \( d = 12.4 \) nm. The wave functions are presented by the probability distributions on a (1 1 1)-plane of In atoms whose value at each atomic site is calculated by summing up the squared amplitudes of all the atomic orbital components on the atomic site and is normalized within each panel by the highest value found in the panel. Panels (a)–(e) show the wave functions of the five lowest conduction band states at the \( \Gamma \)-point, while panels (f)–(j) show the wave functions of the five highest valence band states at the \( \Gamma \)-point.

Figure 6. The same as in figure 5 but for the [1 1 1]-oriented InAs nanowire with a hexagonal cross section of size \( d = 37.1 \) nm.

The other four lowest conduction band states in each nanowire all show donut-shaped probability distributions. These four conduction band states can be grouped into two groups based on their spatial localizations. The second lowest conduction band state (a \( \Gamma_2 \)-symmetric state) and the third lowest conduction band state (a \( \Gamma_5 \)- or a \( \Gamma_6 \)-symmetric state) are in one group and their wave functions are more localized around the center of the nanowire. The fourth lowest conduction band state (again a \( \Gamma_2 \)- or a \( \Gamma_6 \)-symmetric state) and the fifth lowest conduction band state (a \( \Gamma_7 \)-symmetric state) comprise the second group and their wave functions are less localized to the center region of the nanowire and are clearly of a hexagonal shape with six high probability regions localized at the six hexagonal corners.
The wave functions of the valence band states at the Γ-point of the two InAs nanowires with different sizes also show similar spatial distribution characteristics. Nevertheless, the distribution patterns of these valence band states are more complex than their conduction band counterparts. Furthermore, it is interesting to see that the probability distribution of the highest valence band state (a $\Gamma_4$-symmetric state) of a [1 1 1]-oriented InAs nanowire is shaped as a donut with a $2\pi/3$-rotational symmetry, while the second highest valence band state (also a $\Gamma_4$-symmetric state) is a strongly localized, $s$-like state. The third highest valence band state (a $\Gamma_5$- or a $\Gamma_6$-symmetric state) is also a state more localized inside the nanowire with its distribution pattern consisting of a small triangular region of high probability distribution in the center and a region of low but complex probability distribution close to the surface of the nanowire. The fourth highest valence band state (again a $\Gamma_5$- or a $\Gamma_6$-symmetric state) exhibits a donut-shaped probability distribution and is much more localized inside the nanowire when compared with the second-fifth lowest conduction band states. The fifth highest valence band state (a $\Gamma_4$-symmetric state) exhibits a pattern of probability distribution consisting of a highly symmetric region strongly localized in the center of the nanowire and a ring-like region localized in the middle between the center and the surface of the nanowire.

Figures 7 and 8 show the calculated wave functions for the five lowest conduction band states and the five highest valence band states at the Γ-point of the [1 1 1]-oriented InP nanowires with size $d = 12.0\,\text{nm}$ ($n = 25$) and size $d = 36.0\,\text{nm}$ ($n = 75$), respectively. It is seen that the wave functions of the five lowest conduction band states of the InP nanowires have the same spatial probability distribution characteristics as the
InAs nanowires. The same is true for the wave functions of the five highest valence band states of the InP nanowires, except for a minor difference, i.e. the ordering of the probability distribution patterns of the two highest valence band states (two \(\Gamma_4\)-symmetric states) at the \(\Gamma\)-point of the InP nanowire with the smaller size \(d = 12.0\) nm is reversed when compared to the InAs nanowire with size \(d = 12.4\) nm.

