Modeling of tunneling current in ultrathin MOS structure with interface trap charge and fixed oxide charge*

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A model based on analysis of the self-consistent Poisson–Schrodinger equation is proposed to investigate the tunneling current of electrons in the inversion layer of a p-type metal-oxide-semiconductor (MOS) structure. In this model, the influences of interface trap charge (ITC) at the Si–SiO_2 interface and fixed oxide charge (FOC) in the oxide region are taken into account, and one-band effective mass approximation is used. The tunneling probability is obtained by employing the transfer matrix method. Further, the effects of in-plane momentum on the quantization in the electron motion perpendicular to the Si–SiO_2 interface of a MOS device are investigated. Theoretical simulation results indicate that both ITC and FOC have great influence on the tunneling current through a MOS structure when their densities are larger than 10^{12} cm^{-2}, which results from the great change of bound electrons near the Si–SiO_2 interface and the oxide region. Therefore, for real ultrathin MOS structures with ITC and FOC, this model can give a more accurate description for the tunneling current in the inversion layer.

Keywords: tunneling current, ultrathin oxide, interface trap charge, fixed oxide charge

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1. Introduction

As the scale of metal-oxide-semiconductor field effect transistors (MOSFET) quickly approaches the deep submicron regime, an ultrathin gate oxide becomes necessary for future MOSFET devices. However, for such ultrathin gate oxide, direct tunneling current will dominate the gate leakage and the off-state power dissipation of the transistor. Recent studies have shown that the tunneling current can be nearly 100% with a channel length smaller than 5 nm in double-gate silicon n-MOSFETs.[1] The increased tunneling current through thin gate oxide also hinders the extraction of transistor parameters by traditional techniques such as the capacitance–voltage (C–V) method. Therefore, an accurate modeling of tunneling current through the MOS structure is important in transistor technology development.

Tunneling current of conduction band electrons bounded in inversion layers has been extensively studied by solving the self-consistent Poisson–Schrodinger equation.[2–5] Recently, the effect of coupling of channel electrons has been introduced to calculate the tunneling current of electrons in n-MOS structure.[6,7] However, this theoretical model does not take into account electron distribution in energy sub-bands.[7] Interface traps and oxide charges are important parameters in devices. For example, they can alter the threshold voltage of a MOSFET and Si interface potential, and thereby change the reverse surface leakage current in a p–n junction, or alter the avalanche breakdown voltage of a p–n junction. They can invert the silicon, resulting in unwanted current paths between elements in an integrated circuit. Interface traps are defects that occur at the Si–SiO_2 interface, each of which has one or more energy levels within the Si bandgap. These defects can exchange charge with Si, and they can interact with Si conduction by capturing or emitting electrons, and with Si valence by capturing or emitting electrons holes. Fixed oxide charges are located not only at metal–oxide or Si–SiO_2 interfaces, but also deep in the oxide. They are associated with defects in SiO_2 such as impurities and broken bonds. Interface trap charges (ITCs) at the Si–SiO_2 interface and fixed oxide charge (FOC) in the oxide region have been extensively studied in experiments.[8–11] Although a two-dimensional (2D) full-band Monte Carlo simulator has been used to study the impact of interface roughness scattering on electron and hole transport properties in MOSFET's inversion layers,[12] little attention has been paid so far to apply ITC and FOC to model the electric characteristics of the MOS structure. Therefore, in a reliable physical model, ITC and FOC should be presented to evaluate the tunneling current of a real MOS structure. Among the existing models of electron tunneling, none takes ITC and FOC into account.

In this paper, we propose a tunneling electron model, in which the influences of ITC and FOC are taken into account, and we illustrate why the existing models can also provide a relatively accurate calculated result. Here, we use one-band effective mass approximation, which gives an accurate descrip-

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tion of electron tunneling in an inversion layer. The tunneling probability is computed by employing the transfer matrix method. Using this new method, theoretical simulation of the tunneling current for ultrathin MOS structure is closer to reality.

