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Monte Carlo Analysis of Hot Electron Transport and Impact Ionization in Silicon

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A novel impact ionization model which is consistent with a realistic band structure of Si is developed. The present model contains only one and physically transparent parameter, corresponding to the averaged matrix element for the ionization transition. The ionization probability is calculated at every **k**-point in the first Brillouin zone and thus the wave-vector dependence of the ionization probability is explicitly taken into account. Employing the Monte Carlo procedure, the ionization coefficients are calculated and compared with the experimentally available data. It is shown that the value of the parameter closest to the value extracted from the first-principles calculations produces a best-fitting to the experimental ionization coefficients.

1. INTRODUCTION

Impact ionization is recently receiving a renewed interest in connection with the miniaturization of devices in which the range of electron energy and electric field is so large that the hot carrier effects become of critical importance. The hot electron transport can be tackled by the Monte Carlo procedure which provides an exact solution of the Boltzmann transport equation.[1] The impact ionization processes are usually treated by the Keldysh formula[2] which ignores the details of the band structure and thus is not considered to be satisfactory.[3]-[6] In particular, for the wide- and indirect-gap semiconductors like Si, it is essential to take account of a realistic band structure to model impact ionization.

The authors have investigated the impact ionization processes in Si with the wave-vector dependent threshold energies and pointed out the importance of the wave-vector dependence in these processes.[5] Recently, Thoma et al.[6] have developed a new ionization model with an analytical band structure consistent with a realistic density of states of Si. They have also found that the ionization probability cannot be fitted simply by the Keldysh formula.

In the present paper, we develop a novel impact ionization model consistent with a realistic band structure and appropriate for the Monte Carlo procedure. The present model is derived with a band structure obtained from the empirical pseudopotential method [7] and gives the ionization probability *at every k-point* in the first Brillouin zone (BZ) *rather than the electron energy*. The Monte Carlo calculations of the ionization coefficients employing the present ionization model agree very well with the experimental data when the fitting parameter in the ionization probability is close to the value extracted from the first-principles calculation.

In Sec.2, a new model for impact ionization is derived. In Sec.3 the results of the Monte Carlo calculations with the present model are given. Finally, in Sec.4 we draw some conclusions.

2. IMPACT IONIZATION MODEL

Impact ionization is one of the electron-electron interactions taking place between the electrons in the conduction and valence bands. Figure 1 shows a schematic drawing of an impact ionization process and defines the notations of states of electrons involved in the transition, i.e., states 1 and 4 correspond to the initial electrons before the transition and states 2 and 3 to the final states after the transition.

The ionization probability per unit time for an initial electron with wave vector $\mathbf{k}_1$ and band index n_1 is calculated from Fermi's golden rule (after summing over spin degeneracy).

$$w_{ii}(n_1,\mathbf{k}_1) = 2\frac{2\pi}{\hbar}\frac{V^2}{(2\pi)^6}\sum_{\text{bands}}\int d^3k_2 d^3k_3 \; |M|^2 \delta(E_1+E_4-E_2-E_3) \qquad (1)$$

where $|M|^2$ is the matrix element for the transition and

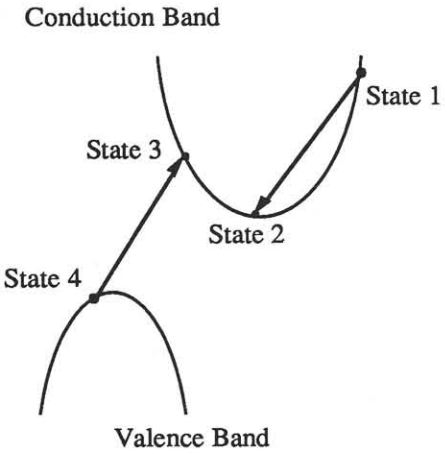

Fig. 1 Schematic drawing of an impact ionization process in Si. States 1 and 4 are the initial electrons before the ionization and states 2 and 3 the final electrons after the ionization.