4. Conclusions

In summary, we present a theoretical study of the electronic structures of the [1 1 1]-oriented, free-standing, zincblende InAs and InP nanowires with hexagonal cross sections by means of the atomistic \(sp^3s^*\) tight-binding method. The band structures and the band state wave functions of these nanowires are calculated and the symmetry properties of the bands and band states are analyzed based on the \(C_3\) double point group. It is shown that all bands of these nanowires are doubly degenerate at the \(\Gamma\)-point and some of these bands will split into non-degenerate bands when the wave vector \(k\) moves away from the \(\Gamma\)-point as a manifestation of spin–splitting due to spin–orbit interaction. It is also shown that the lower conduction bands of these nanowires all show simple parabolic dispersion relations, while the top valence bands show complex dispersion relations and band crossings. The appearance of the band crossings in the top valence bands of the [1 1 1]-oriented InAs and InP nanowires is in strong contrast to the band structures of the [1 0 0]-oriented InAs and InP nanowires with square cross sections in which the top valence bands are seen to go for anti-crossings. The wave functions of the band states of these [1 1 1]-oriented InAs and InP nanowires are presented by probability distributions on cross sections. It is found that all the band states show \(2\pi/3\)-rotation symmetric probability distributions and two degenerate band states at the \(\Gamma\)-point show identical spatial probability distributions. Finally, the effects of quantum confinement on the band structures of the [1 1 1]-oriented InAs and InP nanowires are examined and an empirical formula for the description of quantization energies of the lowest conduction band and the highest valence band is presented. The formula can simply be used to estimate the enhancement of the band gaps of the nanowires at different sizes as a result of quantum confinement. We believe that the results presented in this work will provide important information about the electronic structures of the [1 1 1]-oriented InAs and InP nanowires and useful guidance for the use of these nanowires in novel nano electronic, optoelectronic and quantum devices.

