Effect of an electric field on impact-ionization probability

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Using electric-field-dependent wave functions the transition probability per unit time of the impact ionization has been calculated by time-dependent perturbation analysis. Results of numerical calculations are presented for the case of ionization across the direct band gap of GaAs. It is found that the present calculation yields a remarkable reduction in threshold energy in comparison with previous results obtained using Bloch functions.

I. INTRODUCTION

Carrier multiplication through impact ionization is an essential mechanism in the operation of various semiconductor devices. A number of theories have been presented[1-4] explaining this phenomenon in terms of the threshold energy, the optical-phonon energy, the ionization mean free path, and the mean free path for optical-phonon scattering. However, the threshold energy often used for explaining the experimental data has been chosen rather arbitrarily. On the other hand, recent theoretical calculations[5-7] arrived at the conclusion that plural thresholds of energy should be considered.

In the previous theories where the field effect on the electronic state was neglected, the threshold energy obtained is considerably larger than the band-gap energy. The reason is as follows: The total crystal momentum and the total energy of the system have to be conserved simultaneously before and after the impact transition. In the presence of an electric field, however, the crystal momentum of an electron in the field direction is no longer a good quantum number. As a result the requirement for momentum conservation is relaxed so that a lower value will be expected for the threshold energy. The present author has stressed the important effect of the simultaneous conservation of crystal momentum and energy on the threshold energy for Auger processes.[8,9]

This paper describes a calculation of the transition probability per unit time of the impact ionization on the basis of the field-dependent wave functions and energy levels, i.e., the Stark structure. The calculation is carried out for the simple model of a single-valence-band structure, i.e., the heavy-hole band. The numerical result obtained for GaAs, where excitation across the direct band gap is taken into account, is presented and discussed. It is concluded that the field dependence of the wave functions has a remarkably large effect on the threshold energy.

II. TRANSITION PROBABILITY IN DIRECT-BAND- GAP MATERIALS

In this section we calculate the probability of the impact ionization across the direct band gap, which occurs via the normal process only. Consider an incident energetic electron (1) with an energy of W_1 which is scattered to state (1′) with an energy of $W_{1'}$, producing a pair of an electron (2′) with $W_{2'}$ and a hole (2) with W_2. The scattering is assumed to occur under the Coulomb interaction such that

$$v(\vec{r}_1-\vec{r}_2)=e^2/\epsilon|\vec{r}_1-\vec{r}_2| \ , \tag{2.1}$$

where $\vec{r}_i$ $(i=1,2)$ is the position vector of the ith electron, ϵ the dielectric constant, and e the electronic charge. The screening effect is neglected when considering the high-field case. Using time-dependent perturbation analysis the transition probability per unit time of the above scattering process is given[10] by

$$P(1\to 1',\ 2\to 2')=\frac{2t}{\hbar^2}\frac{\sin\chi}{\chi}[|f(1\,2\,1'\,2')|^2+|g(1\,2\,1'\,2')|^2+|f(1\,2\,1'\,2')-g(1\,2\,1'\,2')|^2]\times 2 \ , \tag{2.2}$$

$$f(1\,2\,1'\,2')=\int \phi_1^*(\vec{r}_1)\,\phi_2^*(\vec{r}_2)\,v(\vec{r}_1-\vec{r}_2)\,\phi_{1'}(\vec{r}_1)\,\phi_{2'}(\vec{r}_2)\,d\vec{r}_1\,d\vec{r}_2 \ , \tag{2.2a}$$

$$g(1\,2\,1'\,2')=\int \phi_1^*(\vec{r}_1)\,\phi_2^*(\vec{r}_2)\,v(\vec{r}_1-\vec{r}_2)\,\phi_{1'}(\vec{r}_2)\,\phi_{2'}(\vec{r}_1)\,d\vec{r}_1\,d\vec{r}_2 \ , \tag{2.2b}$$

and

$$\chi = (t/\hbar)(W_1 + W_2 - W_{1'} - W_{2'}) \ . \qquad (2.2c)$$

In Eqs. (2.2)–(2.2c), $\phi_i(r_j)$ $(i = 1, 2, 1', 2',\ j = 1, 2)$ is the wave function of the jth electron in the ith state, t the time, $\hbar$ Planck's constant, and the factor 2 in Eq. (2.2) arises from the summation over spin.

Equations (2.2a) and (2.2b) are calculated by using the field-dependent wave functions and energy levels which appeared in a number of papers.[11–16] In the crystal-momentum representation, the stationary wave functions in an electric field are directly obtained as an expansion in the complete set of Bloch functions $\psi_n(\vec{k}, \vec{r})$, i.e.,

$$\phi_{\nu n}(\vec{k}_\perp, \vec{r}) = \sum_{k_x} C_{\nu n}(\vec{k})\, \psi_n(\vec{k}, \vec{r}) \qquad (2.3)$$

for the nth energy band, where the x axis has been taken along the field direction. In the above equation $C_{\nu n}(\vec{k})$ is the expansion coefficient, $\vec{k}_\perp$ the wave vector in a plane perpendicular to the field direction, i.e., $\vec{k}_\perp = (0, k_y, k_z)$, and ν an integer specifying the discrete Stark levels as

$$W_{\nu n}(\vec{k}) = \frac{2\pi\nu F}{K_x} + \frac{1}{K_x}\int_{-K_x/2}^{K_x/2} E_n^{(1)}(k_x', \vec{k}_\perp)\, dk_x' \ . \qquad (2.4)$$

In Eq. (2.4), F is an electric field multiplied by the electronic charge, K_x is the width of the Brillouin zone in the x direction, and

$$E_n^{(1)}(\vec{k}) = E_n(\vec{k}) - FX_{nn}(\vec{k}) \ , \qquad (2.5)$$

where $E_n(\vec{k})$ is the energy of an electron in a periodic lattice and we define, in general,

$$X_{nn'}(\vec{k}) = i\int u_n^*(\vec{k}, \vec{r})\, \frac{\partial}{\partial k_x} u_{n'}(\vec{k}, \vec{r})\, d\vec{r} \ , \qquad (2.6)$$

with $u_n(\vec{k}, \vec{r})$ being the modulating part of the Bloch function.