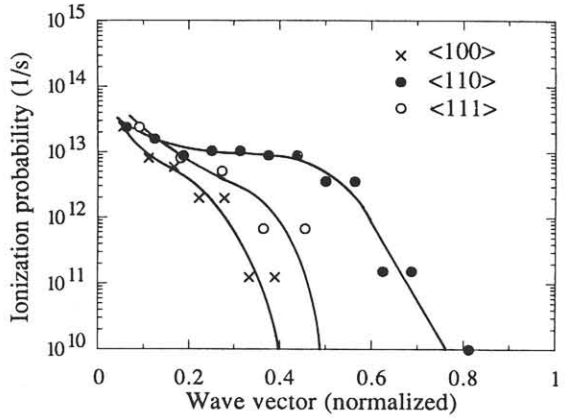

Fig. 2 Ionization probability $w_{ii}(n_1=5,\mathbf{k}_1)$ for the lowest conduction band along three crystallographic directions ; <100>, <110>, and <111>. The wave vector is normalized by the maximum magnitude of $\mathbf{k}_1$ for each direction.

consists of the direct and exchange processes. This is usually dependent of the wave vectors of the electrons and this fact also prevents from detail calculations of the ionization probability. We have investigated in detail the matrix elements and the associated overlap integrals with a realistic band structure. We have found that though these quantities indeed depend on the wave vectors, they do not dominate the wave-vector dependence of the ionization probability, but rather, the conservations of energy and momentum under the realistic band structure play the most dominant role.[8]

Ignoring the wave-vector dependence of the matrix elements and replacing them by a constant F_{ii}, $w_{ii}(n_1,\mathbf{k}_1)$ is approximated by

$$w_{ii}(n_1,\mathbf{k}_1) = \frac{4}{\pi\hbar}\left(\frac{e^2}{a}\right)^2 \frac{(\Delta k)^6}{\delta E} F_{ii}\, g(n_1,\mathbf{k}_1) \qquad (2)$$

$$\approx 6.82 \times 10^{10}\, F_{ii}\, g(n_1,\mathbf{k}_1) \quad (s^{-1})$$

where the weight function $g(n_1,\mathbf{k}_1)$ is defined by

$$g(n_1,\mathbf{k}_1) = \sum_{\text{bands}} \sum_{\mathbf{k}_2,\mathbf{k}_3} \delta_{\mathbf{k}_1+\mathbf{k}_4+\mathbf{G}_o,\,\mathbf{k}_2+\mathbf{k}_3} \qquad (3)$$

Here, $\delta_{\mathbf{k}_1+\mathbf{k}_4+\mathbf{G}_o,\,\mathbf{k}_2+\mathbf{k}_3}$ is the Kronecker delta and $\mathbf{G}_o$ is the reciprocal lattice vector which brings back all $\mathbf{k}$'s to the first BZ. The BZ is discretized with mesh-spacing Δk and the integrals in Eq.(1) are replaced by the sums over $\mathbf{k}_2$ and $\mathbf{k}_3$. δE is the energy interval associated with the energy-conserving delta function in Eq.(1). $\Delta k = 0.1$ in units of $2\pi/a$ and $\delta E = 0.2$ eV are used throughout the study.

It should be noted that the information of the band structure is incorporated through the weight function $g(n_1,\mathbf{k}_1)$. This function is directly related to the energy and momentum conservations with the band structure, and it is this function that introduces the anisotropic character inherent in the ionization processes. Figure 2 shows the ionization probability $w_{ii}(n_1, \mathbf{k}_1)$ for the lowest conduction band (n_1=5) along three different crystallographic directions. The step-like behavior is due to the finite mesh-spacing in the BZ. Strong wave-vector dependence (anisotropy) of the function is clearly seen, and thus it is obvious that the use of a simple isotropic ionization probability like the Keldysh formula cannot be justified.

Notice that the ionization probability is given as a function of the wave vector of the ionizing electron rather than the energy. Comparisons with the conventional models are possible when the wave-vector dependent ionization probability is averaged over the density of states. Figure 3 shows ionization probability thus obtained in comparison with other theoretical findings.[3][6] The present model has a structure around 1.7 eV and this cannot be explained by the simple Keldysh formula. It is interesting to note that a similar structure has been obtained by Thoma et al.[6] This is probably due to the fact that the realistic density of states of Si are, in both cases, taken into account.

