Hole impact ionization enhancement in $Al_xGa_{1-x}Sb$

Y. Jiang, M. C. Teich, and W. I. Wang

Center for Telecommunications Research, Department of Electrical Engineering, Columbia University, New York, New York 10027

The threshold energy and scattering rate for impact ionization in $Al_xGa_{1-x}Sb$ have been calculated for compositions x near the value where the spin-orbit-split gap Δ equals the band gap E_g. We have found that a minimum in the threshold energy for impact ionization near the $\Delta = E_g$ composition cannot explain the enhancement of the hole ionization coefficient, although it has been proposed as a possible mechanism. Rather, an increased scattering rate is responsible for this enhancement. It is caused by a minimum change of momentum in the hole ionization near the threshold and the mixing of an s-like state into the valence-like state induced by a composition disorder in this ternary compound. Our results indicate that the maximum hole ionization coefficient will occur at a composition x that lies between zero and the composition at which $\Delta = E_g$.

I. INTRODUCTION

Avalanche photodiodes (APDs) based on InGaAs/InP material are widely used in 1.3–1.55 μm lightwave communication systems. Unfortunately, they show poor noise performance because the ratio of the hole ionization coefficient to the electron ionization coefficient, $k = \beta / \alpha$, is about 2 in InP. Optimal performance, as is well known, is achieved with $k = 0$ or ∞.[1] APDs with noise performance as good as Si APDs, which are used in 0.8 μm systems and have typical values of $k \sim 0.02$, are desired. $Al_xGa_{1-x}Sb$ which, like InGaAs, has a band-gap wavelength lying in the 1.3–1.55 μm range, shows an enhanced hole ionization coefficient and has very large value of k when the composition x assumes a particular value.[2] In principle, this enables AlGaSb/GaSb-based APDs to achieve a lower excess noise factor, and a higher gain-bandwidth product than InGaAs/InP APDs. Indeed, Kuwatsuka *et al.*[3] recently demonstrated an AlGaSb/GaSb APD with a gain-bandwidth product of 90 GHz, which is the largest ever reported for long-wavelength APDs.

The resonant enhancement of the hole ionization coefficient in $Al_xGa_{1-x}Sb$, near the composition $x = x_0 = 0.065$ where the spin-orbit splitting Δ equals the band gap E_g, was first demonstrated experimentally by Hildebrand *et al.*[2] Vèrié *et al.*[4] demonstrated a similar effect in the $Hg_xCd_{1-x}Te$ system. However, the underlying explanation of the resonant enhancement has been controversial. Hildebrand *et al.* suggested that a minimum in the hole ionization threshold at the $\Delta = E_g$ composition may play an important role in the resonant enhancement, and even proposed that a new expression for the impact-ionization coefficient,

$$\beta \sim \exp\{ - [(E_{th} - E_g)/qF\lambda] \}, \qquad (1)$$

instead of the Shockley lucky drift formula,[5]

$$\beta \sim \exp [- (E_{th}/qF\lambda)], \qquad (2)$$

might be able to explain the resonant effect, where E_{th} is the threshold energy, F is the electrical field, and λ is the carrier mean free path. Kasemset[6] criticized this explanation, point-ing out that Eq. (1) is unphysical, and fitted the experimental data to the Shockley lucky drift formula with hole mean free path as long as 490 Å, suggesting that the long hole mean free path may provide the explanation of the enhancement. Capasso[7] suggested that the hole ionization rate may be enhanced principally by the fact that only a very small momentum, $\Delta k = k_i - k_f$, need be exchanged in the impact-ionization collision for an initial spin-split hole of momentum k_i near the threshold for x near x_0 to a final state of momentum k_f because the long-range nature of the Coulomb interaction leads the impact-ionization collision cross-section to be proportional to $1/\Delta k^4$. But this reasoning cannot explain why in the $Al_xGa_{1-x}Sb$ ternary system the hole ionization decreases when x decreases from x_0 to 0, because $\Delta k = 0$ at the threshold when x decreases from x_0 to 0.