The coefficient $C_{\nu n}(\vec{k})$ in Eq. (2.3) is given by

$$C_{\nu n}(\vec{k}) = \frac{1}{N_x^{1/2}} \exp\left(\frac{i}{F}\int_0^{k_x} [W_{\nu n}(\vec{k}_\perp) - E_n^{(1)}(k_x', \vec{k}_\perp)]\, dk_x'\right), \qquad (2.7)$$

where N_x is the number of the k_x states in the Brillouin zone, neglecting the interband mixing effect arising from the factors $X_{nn'}(\vec{k})$ $(n \neq n')$. The neglect of $X_{nn'}(\vec{k})$ $(n \neq n')$ is reasonable on the basis of the estimations[15,17] that $X_{nn'}$ $(n \neq n')$ is small for a weak field except near points of degeneracy. It should be noted that the impact transition occurs substantially apart from point of degeneracy of the valence band.

Using Eqs. (2.3), (2.6), (2.2a), and (2.2b) and the expansion

$$\psi_n(\vec{k}, \vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{K}} A_n(\vec{K}, \vec{k}) \exp[i(\vec{k} + \vec{K}) \cdot \vec{r}] \ , \qquad (2.8)$$

where V and $\vec{K}$ are the volume of a crystal and the reciprocal-lattice vector, respectively, we obtain by neglecting the umklapp processes[10]

$$f(1\,2\,1'\,2') = \frac{4\pi e^2}{\epsilon V} \sum_{(k_x)} C_1^*(\vec{k}_1)\, C_2^*(\vec{k}_2)\, C_{1'}(\vec{k}_{1'})\, C_{2'}(\vec{k}_{2'})\, D_1(\vec{k}_{1'}, \vec{k}_{2'}, \vec{k}_1, \vec{k}_2)\, \delta_K(\vec{k}_1 + \vec{k}_2 - \vec{k}_{1'} - \vec{k}_{2'}) \qquad (2.9a)$$

and

$$g(1\,2\,1'\,2') = \frac{4\pi e^2}{\epsilon V} \sum_{(k_x)} C_1^*(\vec{k}_1)\, C_2^*(\vec{k}_2)\, C_{1'}(\vec{k}_{1'})\, C_{2'}(\vec{k}_{2'})\, D_2(\vec{k}_{1'}, \vec{k}_{2'}, \vec{k}_1, \vec{k}_2)\, \delta_K(\vec{k}_1 + \vec{k}_2 - \vec{k}_{1'} - \vec{k}_{2'}) \ , \qquad (2.9b)$$

where

$$D_1(\vec{k}_{1'}, \vec{k}_{2'}, \vec{k}_1, \vec{k}_2) = \frac{F(1\,1')\, F(2\,2')}{|\vec{k}_1 - \vec{k}_{1'}|^2} \ , \qquad (2.9c)$$

$$D_2(\vec{k}_{1'}, \vec{k}_{2'}, \vec{k}_1, \vec{k}_2) = \frac{F(1\,2')\, F(2\,1')}{|\vec{k}_1 - \vec{k}_{2'}|^2} \ , \qquad (2.9d)$$

and

$$F(ij) = \int u_i^*(\vec{k}_i, \vec{r})\, u_j(\vec{k}_j, \vec{r})\, d\vec{r} \ . \qquad (2.9e)$$

In Eqs. (2.9a) and (2.9b), $\sum_{(k_x)}$ means taking summation over k_{1x}, k_{2x}, $k_{1'x}$ and $k_{2'x}$, and δ_K is Kronecker's delta.

Now the total rate of impact transition is given by

$$\Re = \sum_{\vec{q}_1\vec{q}_2\vec{q}_{1'}\vec{q}_{2'}} P(1 \to 1',\ 2 \to 2')\, \langle N(\vec{q}_1)\rangle \qquad (2.10)$$

for an incident electron of a quantum state $\vec{q}_1$, where $\vec{q}_i$ $(i = 1, 2, 1', 2')$ denotes a quantum state such as $\vec{q}_i = (\nu_i, \vec{k}_{i\perp})$ for a field-dependent state or $\vec{q}_i = \vec{k}_i$ for a Bloch state, and $\langle N(\vec{q}_1)\rangle$ is the occupation probability.

As shown in Appendix A, the transition probability $\mathcal{P}(E_1)$ per unit time per unit volume per unit energy for an energetic electron having an energy of E_1 is given from Eqs. (2.2), (2.9a), (2.9b), and (2.10) in the form

$$\mathcal{P}(E_1)=\frac{3\sqrt{2}}{\pi^4}\left(\frac{e^2}{\epsilon}\right)^2\frac{m_c^{9/2}}{\hbar^{10}}\frac{1}{1+2\mu}G_0 s_0^2|D|^2(\mathcal{Q}_1+\mathcal{Q}_2)\ , \tag{2.11}$$

$$\mathcal{Q}_1=\int_0^{E_1}dE_{1\perp}\frac{(1+2\alpha E_{1\perp})^{3/2}}{(E_1-E_{1\perp})^{1/2}}\left[E_{1\perp}\left(1-\frac{\mu}{1+2\mu}(1+\alpha E_{1\perp}\right)-E_G\right]\ , \tag{2.11a}$$

$$\begin{aligned}\mathcal{Q}_2=&\frac{2G_0}{3\pi s_0^2}\int_0^{E_1}dE_{1\perp}\int_{-s_0}^{s_0}ds_1\int_{-s_0}^{s_0}ds_2\int_{-s_0}^{s_0}ds_3\frac{(1+2\alpha E_{1\perp})^{3/2}}{(E_1-E_{1\perp})^{1/2}}\frac{1}{(s_1+s_2)^2}\Gamma(s_0-|s_1+s_2-s_3|)\\&\times(1-\cos\{\tfrac{1}{3}[s_1^3+s_2^3+s_3^3+(s_1+s_2-s_3)^3+\beta s_6^3-\beta(s_6+s_1+s_2)^3+\mu(s_3-s_2-s_6)^3\\&+\mu(s_1+2s_2-s_3+s_6)^3]-g(E_{1\perp})(s_1+s_2)\})\ ,\end{aligned} \tag{2.11b}$$

where $\alpha=(1-m_c/m_0)^2E_G^{-1}$, with m_c and m_0 being the effective mass of an electron and the free-electron mass, respectively; $\beta=(1+2\alpha E_{1\perp})^{-1/2}$; $\mu=m_c/m_v$, with m_v being the effective mass of a hole; $G_0=(\hbar^2F^2/2m_c)^{1/3}$; $s_0=G_0K_x/2F$,

$$s_6=2s_0(2m_c/\hbar^2K_x^2)^{1/2}(1+2\alpha E_{1\perp})(E_1-E_{1\perp})^{1/2}\ ;$$

$g(E_{1\perp})$ is defined by Eq. (A11b); and

$$\Gamma(s)=0 \quad \text{for } s<0$$
$$=1 \quad \text{for } s\geq 0\ .$$

Naturally, Eq. (2.11) is meaningless for such a value of E_1 as to give $\mathcal{P}(E_1)<0$.