3. MONTE CARLO SIMULATIONS

The Monte Carlo method used here is conventional and has already been explained in Ref.(5). In addition to the conventional scattering processes for Si, the simulation includes the X-L nonequivalent intervalley scatterings as well. This is essential because the ionization probability is inherenly anisotropic and the high energy electrons should be populated over the entire BZ. Notice that the extreme high field transport (>100 kV/cm) is actually controlled by two para-

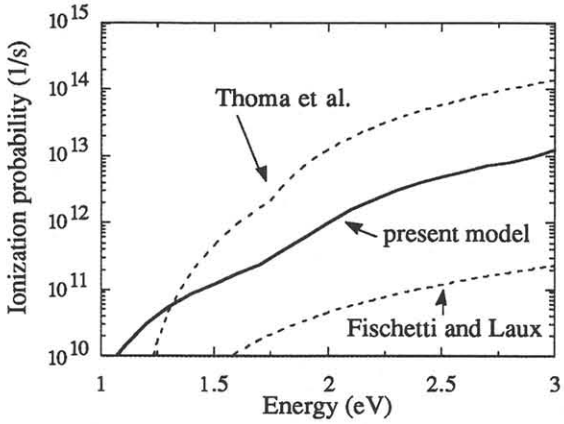

Fig. 3 Ionization probability as a function of electron energy. The probability is averaged over the realistic density of states of Si.

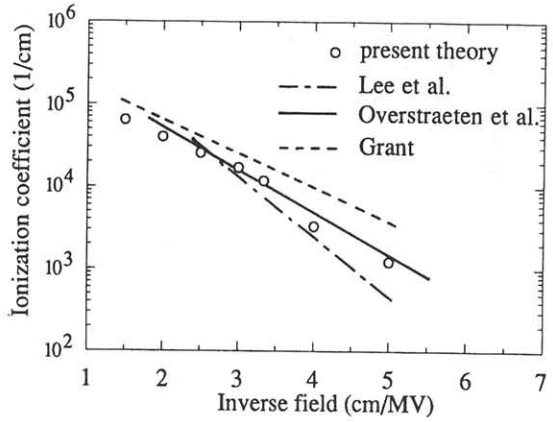

Fig. 4 Ionization coefficients obtained from the Monte Carlo calculations compared with the experimental data.

meters, i.e., the coupling constant D_{XL} of the X-L intervalley scattering and the parameter F_{ii} in the ionization probability (Eq.2).

The impact ionization events are characterized and measured by the ionization coefficients, which are the number of the events per unit drifted path. Figure 4 shows the ionization coefficients versus the inverse of the electric field in comparison with the experimental data.[9)-11)] Recall that F_{ii} directly corresponds to the matrix elements $|M|^2$ in Eq.(1). The value of F_{ii} very close to the value ($\sim 3.4 \times 10^{-3}$) calculated in terms of the wave functions of the pseudopotentials reproduces a very good fit to the experiments, when the coupling constant D_{XL} is equal to 6×10^8 eV/cm. Since no experiments for determining the coupling constant D_{XL} are available, it is a subjective matter to judge the value found above. Experimental evaluations or/and theoretical calculations of D_{XL} are highly desirable.

However, the fact that the present model includes only one and physically more transparent fitting-parameter F_{ii} than the conventional approaches and reproduces a very good fit to the experimental ionization coefficients implies the validity and strongness of the present ionization model.

4. CONCLUSIONS

A new model for the impact ionization processes has been developed and employed in the Monte Carlo calculations for analyzing hot electron transport in Si. The present model takes account of the realistic band structure and the intrinsic anisotropy in the ionization processes. The Monte Carlo calculations have shown that the calculated ionization coefficients agree very well with the experimental data when the parameter corresponding to the matrix element for the transition is close to the value extracted from the first-principles calculations. The present model is, therefore, physically transparent and appropriate to extend for device simulations.

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