Acknowledgments

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References

[1] Hang Q L, Wang F D, Carpenter P D, Zemlyanov D, Zakharov D, Stach E A, Buhro W E and Janes D B 2008 Nano Lett. 8 49
[2] Dayeh S A, Aplin D P R, Zhou X T, Yu P K L, Yu E T and Wang D L 2007 Small 3 326
[3] Nilsson H A, Caroff P, Thelannder C, Lind E, Karlström O and Wernersson L-E 2010 Appl. Phys. Lett. 96 153505
[4] Li Q, Huang S, Pan D, Wang J, Zhao J and Xu H Q 2014 Appl. Phys. Lett. 105 113106
[5] Wang J F, Gudiksen M S, Duan X F, Cui Y and Lieber C M 2001 Science 293 1455
[6] Duan X, Huang Y, Cui Y, Wang J and Lieber C M 2001 Nature 409 66
[7] Wallentin J et al 2013 Science 339 1057
[8] Anttu N, Abgrand A, Asoli D, Heurlin M, Åberg I, Samuelson L and Borgström M 2014 Nano Res. 7 816
[9] Cui Y et al 2013 Nano Lett. 13 4113
[10] Anttu N and Xu H Q 2010 J. Nanosci. Nanotechnol. 10 7183
[11] Boxborg F, Sondergaard N and Xu H Q 2010 Nano Lett. 10 1108
[12] Boxborg F, Sondergaard N and Xu H Q 2012 Adv. Mater. 24 4692
[13] Joyce H J et al 2012 Nano Lett. 12 5325
[14] Jiang X, Xiong Q, Nam S, Qian F, Li Y and Lieber C M 2007 Nano Lett. 7 3214
[15] Mohan P, Motohisa J and Fukui T 2006 Appl. Phys. Lett. 88 133105
[16] Pitanti A, Ercolani D, Sorba L, Roddaro S, Belltram F, Nasi L, Salvianti G and Tredicucci A 2011 Phys. Rev. X 1 011006
[17] Nishio T, Kozakai T, Amaha S, Larsson M, Nilsson H A, Xu H Q, Zhang G, Tateno K, Takayanagi H and Ishibashi K 2011 Nanotechnology 22 445701
[18] Abay S, Nilsson H, Wu F, Xu H Q, Wilson C M and Delsing P 2012 Nano Lett. 12 5622
[19] Abay S, Persson D, Nilsson H, Xu H Q, Fogelström M, Shumeiko V and Delsing P 2013 Nano Lett. 13 3614
[20] Abay S, Persson D, Nilsson H, Wu F, Xu H Q, Fogelström M, Shumeiko V and Delsing P 2014 Phys. Rev. B 89 214508
[21] Mourik V, Zuo K, Frolov S M, Plissard S R, Bakkers E and Kouwenhoven L P 2012 Science. 336 1003
[22] Deng M T, Yu C L, Huang G Y, Larsson M, Caroff P and Xu H Q 2012 Nano Lett. 12 6414
[23] Churchill H O H, Fatemi V, Grove-Rasmussen K, Deng M T, Caroff P, Xu H Q and Marcus C M 2013 Phys. Rev. B 87 241401
[24] Deng M T, Yu C L, Huang G Y, Larsson M, Caroff P and Xu H Q 2014 Sci. Rep. 4 4761
[25] Lee E J H, Jiang X C, Aguado R, Katsaros G, Lieber C M and De Franceschi S 2012 Phys. Rev. Lett. 109 186802
[26] Das A, Ronen Y, Most Y, Oreg Y, Heiblum M and Shtrikman H 2012 Nat. Phys. 8 887
[27] Cahangirov S and Ciraci S 2009 Phys. Rev. B 79 165118
[28] Ning F, Tang L-M, Zhang Y and Chen K-Q 2013 J. Appl. Phys. 114 224304
[29] Ning F, Wang D, Tang L-M, Zhang Y and Chen K-Q 2014 J. Appl. Phys. 116 094308
[30] Ning F, Tang L M, Zhang Y and Chen K Q 2015 Sci. Rep. 5 10813
[31] Lassen B, Willatzen M, Melnik R and Lew L C 2006 J. Mater. Res. 21 2927
[32] Ravi V, Cukaric N, Partoens B, Tadić M and Peeters F M 2012 J. Phys.: Condens. Matter 24 135302
[33] Ravi V, Partoens B and Peeters F M 2012 Phys. Rev. B 86 165439
[34] Wang L-W, Kim J and Zunger A 1999 Phys. Rev. B 59 5678
[35] Persson M P and Xu H Q 2002 Appl. Phys. Lett. 81 1309
[36] Persson M P and Xu H Q 2004 Phys. Rev. B 70 161310
[37] Persson M P and Xu H Q 2004 *Nano Lett.* 4 2409
[38] Persson M P and Xu H Q 2006 *Phys. Rev.* B 73 035328
[39] Persson M P and Xu H Q 2006 *Phys. Rev.* B 73 125346
[40] Liao G H, Luo N, Yang Z H, Chen K Q and Xu H Q 2015 *J. Appl. Phys.* 118 094308
[41] Niquet Y M, Lherbier A, Quang N H, Fernández-Serra M V, Blase X and Delerue C 2006 *Phys. Rev.* B 73 165319
[42] Niquet Y M 2006 *Phys. Rev.* B 74 155304
[43] Lind E, Persson M P, Niquet Y-M and Wernersson L-E 2009 *IEEE Trans. Electron Dev.* 56 201
[44] Xu H Q and Lindefelt U 1990 *Phys. Rev.* B 41 5979
[45] Xu H Q 1992 *Phys. Rev.* B 46 1403
[46] Chadi D and Cohen M L 1975 *Phys. Status Solidi B* 68 405
[47] Vogl P, Hjalmarsen H P and Dow J D 1983 *J. Phys. Chem. Solids* 44 365
[48] Jancu J-M, Scholz R, Beltram F and Bassani F 1998 *Phys. Rev.* B 57 6493
[49] Boykin T B, Klimeck G and Oyafuso F 2004 *Phys. Rev.* B 69 115201
[50] Klimech G, Bowen R C, Boykin T B and Cwik T A 2000 *Superlattices Microstruct.* 27 519
[51] Di Carlo A 2003 *Semicond. Sci. Technol.* 18 R1
[52] Golub G H and Van Loan C F 1996 *Matrix Computations* 3rd edn (Baltimore, MD: Johns Hopkins University Press)
[53] Tinkham M 2003 *Group Theory and Quantum Mechanics* (New York: Dover)
[54] Lax M 2001 *Symmetry Principles in Solid State and Molecular Physics* (New York: Dover)
[55] Yu P Y and Cardona M 2010 *Fundamentals of Semiconductors* 4th edn (New York: Springer)