III. TRANSITION PROBABILITY IN INDIRECT-BAND-GAP MATERIALS

In this section we consider a material having an indirect band gap, where the transition occurs via the umklapp process as well as the normal one. As for the conduction and valence bands we assume a silicon-like band structure, which consists of six equivalent valleys in ⟨100⟩ and other equivalent directions. It is also assumed that the electric field is applied in the ⟨100⟩ direction. Evidently the above assumptions are not prerequisite, but the extension to more general cases is straightforward though the results will be obtained in more complex forms.

In addition to the notations used in the previous section we define $\vec{b}$ as the wave vector measured from a conduction-band minimum and g as the separation between the extrema of the conduction band and the valence band. This gives $\vec{k}=\vec{b}+g\hat{n}$, where $\hat{n}$ is the unit vector from the Brillouin-zone center toward one of the valley minima.

From Eqs. (2.2a) and (2.2b), we obtain, retaining the most contributing terms only,[6]

$$f(1\,2\,1'\,2')=\sum_{(b_x)}C_1^*(\vec{b}_1)\,C_2^*(\vec{b}_2)\,C_{1'}(\vec{b}_{1'})\,C_{2'}(\vec{b}_{2'})\frac{F(1\,1')\,G(2\,2')}{|\vec{k}_1-\vec{k}_{1'}|^2}\delta_K(\vec{k}_1+\vec{k}_2-\vec{k}_{1'}-\vec{k}_{2'})\ . \tag{3.1a}$$

and

$$g(1\,2\,1'\,2')=\sum_{(b_x)}C_1^*(\vec{b}_1)\,C_2^*(\vec{b}_2)\,C_{1'}(\vec{b}_{1'})\,C_{2'}(\vec{b}_{2'})\frac{F(2\,1')\,G(1\,2')}{|\vec{k}_1-\vec{k}_{2'}|^2}\delta_K(\vec{k}_1+\vec{k}_2-\vec{k}_{1'}-\vec{k}_{2'})\ , \tag{3.1b}$$

where $\sum_{(b_x)}$ means taking summation over b_{1x}, b_{2x}, $b_{1'x}$, and $b_{2'x}$,

$$G(i,j)=\sum_{\vec{K}_i}A^*(\vec{K}_i,\vec{k}_i)\,A(\vec{K}_i+\vec{K},\vec{k}_j)\ , \tag{3.1c}$$

and $C_i(\vec{b})$, $A(\vec{K},\vec{k})$, and $F(ij)$ are defined by Eq. (2.7) with $\vec{k}$ replaced with $\vec{b}$, by Eq. (2.8), and by Eq. (2.9e), respectively.

By a similar procedure as adopted in Sec. II we obtain

$$f(1\,2\,1'\,2')=\frac{4\pi e^2}{\epsilon V}D_f\sum_{(bx)}C_1^*(\vec{b}_1)\,C_2^*(\vec{b}_2)\,C_{1'}(\vec{b}_{1'})\,C_{2'}(\vec{b}_{2'})\,\delta_K(\vec{k}_1+\vec{k}_2-\vec{k}_{1'}-\vec{k}_{2'}+\vec{K}) \tag{3.2a}$$

and

$$g(1\,2\,1'\,2')=(D_g/D_f)f(1\,2\,1'\,2')\ , \tag{3.2b}$$

where

$$D_f=F(11')\,G(22')/|\vec{k}_1-\vec{k}_{1'}|^2$$

and

$$D_g=F(21')\,F(12')/|\vec{k}_1-\vec{k}_{2'}|^2\ ,$$

both of which are evaluated at $\vec{b}_{1'}=\vec{b}_{2'}=0$ and at $\vec{b}_1$ satisfying $E_1(\vec{b}_1)=E_G$. In Eqs. (3.2a) and (3.2b) we have the normal process when $\vec{K}=0$ and the umklapp process when $\vec{K}\neq 0$.

Considering a pair of valleys in the $\langle 100\rangle$ and $\langle\bar{1}00\rangle$ directions and other two equivalent pairs for the transition processes, we obtain

$$f(1\,2\,1'\,2')=\frac{4\pi e^2}{\epsilon V}\,D_f(Z)\sum_{(bx)}C_1^*(\vec{b}_1)\,C_2^*(\vec{b}_2)\,C_{1'}(\vec{b}_{1'})\,C_{2'}(\vec{b}_{2'})\,\delta_K(\vec{b}_1+\vec{b}_2-\vec{b}_{1'}-\vec{b}_{2'}+Z\hat{n}) \tag{3.3a}$$

and

$$g(1\,2\,1'\,2')=[D_g(Z)/D_f(Z)]\,f(1\,2\,1'\,2')\,, \tag{3.3b}$$

where $Z=K_x-3g$, K_x-g, or g. The case of $\hat{n}$ parallel to the field and the case of $\hat{n}$ perpendicular to it must be treated in different ways. Quite analogously to the procedures adopted in Sec. II, we finally obtain

$$\mathcal{P}(E_1)=\frac{3\sqrt{2}}{2\pi^4}\left(\frac{e^2}{\epsilon}\right)^2\frac{m_c^{9/2}}{\hbar^{10}}\,\frac{1}{1+2\mu}\,G_0\,s_0^2\sum_Z(|D_f(Z)|^2+|D_g(Z)|^2)[H_1(Z)+2H_2(Z)]\,, \tag{3.4}$$