2. Theoretical model

In order to investigate electron tunneling in the inversion layer, p-Si/SiO_2/n^+-poly silicon structure is studied when positively biased gate voltage is applied. In Fig. 1, a schematic band diagram is shown for such a structure. The origin of the coordinate system is set at the oxide–semiconductor interface. Taking into account the conservation of the longitudinal momentum of the electron, the equation for such a MOS structure is given by[6,7]

$$\left[-\frac{\hbar^2}{2m_{\perp-\mathrm{Si}}}\frac{\partial^2}{\partial z^2}+V(z)\right]\psi(z)=E_{\perp-\mathrm{Si}}\psi(z), \tag{1}$$

$$\left\{-\frac{\hbar^2}{2m_{\mathrm{ox}}}\frac{\partial^2}{\partial z^2}+\left[V(z)-\frac{\hbar^2k_{\mathrm{r}}^2}{2m_{//-\mathrm{Si}}}\left(1-\frac{m_{//-\mathrm{Si}}}{m_{\mathrm{ox}}}\right)\right]\right\}\psi(z) = E_{\perp-\mathrm{Si}}\psi(z), \tag{2}$$

where $m_{\|-\mathrm{Si}}$ and $m_{\perp-\mathrm{Si}}$ are the longitudinal and transverse effective masses of channel electrons in the substrate region, respectively. The term $h^2k_{\mathrm{r}}^2/m_{\|-\mathrm{Si}}$ is the transverse energy of a channel electron in a plane parallel to the Si–SiO_2 interface. The $\psi(z)$ and $E_{\perp-\mathrm{Si}}$ are the electron wave function and the transverse energy, respectively. Furthermore, the electron wave function $\psi(z)$ in the region $(-t_{\mathrm{ox}} \le z \le L)$ must satisfy the following boundary condition:

$$\psi|_{z=-t_{\mathrm{ox}}}=0\psi|_{z=L}=0, \tag{3}$$

$$\frac{1}{m_{\perp-\mathrm{Si}}}\frac{\mathrm{d}\psi}{\mathrm{d}z}|_{z=0^+}=\frac{1}{m_{\mathrm{ox}}}\frac{\mathrm{d}\psi}{\mathrm{d}z}|_{z=0^-}. \tag{4}$$

The Poisson equation in the z direction is written as

$$\frac{\mathrm{d}^2V(z)}{\mathrm{d}z^2}=\frac{q^2}{\varepsilon_{\mathrm{Si}}}\left(p(z)-n(z)-N_{\mathrm{A}}\right), \tag{5}$$

$$\frac{\mathrm{d}^2V(z)}{\mathrm{d}z^2}=\frac{q^2}{\varepsilon_{\mathrm{Si}}}\left(N_{\mathrm{f}}\delta(z+t_{\mathrm{f}})-n(z)\right), \tag{6}$$

where $\varepsilon_{\mathrm{Si}}$ and $\varepsilon_{\mathrm{ox}}$ are the permittivity of Si and SiO_2, respectively, $n(z)$ is the free-electron concentration in the conduction band, and N_{f} is the fixed oxide charge unit area situated at $z=-t_{\mathrm{f}}$. The ionized acceptor and hole concentrations have been neglected when electrons are dominant in the accumulation layer. The change of the oxide effective potential barrier height results from the influence of coupling of the transverse and longitudinal effective masses of channel electrons. Therefore, the oxide effective potential barrier $V_{\mathrm{eff}}(z)$ is given by[6]

$$V_{\mathrm{eff}}(z) = V(z)-\frac{\hbar^2k_{\mathrm{r}}^2}{2m_{//-\mathrm{Si}}}\left(1-\frac{m_{//-\mathrm{Si}}}{m_{\mathrm{ox}}}\right)$$

$$= V(z)-\alpha k_{\mathrm{B}}T\left(1-\frac{m_{//-\mathrm{Si}}}{m_{\mathrm{ox}}}\right), \tag{7}$$

where $V(z)$ is the oxide potential barrier height, α is a parameter characterizing the relation between the electron temperature T_{c} in the plane parallel to the Si–SiO_2 interface, and the device temperature T_{c} ($\alpha = T_{\mathrm{c}}/T$). The value of α will change when an external voltage is applied to the MOS structure.

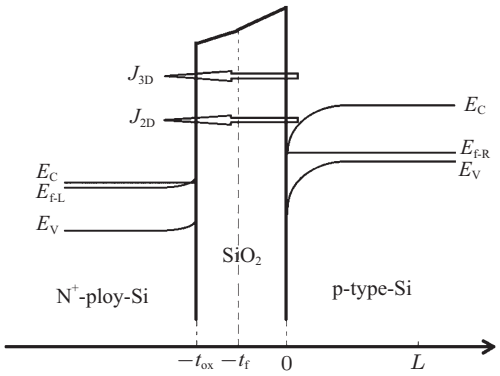

Fig. 1. Schematic band diagram of p-Si/SiO_2/n^+-poly Si structure.