Brennan *et al.*[8] have performed a Monte Carlo simulation of the hole ionization in $Al_xGa_{1-x}Sb$ for compositions x in which Δ is equal to or smaller than E_g. They find that in order to fit the hole ionization data at x near the value of x_0 obtained in Ref. 2, a very large value of the impact-ionization scattering rate must be assumed near the bottom of the split-off band. They also find that the minimum in the hole ionization threshold at the $\Delta = E_g$ composition accounts for only a small part of the resonant enhancement of the hole ionization coefficient. However, they do not provide an explanation of why the impact-ionization cross section takes on such a large value.

The ionization coefficient is determined both by the possibility that a carrier can initiate impact ionization (or impact-ionization scattering rate), and by the distribution of the carriers that can participate in the ionization interaction; this distribution is determined by the ionization threshold energy. Usually, most of the impact ionizations are initiated by carriers at or just above the threshold. The threshold and the scattering rate are very important in determining the impact-ionization rate of a material.

We calculated the ionization threshold energies for electrons and holes, and the hole ionization scattering rate, in the $Al_xGa_{1-x}Sb$ system for compositions x near the resonant

composition. The result of the threshold calculation is presented in Sec. II. Section III provides the results of the scattering-rate calculation. We find that $\Delta k = 0$ at threshold, by itself, is not the reason for the enhancement of the hole ionization; furthermore, $\Delta k = 0$ at threshold and the mixing of the s-like state into the valence-band state induced by a composition disorder in the ternary alloy, enhance the ionization scattering rate. This in turn, causes the enhancement of the hole ionization coefficient.

II. IMPACT IONIZATION THRESHOLD ENERGY

Unlike AlGaAs, AlGaSb (and a few other Sb-related compound semiconductors) have a very large spin-orbit-split gap. The GaSb band structure has $\Delta > E_g$. AlSb has $\Delta < E_g$ (Γ point). As x increases from 0 to 1, the value of Δ for $Al_x Ga_{1-x} Sb$ decreases slowly from 0.8 to 0.75 eV while E_g increases from 0.73 to 2.22 eV at the Γ point. For $Al_x Ga_{1-x} Sb$, $\Delta = E_g$ at $x = x_0 = 0.065$, $\Delta > E_g$ for $0 \leqslant x \leqslant x_0$, and $\Delta < E_g$ for $x_0 < x \leqslant 1$.

Our calculation of the GaSb and AlSb band structures is based on the k·p method.[9] The parameters used are from the *Handbook of Electronic Materials*[10] except that the band gap of GaSb is chosen to be 0.726 eV. The energy bands for $Al_x Ga_{1-x} Sb$ are obtained from a linear interpolation between those of GaSb and AlSb.

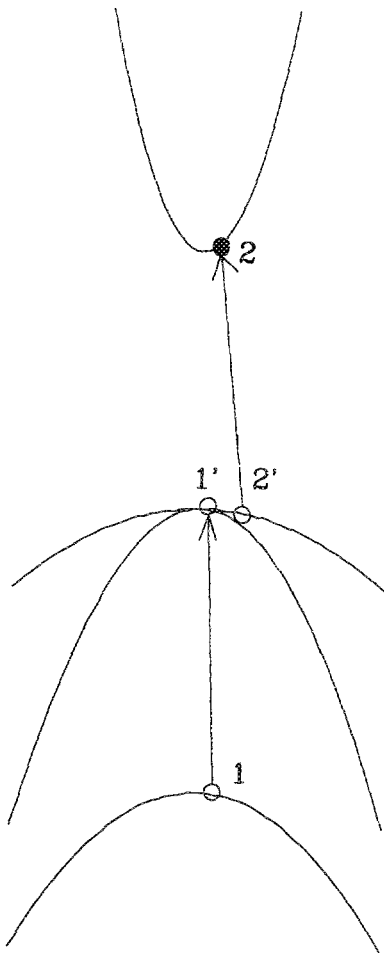With the parameters we use, the composition at which the band gap equals the split-off energy is $x_0 = 0.049$ instead of the more precisely calculated value of 0.065 reported in Ref. 2. But this value does not affect the theoretical calculation that explains the enhancement of the hole ionization coefficient.