$$H_1(Z)=\mathcal{Q}_1+\mathcal{Q}_2(Z)\,, \tag{3.4a}$$

and

$$H_2(Z)=\mathcal{Q}_1^+(Z)+\mathcal{Q}_2^+(Z)\,, \tag{3.4b}$$

where $\mathcal{Q}_1$ is the same as that given by Eq. (2.11a), $\mathcal{Q}_2(Z)$ is obtained in Eq. (2.11b) by replacing $\mu(s_3-s_2-s_6)^3$ and $\mu(s_1+2s_2-s_3+s_6)^3$ with $\mu(s_3-s_2-s_6+s_Z)^3$ and $\mu(s_1+2s_2-s_3+s_6+s_Z)^3$, respectively, where $s_Z=(\hbar^2/2m_cF)^{1/3}Z$, and $\mathcal{Q}_1^+(Z)$ and $\mathcal{Q}_2^+(Z)$ are obtained in Eqs. (2.11a) and (2.11b) by replacing E_G with

$$E_G+\frac{\mu}{1+2\mu}\,\frac{\hbar^2}{2m_c}Z^2.$$

Any negative values of $H_1(Z)$ and $H_2(Z)$ are meaningless and must be put equal to zero.

IV. WEAK-FIELD APPROXIMATION

In this section we discuss a relation of the field-dependent impact ionization probability to the field-free one. The discussion is restricted hereafter to the case of the normal process for ionization across a direct band gap. The extension to other possible cases is straightforward.

Noting Eq. (2.4) and the relation

$$\int d\nu\,\exp[i(2\pi\nu/K_x)k]=K_x\,\delta(k)\,,$$

the integration over ν in Eq. (A6) can be performed, yielding

$$\mathcal{R}=\frac{2}{\hbar}\left(\frac{4\pi e^2}{\epsilon V}\right)^2\left(\frac{V}{(2\pi)^3}\right)^3\frac{1}{F}\int d\vec{k}_{1\perp}\int d\vec{k}_{1'\perp}\int d\vec{k}_{2'\perp}\int dk_1\int dk_3\int dk_5\int dk_6$$
$$\times\,\mathcal{G}_3\,\Phi(-k_2,\,-k_4,\,k_6,\,k_1,\,k_3,\,-k_5,\,\vec{k}_{1\perp},\,\vec{k}_{1'\perp},\,\vec{k}_{2'\perp})\langle N(k_5,\,\vec{k}_{1\perp})\rangle\,, \tag{4.1}$$

where

$$\mathcal{G}_3=\exp\left[\frac{i}{F}\left((E_\perp-E_G)(k_5+k_6)+\frac{\hbar^2}{6m_c}(k_1^3+k_2^3+k_3^3+k_4^3)+\frac{\hbar^2}{6m_1}(k_5^3+k_6^3)+\frac{\hbar^2}{6m_v}(k_7^3+k_8^3)\right)\right]\,, \tag{4.1a}$$

with

$$k_2=-(k_5+k_6+k_1),\quad k_4=-(k_5+k_6+k_3)\,, \tag{4.1b}$$

and

$$E_\perp=E_{1\perp}-\frac{\hbar^2}{2m_v}k_{2\perp}^2-\frac{\hbar^2}{2m_c}(k_{1'\perp}^2+k_{2'\perp}^2). \tag{4.1c}$$

Equation (4.1a) can be rewritten with the aid of Eq. (4.1b) as

$$\mathcal{G}_4=\exp\left[-\frac{i}{F}\left(\frac{\hbar^2}{6\lambda_1}(k_5+k_6)^3-\frac{\hbar^2}{2\lambda_2}|k_7|(k_5+k_6)^2\right.\right.$$
$$\left.\left.+(E_x+E_\perp-E_G)(k_5+k_6)\right)\right]\,, \tag{4.2}$$

where

$$E_x = \frac{\hbar^2}{2m_1} k_5^2 - \frac{\hbar^2}{2m_v} k_7^2 - \frac{\hbar^2}{2m_c} (k_1^2 + k_3^2) , \tag{4.2a}$$

$$\frac{1}{\lambda_1} = \frac{2}{m_c} - \frac{1}{m_1} + \frac{1}{m_v} , \quad \text{and} \quad \frac{1}{\lambda_2} = \left(\frac{1}{m_c} (k_1 + k_3) + \frac{1}{m_v} k_7 + \frac{1}{m_1} k_5 \right) \Big/ |k_7| , \tag{4.2b}$$

Defining a new variable

$$s = -(k_5 + k_6)/c$$

with

$$c = (2\lambda_1 F/\hbar^2)^{1/3}$$

and restoring the original notation according to

$$k_1 \rightarrow k_{1'x} , \quad k_3 \rightarrow k_{2'x} , \quad k_5 \rightarrow k_{1x} , \quad k_7 \rightarrow k_{2x} ,$$

we obtain

$$\mathcal{R} = \frac{2}{\hbar} \left(\frac{4\pi e^2}{\epsilon \bar{V}} \right)^2 \left(\frac{\bar{V}}{(2\pi)^3} \right)^3 \int d\vec{k}_1 \int d\vec{k}_{1'} \int d\vec{k}_{2'} \frac{1}{\hbar\Omega} \int_{-(K_x - k_{1x})c^{-1}/2}^{(K_x + k_{1x})c^{-1}/2} \exp\left[i \left(\tfrac{1}{3} s^3 + \left(\frac{\Omega_0}{\Omega} \right)^{1/2} s^2 + \frac{E_1 + E_2 - E_{1'} - E_{2'}}{\hbar\Omega} s \right) \right]$$

$$\times \langle N(\vec{k}_1) \rangle \Phi(k_{1'x} - cs, \; k_{2'x} - cs, \; k_{1x} - cs, \; k_{1'x} , \; k_{2'x} , \; k_{1x} , \; \vec{k}_{1'\perp} , \; \vec{k}_{2'\perp} , \; \vec{k}_{1\perp}) , \tag{4.3}$$

where

$$\hbar\Omega = \left(\frac{\hbar^2 F^2}{2\lambda_1} \right)^{1/3} , \quad \hbar\Omega_0 = \frac{\hbar^2 k_{2x}^2}{2\lambda_1} \left(\frac{\lambda_1}{\lambda_2} \right)^2 , \quad k_{2x} = k_{1'x} + k_{2'x} - k_{1x} ,$$

with E_i $(i = 1, 2, 1', 2')$ being the energy of an electron in a periodic lattice.