Assume that the effective potential $\Phi(z)$ satisfies the boundary condition[13–15]

$$V|_{z=-t_{\mathrm{OX}}}=V_{\mathrm{g}}-V_{\mathrm{FB}}, \quad V|_{z=L}=0, \tag{8}$$

$$\varepsilon_{\mathrm{Si}}\frac{\mathrm{d}V}{\mathrm{d}z}\bigg|_{z=0^+}-\varepsilon_{\mathrm{ox}}\frac{\mathrm{d}V}{\mathrm{d}z}\bigg|_{z=0^-}=N_{\mathrm{s}}, \tag{9}$$

where N_{s} is the interface trap charge unit area, V_{g} the applied gate voltage, and V_{FB} the flat-band voltage. The quantum calculation of the carrier concentration is performed by summing the contribution of each sub-band. In the 2D case, the density of states is independent of the energy. The electron charge density along the MOS structure is given by

$$n(z) = \frac{\eta m_{//-\mathrm{Si}}k_{\mathrm{B}}T}{\pi\hbar^2} \times\sum_i \ln\left[1+\exp\left(\frac{E_{\mathrm{f}}-E_{\mathrm{j}}}{k_{\mathrm{B}}T}\right)\right]\left|\psi_{\mathrm{ij}}(z)\right|^2, \tag{10}$$

where η is the valley degeneracy factor, and E_{f} is the Fermi energy level of the semiconductor.

The calculation approach to discretizing Poisson–Schrodinger equations uses the finite difference method.[16,17] Real space is divided into discrete mesh points, and the wave functions $\psi(z)$ and $V(z)$ are calculated within these discrete spaces. The Poisson equation at the Si–SiO_2 interface is solved by a boundary condition capturing method.[18,19] Finally, an iteration procedure is used to obtain the self-consistent solution of the Poisson–Schrodinger equations. The electron charge density and the corresponding potential are obtained along the MOS structure.

For the carrier confined in the quasi-bound states in the inversion layer, the lifetime of the n-th sub-band state is given approximately by[2,15]

$$\frac{1}{\tau_n(E_n)} = \frac{T(E_n)}{\int_0^{Z_n} \sqrt{2m_{\perp-\mathrm{Si}}/(E_n - V(z))}\,\mathrm{d}z}, \tag{11}$$

where E_n is the sub-band energy for the n-th quasi-bound state, Z_n is the classical turning point for the n-th bound state, and $T(E)$ is the transmission probability of a particle. The transmission probability is determined by using the transfer matrix method.

For the extended states following the Fermi–Dirac distribution, the tunneling current from the extended states is given by[6,20]

$$J_{3\mathrm{D}} = \int_0^{\infty} \frac{qm_{\perp-\mathrm{Si}}k_{\mathrm{B}}T}{2\pi^2\hbar^3} T(E_\perp) \times \ln\left[\frac{1+\exp(E_{\mathrm{f-L}} - E_\perp)}{1+\exp(E_{\mathrm{f-R}} - E_\perp - qV)}\right] \mathrm{d}E_\perp, \tag{12}$$

where $E_{\mathrm{f-L}}$ and $E_{\mathrm{f-R}}$ are the Fermi levels of the left contact and the right contact, respectively, and V is the potential drop from the oxide gate region and the Si substrate region. In the calculation, the maximum of the transverse electron energy was set as $30k_{\mathrm{B}}T$ above the conduction band.

For the bound states, we assume the value of the quasi-Fermi level is equal to that in bulk Si, even when the tunneling current is nonzero. With these approximations, the tunneling current from the bound states is written as[2,15]

$$J_{2\mathrm{D}} = \frac{\eta q m_{//-\mathrm{Si}}k_{\mathrm{B}}T}{\pi\hbar^2} \sum_i \frac{1}{\tau_i(E_i)} \times \ln\left[\frac{1+\exp(E_{\mathrm{f-L}} - E_i)}{1+\exp(E_{\mathrm{f-R}} - E_i - qV)}\right]. \tag{13}$$

Finally, the total tunneling current J is obtained by summing the 2D and 3D contributions.

