Band Structure Calculation of Si and Ge by Non-Local Empirical Pseudo-Potential Technique

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Abstract In this paper, the principle of spatial nonlocal empirical pseudopotential and its detailed calculation procedure is presented. Consequently, this technique is employed to calculate the band structures of Silicon and Germanium. By comparing the results with photoemission experimental data, the validity and accuracy of this calculation are fully conformed for valence or conductance band, respectively. Thus it can be concluded that the spin-orbit Hamiltonian will only affect the energy band gap and another conductance or valence band structure. Therefore, this nonlocal approach without spin-orbit part is adequate for the device simulation of only one carrier transport such as metal oxide semiconductor field effect transistors (MOSFET)'s, and it can significantly reduce the complication of band structure calculation.

Key words band structure; pseudo-potential; brillouin zone; Silicon; Germanium

As the advance of modern microelectronics and optical-electronics, it is necessary to account for the accurate band structure for modeling scattering rate, density of state and other solid state characteristics which are essential for simulating the transport characteristics of semiconductor materials and nano-scaled devices[1,2]. The band structure of semiconductors may be obtained by using a variety of methods, known as tight-binding, kp, local and non-local pseudopotentials, etc. For semiconductors, it is necessary to adopt pseudopotential method to calculate their band structures for which is suitable for the simulation of carrier transport characteristics[3]. Although the nonlocal pseudopotential calculation of band structure can get the accurate results, it is complicate for the spin-orbit consideration[3-5]. In this paper, the detailed steps to solve a band structure problem with the nonlocal empirical pseudopotential approach are reviewed and this technique is applied to solve the Si and Ge band structure eigenvalues corresponding to valence and conduction band. After comparing the results with existing photoemission experimental data, the validity and accuracy of this calculation is fully conformed, thus it can be concluded that this nonlocal approach without spin-orbit part is adequate for the device simulation of only one carrier transport such as MOSFET’s, and it can reduce the CPU cost of band structure calculation significantly.

1 Principle

The pseudopotential method assume a “reasonable form” of the potential due to the atom from nucleus up to core electrons. The band structure of crystal can be obtained by solving the Schrödinger equation to obtain the allowed values of energy $E$ for a given value of wave vector $k$ for the valence electrons.

$$\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V(r)\psi(r) = E\psi(r)$$

and pseudopotential hamiltonian $H$ is defined as

$$H = \frac{\hbar^2}{2m^*} \nabla^2 + V(r)$$

where $m^*$ is an effective mass. According to Block’s theorem, the wavefunction and potential $V(r)$ are periodic with lattice, they can be expanded in terms of reciprocal lattice vectors as follows

$$\psi(r) = e^{ikr} u_i(r)$$

and

$$u_i(r) = \sum A_g e^{G r}$$

where $u_i(r)$ is a periodic function with the lattice, $A_g$ is the expansion parameter and $G$ are reciprocal lattice vectors.

The potential $V(r)$ is then expanded in reciprocal...
lattice vectors by using Fourier transform.

\[ V(r) = \sum_\text{G} V_\text{v}(\text{G}) e^{i r \cdot \text{G}} \]  

(5)

\[ V_\text{v}(\text{G}) = \frac{1}{\Omega_\text{G}} \int e^{i r \cdot \text{G}} V(r) dr \]  

(6)

where \( \Omega_\text{G} \) is the atomic volume. For convenience it can be expressed in terms of symmetric part \( V^+ (\text{G}) \) and anti-symmetric part \( V^- (\text{G}) \) [3]:

\[ V(r) = \sum_\text{G} \left[ V^+ (\text{G}) \cos (\text{G} \cdot \tau) + i V^- (\text{G}) \sin (\text{G} \cdot \tau) \right] \times \exp (-j \text{G} \cdot r) \]  

(7)

where \( \tau = 0.125a(1,1,1) \), \( a \) is the lattice constant. For diamond structure semiconductors, the anti-symmetric form factors \( V^- (\text{G}) \) are zero. The above series usually converges rapidly enough so that only several form factors are needed for each atom.