Since Φ is the slowly varying function of k_i's, for an extremely low field we can neglect the c dependence of Φ in the integration over s noting that c tends to zero as F approaches zero. This we obtain

$$\mathcal{R} = \frac{4\pi}{\hbar} \left(\frac{4\pi e^2}{\epsilon V} \right)^2 \left(\frac{\bar{V}}{(2\pi)^3} \right)^3 \int d\vec{k}_1 \int d\vec{k}_{1'} \int d\vec{k}_{2'} \frac{1}{\hbar\Omega} B_i \left(\frac{E_1 + E_2 - E_{1'} - E_{2'}}{\hbar\Omega} , \left(\frac{\Omega_0}{\Omega} \right)^{1/2} , \; c \right)$$

$$\times (|D_1|^2 + |D_2|^2 + |D_1 - D_2|^2) \langle N(\vec{k}_1) \rangle , \tag{4.4}$$

where

$$B_i(a, b, c) = \frac{1}{2\pi} \int_{-(K_x - k_{1x})c^{-1}/2}^{(K_x + k_{1x})c^{-1}/2} \exp[i(\tfrac{1}{3} s^3 - bs^2 + as)] \, ds , \tag{4.4a}$$

and D_i $(i = 1, 2)$ is now a function of k_{ix} $(i = 1, 2, 1', 2')$. Equation (4.4) is the convolution expression for the electric-field effect in the weak-field approximation.

For $K_x > 2|k_{1x}|$, we have

$$\lim_{\Omega \to 0} \frac{1}{\hbar\Omega} B_i \left(\frac{E_1 + E_2 - E_{1'} - E_{2'}}{\hbar\Omega} , \left(\frac{\Omega_0}{\Omega} \right)^{1/2} , \; c \right) = \delta(E_1 + E_2 - E_{1'} - E_{2'}) , \tag{4.5}$$

so that the effect of the electric field can be represented by replacing the δ function in the zero-field expression (A2) with a function of unit area of finite width. The field therefore lowers the threshold by a magnitude of the order of $\hbar\Omega$ in comparison with the zero field case.

We can not derive a simpler formula for the transition probability $\mathcal{P}(E_1)$ either from Eq. (2.11) or from Eq. (4.4). In the special case of the zero field, however, we can obtain from Eq. (A2) the approximate expression for $\mathcal{P}(E_1)$ as

$$\mathcal{P}_0(E_1) = \frac{4\sqrt{2}}{\pi^2} \left(\frac{e^2}{\epsilon} \right)^2 \frac{m_c^{4\,1/2}}{\hbar^{10}} |D|^2 \frac{1}{(1 + 2\mu)^{3/2}} [E_1(1 + \alpha E_1)]^{1/2} (1 + 2\alpha E_1) \left[E_1 \left(1 - \frac{\mu}{1 + 2\mu} (1 + \alpha E_1) \right) - E_G \right]^2 , \tag{4.6}$$

where the suffix 0 indicates the zero field case and D $(= D_1 = D_2)$ is evaluated for $\vec{k}_{1'} = \vec{k}_{2'} = 0$ and $E_1(\vec{k}_1) = E_G$.

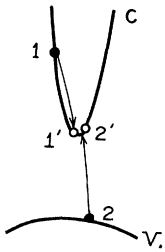

FIG. 1. Schematic illustration of impact transition in the energy scheme of a periodic lattice.

TABLE I. Material parameters of GaAs.

m_c/m_0	0.067
m_v/m_0	0.50
E_G (eV)	1.40
ϵ	12.5
lattice constant (Å)	5.64191

V. NUMERICAL RESULTS AND DISCUSSIONS

In this section we describe the numerical results obtained by applying the theory in Sec. II to GaAs, for which only the direct band gap is considered. For the evaluation of $|D|^2$ in Eq. (2.11), the relation[18-20]

$$|F(2i)|^2 = \alpha_{cv}|\vec{k}_i - \vec{k}_2|^2/(E_i - E_2)$$

is used and $|F(1i)|^2$ is calculated directly from the $\vec{k}\cdot\vec{p}$ perturbation theory.[21]

The fourfold integral in Eq. (2.11b) is evaluated by a Monte Carlo calculation. Since the integrand is a rapidly varying function of s_1, s_2, and s_3, the calculation for a low field, especially for a field below 5×10^5 V/cm, requires long computing time because of the large magnitude of s_0. For the zero field, however, the calculation is facilitated with Eq. (4.6).

Figure 2 shows the result of the numerical calculation of the transition probability $\mathcal{P}(E)$ at 300 K for fields applied in ⟨100⟩ direction. It is seen that the threshold energy decreases with increasing field. This is the direct consequence of the relaxation of the crystal momentum in the field direction. The threshold energy is pronouncedly reduced even below the band-gap energy as a result of tunneling of electrons into the forbidden gap. Consequently, taking the threshold value of $1.5E_G$, as has often been done, seems to be quite unreasonable.

The threshold energy also decreases with increasing field in the case of the indirect band gap. As for the indirect band gap the term except $H_1(Z)$ vanishes in the vicinity of the lowest threshold energy. Since $\mathfrak{L}_2(Z)$ in Eq. (3.4a) is nearly equal to $\mathfrak{L}_2$ in Eq. (2.11), no situations distinct from the case of the direct band gap are expected in the case of the indirect band gap.

In all the discussions we did not take into account the collision broadening of the Stark levels due to phonons and/or crystal imperfections. Especially for an energetic electron, the effect of phonon scattering may be important. The level broadening will relax the requirement for the conservation of the energy as well as of the crystal momentum, and eventually may enhance the lowering of the threshold energy.