3. Tunneling current–voltage characterization

3.1. Influence of the interface trap charge at the Si–SiO$_2$ interface

The channel electron momentum of a conventional MOS structure in the ballistic region cannot reach a high value, so the coupling effect of the transverse and longitudinal electron effective mass is weak.[7] Therefore, the parameter α can be taken to be a small value. First, regardless of ITC at the Si–SiO$_2$ interface, Fig. 2 shows the calculated tunneling current for p-Si/SiO$_2$/n$^+$-poly-Si structure with different oxide thicknesses, and shows experimental results extracted from Ref. [21]. When the gate voltage V_{g} is larger than 0.6 V, the calculation results are in good agreement with the experimental results. However, the calculated results do not agree with the experimental results in the case of $V_{\mathrm{g}} < 0.6$ V, which may result from defects or oxide charges in real p-Si/SiO$_2$/n$^+$-poly-Si structures. When the tunneling current is weak, these defects and oxide charges may play an important role in the tunneling current. When ITC at the Si–SiO$_2$ interface is taken into account, the tunneling currents calculated using this model are shown in Fig. 3(a). With the increase of density of ITC, the tunneling current decreases. When the density N_{s} of ITC is smaller than 10^{12} cm^{-2}, there is no significant change compared with the calculated tunneling current I_{tc}, regardless of ITC at the Si–SiO$_2$ interface. Measurements[22] on clean surfaces in an ultra-high-vacuum system confirm that N_{s} can be very high: on the order of the density of surface atoms ($\sim 10^{15}$ cm^2). For today's MOS capacitors having thermally grown SiO$_2$ on Si, most of the interface trap charge can be neutralized by low-temperature annealing. The total surface traps can be as low as 10^{12} cm^{-2}, which is in good agreement with the result calculated using our proposed model. For N_{s} greater than -5×10^{12} cm^{-2} and V_{g} lower than 1.0 V, the I_{tc} decreases rapidly. These results may result from the decrease of the density of electrons bound in Si substrate near the Si–SiO$_2$ interface. However, for V_{g} greater than 1.5 V, I_{tc} varies slightly with the increase of N_{s}. When V_{g} is low, the number of electrons in the silicon inversion layer is very small, and it increases rapidly with the increase of V_{g}. However, it increases slightly when V_{g} is large. Therefore, ITC has a great influence on tunneling current in the case of low V_{g}, whereas it has little influence in the case of large V_{g}.

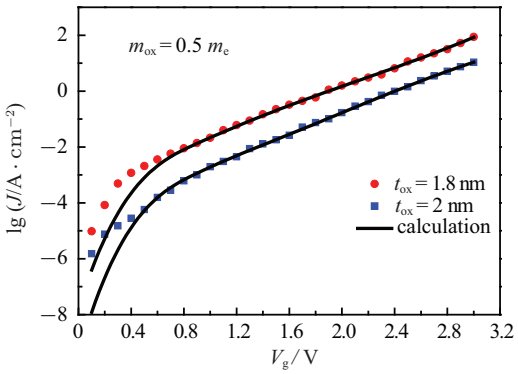

Fig. 2. (color online) Solid lines: calculated tunneling current–voltage characteristics for p-Si/SiO$_2$/n$^+$-poly-Si structure with different oxide thicknesses regardless of interface trap charge at the Si–SiO$_2$ interface. The doping concentrations of n$^+$-poly-Si and p-Si substrate are 10^{20} and 5×10^{17} cm^{-3}, respectively. Discontinuous symbols: experimental data extracted from Ref. [21].

Considering different negative surface charge densities at the Si–SiO$_2$ interface, the density distributions of electrons in the silicon inversion layer are shown in Fig. 3(b). With the increase of negative interface trap charge density, fewer and fewer electrons accumulate in the Si substrate near the Si–SiO$_2$ interface. When a voltage is applied, the Fermi level moves up or down with respect to the interface-trap levels and a change of charge occurs in the interface traps. This

change of charge affects the tunneling current and alters the ideal current–voltage (I–V) curve. When positive voltage is applied to p-type MOS structure, the energy band is bent down near the Si–SiO_2 interface. Negative ITC can weaken the degree of band bending, which results in decreasing density of electrons bound near the Si–SiO_2 interface. When the density of ITC is smaller than 10^{12} cm^{-2}, the density of electrons bound in the Si substrate near the Si–SiO_2 interface has no significant change compared with the calculation that was made without regard to the ITC effect.