In order to accurately calculate the band structure, the energy dependent nonlocal and spin-orbit part of hamiltonian should be accounted for. The nonlocal angular momentum dependent pseudopotential is expressed as [4,5]

\[ V_{\text{nl}}(r, E) = \sum_j A_j(E) f_j(r) \hat{P}_j \]  

(9)

where \( A_j(E) \) is the energy dependent well depth, \( \hat{P}_j \) denoting the angular momentum projector. The nonlocal part of the atomic potential with \( l \) symmetry \( f_j(r) \) is written as

\[ f_j(r) = \begin{cases} \Theta(r - R_l) & \text{in Si} \\ \exp (-r^2/R_l^2) & \text{in Ge} \end{cases} \]  

where \( r \) is the absolute value of \( r \). According to Ref. [3], the core form factor \( f_j(r) \) is represented by a Heaviside step function \( \Theta(x) = 1 \) for \( x \geq 0 \) and 0 otherwise) in Si and by a Gaussian function in Ge. For Si only \( l = 0 \) contribution whereas for Ge only \( l = 2 \) contribution is include explicitly in the above equation.

The spin-orbit hamiltonian is much more complicated and not listed here. Then, the energy eigenvalues and eigenvectors are found by solving the secular equation

\[ \det [H_{\text{kk}}(k) - E(k) \delta_{\text{kk}}] = 0 \]  

(11)

where \( k \) is the wave vector in the first brillouin zone and \( K = k + G, \ K' = k + G' \), \( G' \) is also the reciprocal lattice vector.

2 Methods of Calculation

As mentioned in above section, the matrix element of spatial part of the hamiltonian is given as [6]

\[ H_{\text{kk}} = \frac{\hbar^2}{2m} K_j^2 \delta_{\text{kk}} + \left[ V^+(k - K') + V^- (k, K') \right] \times \cos [(k - K') \cdot \tau] \]  

(12)

and the nonlocal part is expressed as

\[ V^- (k, K') = \frac{4\pi}{\Omega_k} \sum_{l=0,2} A_l(2l+1) P_l(\cos \theta_{kk'}) F_l (k, K') \]  

(13)

where \( P_l(x) \) is the Legendre polynomials, and \( \theta_{kk'} \) denote the angle between \( K \) and \( K' \). \( A_l \) are parameters.

\[ F_l (k, K') = \int_{-1}^1 j_l(kr) j_l(k'r) j_l(k'R) dr \]  

(14)

where \( j_l(x) \) is the sphere Bessel function.

Transform the sphere Bessel function to ordinary Bessel function \( J_l(x) \) as follows

\[ j_l(x) = \sqrt{\frac{\pi}{2x}} J_{l + \frac{1}{2}}(x) \]  

(15)

and use the following equation for the integrals of Bessel functions [7]

\[ \int_0^\infty t \exp(-p^2 t^2) J_l(at) J_m(bt) dt = \frac{1}{2p^2} \exp\left(-\frac{a^2 + b^2}{4p^2}\right) I_m\left(\frac{ab}{2p}\right) \]  

(16)

and expand the modified Bessel functions of the first kind \( I_n(x) \) as

\[ I_n(x) = \text{exp}(x) \sum_{m=0}^\infty \frac{x^{n+2m}}{2^{n+2m} n! (m+n+1)} \]  

(17)

Then the computing procedure for Eq.(14) can be given as

\[ F_l (k, K') = \frac{\pi R^2}{4\sqrt{KK'}} \exp\left(-\frac{R^2}{4(K^2 + K'^2)}\right) \times \sum_{n=0}^\infty \frac{(KK')^2 / 2^{m+2n}}{2^{m+2n} n! (m+n+1)} \]  

(18)

where \( K \) and \( K' \) are the absolute values of \( K \) and \( K' \). Thus the way to calculate the nonlocal hamiltonian part in Eq.(13) is obtained.