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APPENDIX A

It is convenient for the later discussion to investigate the conventional case at first, where the field dependence of the electronic states is not taken into account. Using Bloch functions for $\phi_i(\vec{r}_j)$ in Eqs. (2.2a) and (2.2b), we obtain immediately

$$f_0(121'2') = (4\pi e^2/\epsilon V)D_1(\vec{k}_{1'}, \vec{k}_{2'}, \vec{k}_1, \vec{k}_2)\delta_K(\vec{k}_1+\vec{k}_2-\vec{k}_{1'}-\vec{k}_{2'}) \tag{A1a}$$

and

$$g_0(121'2') = (4\pi e^2/\epsilon V)D_2(\vec{k}_{1'}, \vec{k}_{2'}, \vec{k}_1, \vec{k}_2)\delta_K(\vec{k}_1+\vec{k}_2-\vec{k}_{1'}-\vec{k}_{2'}) \tag{A1b}$$

in place of $f(121'2')$ and $g(121'2')$ in Eq. (2.2), where the suffix 0 refers to the zero-field case. Using the above functions and replacing the summation $\sum_{(\vec{k})}$ with the integral $[V/(2\pi)^3]\int d\vec{k}\ldots$, we obtain the total rate of the transition for the zero-field case in the form

$$\mathfrak{R}_0 = \frac{4\pi}{\hbar}\left(\frac{4\pi e^2}{\epsilon V}\right)^2\left(\frac{V}{(2\pi)^3}\right)^3\int d\vec{k}_1\int d\vec{k}_{1'}\int d\vec{k}_{2'}(|D_1|^2+|D_2|^2+|D_1-D_2|^2)\langle N(\vec{k}_1)\rangle\,\delta(E_1+E_2-E_{1'}-E_{2'}), \tag{A2}$$

where δ is the Dirac δ function.

For the field-dependent case, we obtain with the use of Eqs. (2.2), (2.9a), (2.9b), and (2.10) in the form

$$\mathcal{R}=\frac{4\pi}{\hbar}\left(\frac{4\pi e^2}{\epsilon V}\right)^2\left(\frac{V}{(2\pi)^3}\right)^3\frac{2\pi}{L_x}\frac{1}{K_x^4}\sum_{\substack{\nu_1\nu_2\\ \nu_1'\nu_2'}}\int d\vec{k}_{1\perp}\int d\vec{k}_{1'\perp}\int d\vec{k}_{2'\perp}$$

$$\times[\,|\,\mathcal{g}_1 D_1|^2+|\,\mathcal{g}_1 D_2|^2+|\,\mathcal{g}_1(D_1-D_2)|^2\,]\,\langle N(\vec{q}_1)\rangle\delta(W_1+W_2-W_{1'}-W_{2'}), \tag{A3}$$

where L_x is the length of a crystal in the x direction, $dk_{i\perp}=dk_{iy}\,dk_{iz}$, and $\mathcal{g}_1$ is the integration operator acting on D_1 and D_2, defined as

$$\mathcal{g}_1=\int dk_{1x}\int dk_{1'x}\int dk_{2'x}\,C_1^*(\vec{k}_1)C_2^*(\vec{k}_2)C_{1'}(\vec{k}_{1'})C_{2'}(\vec{k}_{2'})\,\delta_K(k_{1x}+k_{2x}-k_{1'x}-k_{2'x}). \tag{A3a}$$

For the calculation of Eq. (A3a), we use the following relations:

$$E_i(\vec{k}_i)=(\hbar^2/2m_c)k_i^2\quad(i=1',2'), \tag{A4a}$$

$$E_2(\vec{k}_2)=-E_G-(\hbar^2/2m_v)k_2^2, \tag{A4b}$$

and

$$E_1(\vec{k}_1)=E_{1\perp}(\vec{k}_{1\perp})+(\hbar^2/2m_1)\,k_{1x}^2, \tag{A4c}$$

where m_c and m_v are the masses of an electron and a hole, respectively, at $\vec{k}=0$,

$$m_1=m_c[1+(2\alpha\hbar^2/m_c)\,k_{1\perp}^2]^{1/2}, \tag{A4d}$$

$$E_{1\perp}(\vec{k}_{1\perp})=\left[\left(1+\frac{2\alpha\hbar^2}{m_c}\,k_{1\perp}^2\right)^{1/2}-1\right]\Big/\,2\alpha, \tag{A4e}$$

with $\alpha=(1-m_c/m_0)^2E_G^{-1}$ (m_0 being the free-electron mass), $k_{1\perp}^2=k_{1y}^2+k_{1z}^2$, and E_G is the band-gap energy. The energy is measured from the bottom of the conduction band. Equations (A4c)–(A4e) are obtained using the relation[22]

$$(\hbar^2/2m_c)\,k_1^2=E_1(1+\alpha E_1), \tag{A5}$$

from which E_1 is approximately estimated for $\hbar^2k_{1x}^2/2m_c\ll\frac{1}{4}E_G$. Further, we neglect the second term in Eq. (2.5), which vanishes for a crystal with a center of inversion or may be small for a weak field even in a crystal without it. This simplification is not essential in carrying out the calculation.

Defining the new variables according to the relation

$$k_{1'x}=k_1\ \text{and}\ -k_2,$$

$$k_{2'x}=k_3\ \text{and}\ -k_4,$$

$$k_{1x}=-k_5\ \text{and}\ k_6,$$

$$k_{2x}=k_7\ \text{and}\ -k_8,$$

Equation (A3) can be rewritten[16]

$$\mathcal{R}=\frac{4\pi}{\hbar}\left(\frac{4\pi e^2}{\epsilon V}\right)^2\left(\frac{V}{(2\pi)^3}\right)^3\frac{2\pi}{L_x}\frac{1}{K_x^4}\int d\nu_1\int d\nu_2\int d\nu_{1'}\int d\nu_{2'}\int d\vec{k}_{1\perp}\int d\vec{k}_{1'\perp}\int d\vec{k}_{2'\perp}$$

$$\times\mathcal{g}_2\,\Phi(-k_2,-k_4,k_6,k_1,k_3,-k_5,\vec{k}_{1\perp},\vec{k}_{1'\perp},\vec{k}_{2'\perp})\,\langle N(k_5,\vec{k}_{1\perp})\rangle$$

$$\times\delta_K(\vec{k}_{1\perp}+\vec{k}_{2\perp}-\vec{k}_{1'\perp}-\vec{k}_{2'\perp})\,\delta(W_1+W_2-W_{1'}-W_{2'}), \tag{A6}$$

where the summation over ν has been replaced with the integral over ν. The integration operator $\mathcal{g}_2$ acting on $\Phi\,\langle N(k_5,\vec{k}_1)\rangle$ is defined as