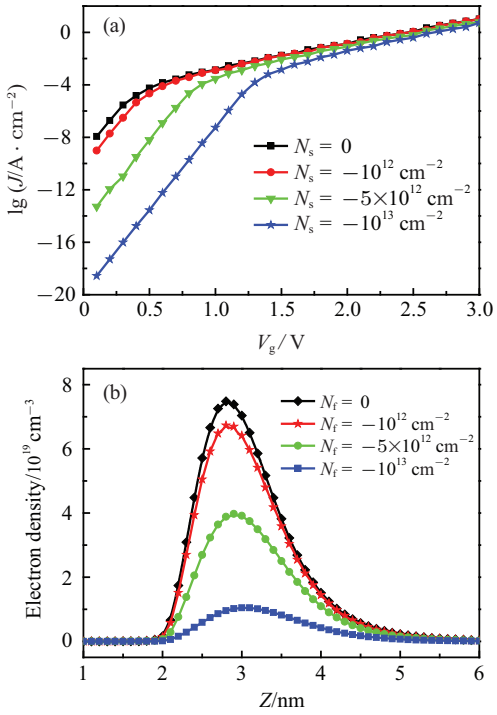

Fig. 3. (color online) (a) Tunneling current density as a function of applied gate voltage with different negative surface charge densities with $t_{ox} = 2$ *nm*; (b) density distribution of electrons in silicon inversion layer in the case of considering different negative surface charge density N_s at Si–SiO_2 interface. The applied gate voltage V_g is 1.5 V, $t_{ox} = 2$ nm, and the doping concentration of p-Si substrate and n$^+$-ploy-Si are 10^{17} and 5×10^{19} cm^{-3}, respectively.

3.2. Influence of fixed oxide charge in oxide gate region

The calculated tunneling current–voltage curves for p-Si/SiO_2/n$^+$-poly-Si structure with different positive FOC in the oxide region are shown in Fig. 4(a). In the calculation, the effect of ITC is not considered, and FOC is assumed to be located at $t_f = 1.0$ nm. The tunneling current increases with the increase of FOC density when the effect of FOC is considered. For the density N_f of FOC smaller than 10^{12} cm^{-2}, tunneling current has no significant change compared with I_{tc} calculated without regard to the FOC effect. For N_s greater than 5×10^{12} cm^{-2}, I_{tc} increases rapidly. These results may result from an increase in injected electrons in the Si substrate near the Si–SiO_2 interface. In general, unlike interface trap charges, fixed oxide charges are independent of gate voltage, so they cause a parallel shift in the gate-bias direction, as indicated in Fig. 4(a). The density distributions of electrons in the silicon inversion layer, considering different positive fixed oxide charges, are shown in Fig. 4(b). When the density of FOC is below 10^{12} cm^{-2}, the distribution of electrons has no significant change compared with the case of the FOC effect being ignored. The number of electrons in the silicon inversion layer increases with the increase of FOC. Therefore, the increase of tunneling current induced by FOC can be attributed to the injected electrons in the Si substrate near the Si–SiO_2 interface.

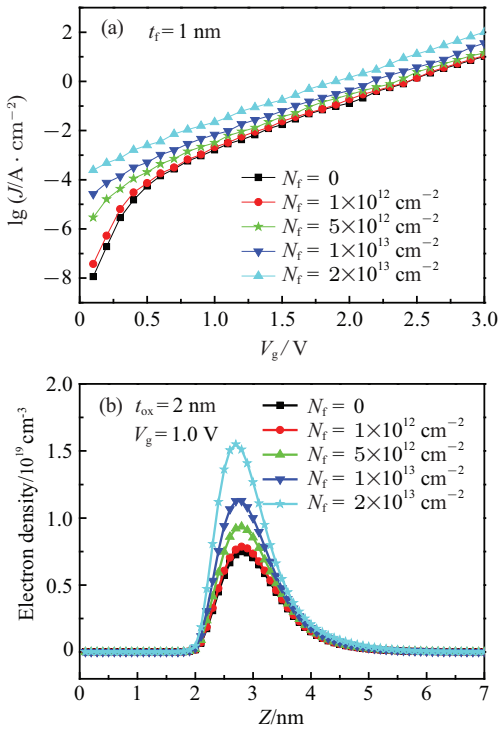

Fig. 4. (color online) (a) Calculated tunneling current–voltage for p-Si/SiO_2/n$^+$-poly-Si structure with different positive fixed oxide charges in oxide region; (b) density distribution of electrons in silicon inversion layer in the case of considering different positive fixed oxide charge N_f located at $t_f = 1.0$ nm in oxide region.