3 Results and Discussions

In this work, the above scalar equation is solved to get the eigenvalues in the 1/48 irreducible wedge of the first brillouin zone shown in Fig.1, by using the parameters listed in Tab.1. the outcome of the program
for the band structures is shown in Fig.2. The results of valence band are quite similar for Si and Ge from Fig.2, but conductance band structures of Si and Ge are completely different, there are 2 valleys for Si but 3 valleys for Ge.

Detailed comparisons of critical point energies calculated by this pseudopotential method and measured by photoemission experiments for Si and Ge are given in Tab.2\(^3\),\(^8\). Over all, the agreement is quite satisfactory for Si in both conductance and valence band and Ge in only conductance band. The chief difference resides in the valence band symmetry energy. The reason for this can be traced back to the nonlocal treatment of pseudopotential. Although the valence electron configuration of germanium and silicon are both \(s^2p^2\), significant difference exist for the core charge configuration, larger number of core electrons reflects the more effective spin-orbit effect for Ge. As a result, the band structure of Ge shows more metallic character and the spin-orbit term should be accounted for in order to get the accurate band structure. However, the spin-orbit Hamiltonian is much more complicate and costs much more CPU time comparing with the spatial nonlocal Hamiltonian calculation\(^6\). With this consideration, large numbers of calculation has been carried out, and we find this spatial nonlocal approach can accurately modeling the structure of conductance band or valence band separately for Ge by using different parameters, even it has the defect of imprecise whole band and energy gap calculation. Therefore, this simple pseudopotential approach can be used to modeling the conductance or valence band structure for the device simulation with only one kind of carriers, such as MOSFET.

Fig.3 shows the contour line of equal energy surface for the first conductance band of Si (a) and Ge (b) and the first valence band of Si (c) and Ge (d) corresponding to the \(k_x-k_y\) cross section shown in Fig.1. From Fig.3a and Fig.3b, we find that the \(X\) and even \(L\) valleys are elliptic for both Si and Ge, but there is another warp \(\Gamma\) valley for Ge and which make the transport characteristics of electron difficult to solve by a simple valley model. From Fig.3c and Fig.3d, it is found that these first valence band structures are quite similar, the difference of warping has a strong impact on the hole mobility.

<table>
<thead>
<tr>
<th>Material</th>
<th>Lattice constant /0.1 μm</th>
<th>Form factor ((\text{Ry}))</th>
<th>Nonlocal parameters</th>
</tr>
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<tr>
<td></td>
<td></td>
<td>(V^s(3))</td>
<td>(V^s(4))</td>
</tr>
<tr>
<td>Si</td>
<td>5.43</td>
<td>-0.2240</td>
<td>0</td>
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<tr>
<td>Ge</td>
<td>5.65</td>
<td>-0.2378</td>
<td>-0.1600</td>
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Fig.2  Band structures calculated by the spatial nonlocal empirical pseudopotential
Conclusions

In this paper, explicit formulas and detailed steps are presented to solve a band structure problem with the nonlocal empirical pseudopotential approach, this spatial nonlocal Hamiltonian is applied it to solve the Si and Ge band structure eigenvalues corresponding to valence and conduction band. The validity and accuracy of this calculation is fully conformed for

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<th>level</th>
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<th>Experiment</th>
<th>Ge</th>
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</tbody>
</table>

Fig.3 Contour line of equal energy surface corresponding to the kx-ky cross section shown in Fig.1

4 Conclusions

In this paper, explicit formulas and detailed steps are presented to solve a band structure problem with the nonlocal empirical pseudopotential approach, this spatial nonlocal Hamiltonian is applied it to solve the Si and Ge band structure eigenvalues corresponding to valence and conduction band. The validity and accuracy of this calculation is fully conformed for
valence or conductance band respectively by comparing the results with existing experimental data. Thus it can be concluded that the spin-orbit Hamiltonian will only affect the energy band gap and another conductance or valence band structure, and this spatial nonlocal approach is adequate for the device simulation of only one carrier transport such as MOSFET’s. In this case, it can significantly reduce the computational cost of band structure calculation.

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References


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