$$\mathcal{g}_2=\int_{-K_x/2}^{K_x/2}dk_1\int_{-K_x/2}^{K_x/2}dk_2\int_{-K_x/2}^{K_x/2}dk_3\int_{-K_x/2}^{K_x/2}dk_4\int_{-K_x/2}^{K_x/2}dk_5\int_{-K_x/2}^{K_x/2}dk_6\exp\Bigg(i\,\frac{2\pi}{K_x}[(\nu_2-\nu_{1'})(k_1+k_2)$$

$$+(\nu_2-\nu_{2'})(k_3+k_4)+(\nu_2-\nu_1)(k_5+k_6)]+\frac{i}{F}[(\overline{E}_{2x}-\overline{E}_{1'x})(k_1+k_2)+(\overline{E}_{2x}-\overline{E}_{2'x})(k_3+k_4)+(\overline{E}_{2x}-\overline{E}_{1x})(k_5+k_6)]$$

$$+\frac{\hbar^2}{6m_c}(k_1^3+k_2^3+k_3^3+k_4^3)+\frac{\hbar^2}{6m_1}(k_5^3+k_6^3)+\frac{\hbar^2}{6m_v}(k_7^3+k_8^3)\Bigg). \tag{A6a}$$

In Eqs. (A6) and (A6a) we have the relations

$$k_7=k_1+k_3+k_5,\quad k_8=k_2+k_4+k_6, \tag{A6b}$$

$$\overline{E}_{ix}=\frac{1}{K_x}\int_{-K_x/2}^{K_x/2}\frac{\hbar^2}{2m_i}\,k_{ix}^2\,dk_{ix}, \tag{A6c}$$

and

$$\Phi=D_1^*D_1+D_2^*D_2+(D_1^*-D_2^*)(D_1-D_2), \tag{A6d}$$

where $D_i=D_i(k_1,k_3,-k_5,k_7)$ and $D_i^*=D_i^*(-k_2,-k_4,k_6,-k_8)$ for D_i's defined by Eq. (2.9c) and (2.9d).

Now we simplify the calculation by considering D_1 and D_2 to be slowly varying functions of k_i's in comparison with the rest of the integrand in Eq. (A6). Then D_1 and D_2 are evaluated at $\vec{k}_{1'} = \vec{k}_{2'} = 0$ and at $\vec{k}_1$ satisfying $E_1(\vec{k}_1) = E_G$. This will be a reasonable approximation as far as an incident electron has a kinetic energy close to the band gap energy. Consequently we put $D_1 = D_2 = D$, resulting in the relation $f(121'2') = g(121'2')$.

By definition of

$$s_i = (\hbar^2/2m_c F)^{1/3} k_i ,$$

we obtain

$$\mathcal{R} = \frac{8\pi}{\hbar}\left(\frac{4\pi e^2}{\epsilon V}\right)^2 \left(\frac{V}{(2\pi)^3}\right)^3 \frac{2\pi}{L_x}\frac{1}{K_x^4}|D|^2\left(\frac{2m_c F}{\hbar^2}\right)^2 \int d\nu_1 \int d\nu_2 \int d\nu_{1'} \int d\nu_{2'}$$

$$\times \int d\vec{k}_{1\perp} \int d\vec{k}_{1'\perp} \int d\vec{k}_{2'\perp}\, \vartheta_0 \langle N(k_5, \vec{k}_{1\perp})\rangle \delta_K(\vec{k}_{1\perp} + \vec{k}_{2\perp} - \vec{k}_{1'\perp} - \vec{k}_{2'\perp})\, \delta(W_1 + W_2 - W_{1'} - W_{2'}) , \tag{A7}$$

where

$$\vartheta_0 = \int_{-s_0}^{s_0} ds_1 \int_{-s_0}^{s_0} ds_2 \int_{-s_0}^{s_0} ds_3 \int_{-s_0}^{s_0} ds_4 \int_{-s_0}^{s_0} ds_5 \int_{-s_0}^{s_0} ds_6 \cos\left(\frac{G_2 - G_{1'}}{G_0}(s_1 + s_2) + \frac{G_2 - G_{2'}}{G_0}(s_3 + s_4) + \frac{G_2 - G_1}{G_0}(s_5 + s_6)\right.$$

$$\left. + \tfrac{1}{3}(s_1^3 + s_2^3 + s_3^3 + s_4^3) + \frac{m_c}{m_1}(s_5^3 + s_6^3) + \mu(s_1 + s_3 + s_5)^3 + \mu(s_2 + s_4 + s_6)^3\right) \tag{A7a}$$

with

$$s_0 = \tfrac{1}{2}(\hbar^2/2m_c F)^{1/3} K_x ,$$

$$G_0 = (\hbar^2 F^2/2m_c)^{1/3} ,$$

$$\mu = m_c/m_v ,$$

and

$$G_i = 2\pi\nu_i F/k_x + \bar{E}_{ix} .$$

It is convenient to define new variables of integration $\vec{j}$ and $\vec{h}$ as

$$\vec{j} = \vec{k}_{1'\perp} + \vec{k}_{2'\perp} - [2\mu/(1+2\mu)]\vec{k}_{1\perp} \tag{A8a}$$

and

$$\vec{h} = \vec{k}_{1'\perp} - \vec{k}_{2'\perp} . \tag{A8b}$$

We obtain

$$W_1 + W_2 - W_{1'} - W_{2'} = \frac{\hbar^2}{2m_c}\left(\left(\tfrac{1}{2} + \mu\right) j^2 + \tfrac{1}{2} h^2 + \frac{\mu}{1+2\mu} k_{1\perp}^2 - \frac{2m_c}{\hbar^2}[E_{1\perp}(\vec{k}_{1\perp}) - G_s]\right) , \tag{A8c}$$

with

$$G_s = G_{1'} + G_{2'} - G_1 - G_2 + E_G .$$

For an incident electron with an energy $E_1(\vec{k}_1)$, $\mathcal{R}$ is given by