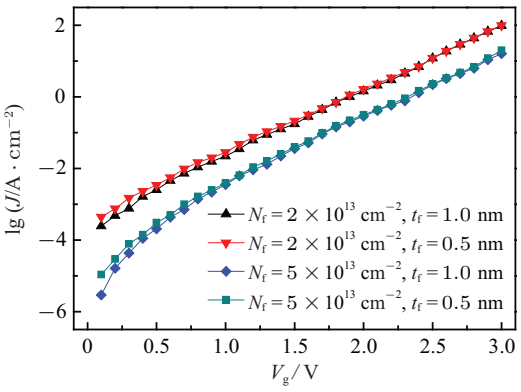

Fig. 5. (color online) Calculated tunneling current-voltage for p-Si/SiO_2/n$^+$-poly-Si structure with positive fixed oxide charge located in different positions in the oxide region.

The origin of fixed oxide charge is generally considered to be excess silicon (trivalent silicon) or the loss of an electron from excess oxygen centers (nonbridging oxygen) near the Si–SiO_2 interface. It is generally positive and its density is not greatly affected by the oxide thickness or by the type or concentration of impurities in the silicon. The influence of FOC position on tunneling current is shown in Fig. 5. For FOCs located at 0.5 and 1.0 nm in the oxide region, respectively, the calculated tunneling currents are almost the same. Therefore, the tunneling current is independent of the FOC position in the oxide region.

4. Conclusion

In the proposed model, the influences of interface trap charge and fixed oxide charge are taken into account, and one-band effective mass approximation is used. The tunneling probability is obtained by employing the transfer matrix method. On the other hand, the effects of in-plane momentum on the quantization in the electron motion perpendicular to the Si–SiO_2 interface of a MOS device are prescribed. Theoretical simulation results indicate that both ITC and FOC have great influence on the tunneling current through a MOS structure when their densities are larger than 10^{12} cm^{-2}, which results from a great change of electrons bound near the Si–SiO_2 interface and oxide region. Therefore, for a real ultrathin MOS structure with ITC and FOC, this model can give a more accurate description for the tunneling current in the inversion layer.

References

[1] Jiang X W and Li S S 2012 *Chin. Phys.* B **21** 027304
[2] Simonetti O, Maurel T and Jourdain M 2002 *J. Appl. Phys.* **92** 4449
[3] Nakhmedov E P, Wieczorek K, Burghardt H and Radehaus C 2005 *J. Appl. Phys.* **98** 024506
[4] Nadimi E, Radehaus C, Nakhmedov E P and Wieczorek K 2006 *J. Appl. Phys.* **99** 104501
[5] Pourghaderi M A, Magnus W, Soree B, Meuris M, Meyer K D and Heyns M 2009 *Phys. Rev.* B **80** 085315
[6] Mao L F 2007 *IEEE Electron Dev. Lett.* **28** 161
[7] Mao L F 2007 *Appl. Phys. Lett.* **91** 123519
[8] Margaritondo G 1999 *Rep. Prog. Phys.* **62** 765
[9] Arnold E 1995 *Appl. Phys. Lett.* **66** 3027
[10] Pei L R, Duscher G, Steen C and Pichler P 2008 *J. Appl. Phys.* **104** 043507
[11] Huang A P, Zheng X H, Xiao Z S, Yang Z C, Wang M, Paul K C and Yang X D 2011 *Chin. Phys.* B **20** 097303
[12] Du G, Liu X Y, Xia Z L,Yang J F and Han R Q 2010 *Chin. Phys.* B **19** 057304
[13] Aktsipetrov O A, Fedyanin A A, Mishina E D and Rubtsov A N 1996 *Phys. Rev.* B **54** 1825
[14] Laikhtman B and Solomon P M 2005 *Phys. Rev.* B **72** 125338
[15] Rana F, Tiwari S and Buchanan D A 1996 *Appl. Phys. Lett.* **69** 1104
[16] Snider G L, Tan I H and Hu E L 1990 *J. Appl. Phys.* **68** 2849
[17] Tan I H, Snider G L and Hu E L 1990 *J. Appl. Phys.* **68** 4071
[18] Liu X D, Fedkiw R P and Kang M 1999 *J. Comput. Phys.* **154** 393
[19] Chern I L and Shu Y C 2007 *J. Comput. Phys.* **225** 2138
[20] Ando Y and Itoh T 1987 *J. Appl. Phys.* **61** 1497
[21] Yang N, Henson W K, Hauser J R and Wortman J J 1999 *IEEE Trans. Electron Dev.* **46** 1464
[22] Allen F G and Gobeli G W 1962 *Phys. Rev.* **127** 150