$$\mathcal{R} = 4\left(\frac{4\pi e^2}{\epsilon}\right)^2 \left(\frac{1}{2\pi}\right)^5 \frac{V}{L_x}\frac{m_c^2}{\hbar^5}|D|^2 \frac{1}{K_x^4}\left(\frac{2m_c F}{\hbar^2}\right)^{5/3} \frac{1}{1+2\mu} \int_0^{K_x/2} dk_{1x} \int d\nu_1 \int d\nu_2 \int d\nu_{1'} \int d\nu_{2'} \int k_{1\perp}\, dk_{1\perp}$$

$$\times I_0\left(E_{1\perp}(\vec{k}_{1\perp}) - \frac{\mu}{1+2\mu}\frac{\hbar^2}{2m_c} k_{1\perp}^2 - G_s\right)\langle N(E_1)\rangle , \tag{A9}$$

where

$$I_0 = \int_{-s_0}^{s_0} ds_1 \int_{-s_0}^{s_0} ds_2 \int_{-s_0}^{s_0} ds_3 \int_{-s_0}^{s_0} ds_4 \int_{-s_0}^{s_0} ds_5 \cos\left[\frac{G_2 - G_{1'}}{G_0}(s_1 + s_2) + \frac{G_2 - G_{2'}}{G_0}(s_3 + s_4) + \frac{G_2 - G_1}{G_0}(s_5 + s_6)\right.$$

$$\left. + \tfrac{1}{3}\left(s_1^3 + s_2^3 + s_3^3 + s_4^3 + \frac{m_c}{m_1}(s_5^3 + s_6^3) + \mu(s_1 + s_3 + s_5)^3 + \mu(s_2 + s_4 + s_6)^3\right)\right] \tag{A9a}$$

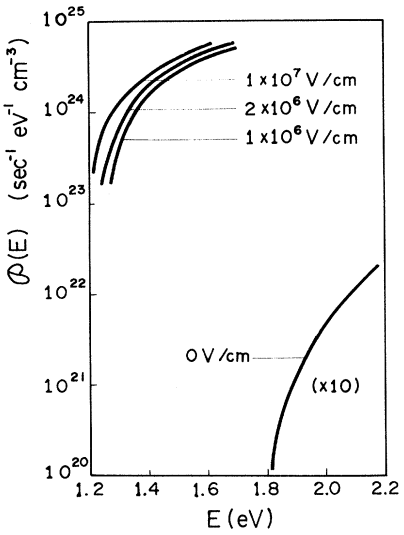

FIG. 2. Transition probability $\mathcal{P}(E)$ per unit time per unit volume per unit energy of impact ionization in GaAs as a function of energy of an incident electron with the field as a parameter.

with $s_6 = 2s_0 k_{1x}/K_x$. In Eq. (A9) the original notation is restored according to $k_5 \to -k_{1x}$. The integration should be performed in the range where the quantity in the square bracket is positive. Defining

$$\xi = (G_2 - G_{1'})/G_0 ,$$

$$\eta = (G_2 - G_{2'})/G_0 ,$$

and

$$\zeta = (G_2 - G_1)/G_0 ,$$

we make the transformation

$$\iiiint d\nu_1\, d\nu_2\, d\nu_{1'}\, d\nu_{2'} \ldots$$

$$= (K_x/2\pi F)^4 G_0^3 \iiiint dG_{2'}\, d\xi\, d\eta\, d\zeta \ldots .$$

Let us define the transition probability $\mathcal{P}(E_1)$ per unit time per unit volume per unit energy for an incident electron having an energy of E_1 as

$$\mathcal{R} = V \int \mathcal{P}(E_1) \langle N(E_1) \rangle\, dE_1 . \tag{A10}$$

Noting Eqs. (A4c)–(A4e) and $L_x^{-1} \int dG_{2'} = F$, we obtain from Eq. (A9)

$$\mathcal{P}(E_1) = 32\sqrt{2} \left(\frac{1}{2\pi}\right)^7 \left(\frac{e^2}{\epsilon}\right)^2 \frac{m_c^{9/2}}{\hbar^{10}}\, G_0\, \frac{1}{1+2\mu}\, |D|^2 \int_0^{E_1} dE_{1\perp}\, \frac{(1+2\alpha E_{1\perp})^{3/2}}{(E_1 - E_{1\perp})^{1/2}}\, I(E_{1\perp}) , \tag{A11}$$

where

$$I(E_{1\perp}) = \int_{-\infty}^{\infty} d\xi \int_{-\infty}^{\infty} d\eta \int_{-\infty}^{\infty} d\zeta \int_{-s_0}^{s_0} ds_1 \int_{-s_0}^{s_0} ds_2 \int_{-s_0}^{s_0} ds_3 \int_{-s_0}^{s_0} ds_4 \int_{-s_0}^{s_0} ds_5$$
$$\times \cos\{\xi(s_1+s_2) + \eta(s_3+s_4) + \zeta(s_5+s_6) + \tfrac{1}{3}[s_1^3 + s_2^3 + s_3^3 + s_4^3 + \beta(s_5^3 + s_6^3)$$
$$+ \mu(s_1+s_3+s_5)^3 + \mu(s_2+s_4+s_6)^3]\}[g(E_{1\perp}) + \xi + \eta - \zeta]\, G_0 \tag{A11a}$$

with

$$g(E_{1\perp}) = \left[E_{1\perp}\left(1 - \frac{\mu}{1+2\mu}\,(1+\alpha E_{1\perp})\right) - E_G\right] \Big/ G_0 \tag{A11b}$$

and

$$\beta = (1+2\alpha E_{1\perp})^{-1/2} .$$

Now let us transform Eq. (A11a) into a more tractable form. In place ot the integration

$$\int_{-\infty}^{\infty} d\xi \int_{-\infty}^{\infty} d\eta \int_{-\infty}^{\infty} d\zeta \ldots ,$$

we first perform the integration

$$\int_{-\xi_0}^{\xi_0} d\xi \int_{-\xi_0}^{\xi_0} d\eta \int_{-\xi_0}^{\xi_0} d\zeta \ldots ,$$

and then we make ξ_0 and ζ_0 infinite. Defining new variables $\sigma_1 = \frac{1}{2}(\xi + \eta)$ and $\sigma_2 = \frac{1}{2}(\xi - \eta)$, the integration is performed noting that the value of $[g(E_{1\perp}) + \sigma_1 - \zeta]$ should never be negative. After further integration over s_4 and s_5 we finally obtain the results given by Eq. (2.11)–(2.11b).

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