The threshold energy is the lowest energy that a carrier must have to initiate an impact ionization while conserving energy and momentum. Figure 1 shows a split-off hole initiated impact-ionization. The split-off hole with momentum k_1 is scattered to a new heavy-hole state of momentum k'_1, creating an electron-hole pair with momentum k_2 and k'_2. The discussion below holds for both electron- and hole-initiated impact ionization.

In the process both momentum and energy are conserved:

$$k_1 = k'_1 + k'_2 - k_2, \tag{3}$$

$$E_1(k_1) = E_{1'}(k'_1) + E_{2'}(k'_2) - E_2(k_2). \tag{4}$$

Using the Lagrange multiplier method, we can obtain from (3) and (4) at the threshold,

$$\nabla_{k'_1} E_{1'}(k'_1) = \nabla_{k_2} E_2(k_2) = \nabla_{k'_2} E_{2'}(k'_2), \tag{5}$$

which is sometimes called Anderson and Crowell criteria[11] and is useful for numerical calculation. We must keep in mind that the validity of Eq. (5) depends on the continuity of the energy bands, which is not satisfied at the band edges. The hole ionization threshold energy calculation in Ref. 6 does not account for the invalidity of Eq. (5) at band edges, leading to an invalid calculation of the threshold energy.

We calculated the ionization threshold energies of $Al_x Ga_{1-x} Sb$ for $x \leqslant 0.2$. For $Al_x Ga_{1-x} Sb$ with $x > 0.025$, there is no electron ionization threshold in the (111) direction. The phenomenon that causes a reduction of the electron ionizations in the (111) direction, was first found in GaAs.[12] The electron ionization energies in (100) direction

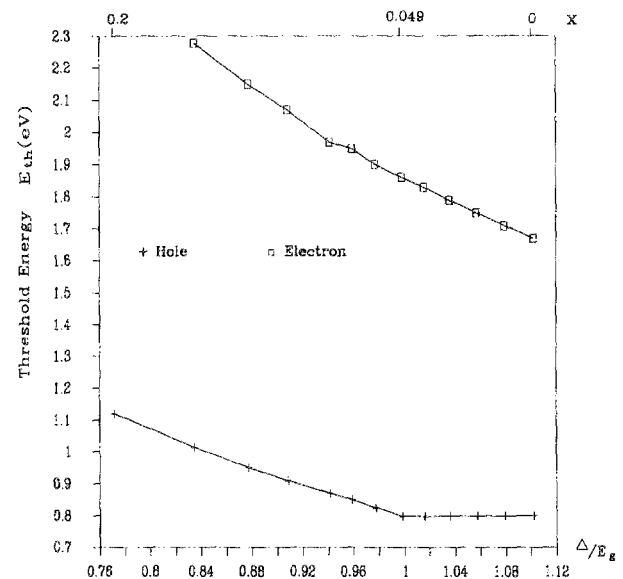FIG. 1. Split-off hole-initiated impact-ionization process.

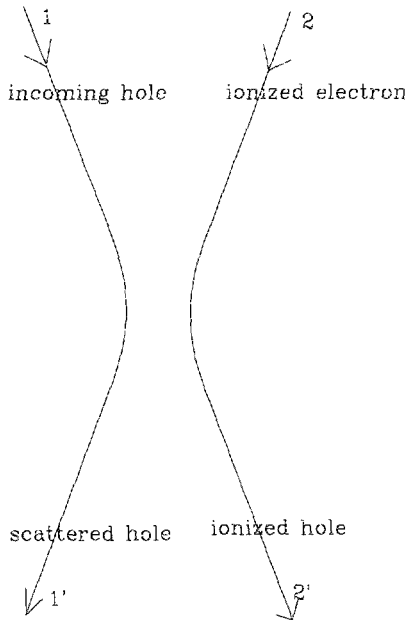FIG. 2. Threshold energy of impact ionization in AlGaSb.

FIG. 3. Hole initiated impact-ionization scattering diagram.

are higher than those reported in Ref. 2, which were calculated based on the assumption of the parabolic bands.

The spin-orbit split-off-hole initiated impact ionization achieves a much lower threshold energy than does the light-hole or the heavy-hole initiated impact ionization. For $\Delta \gg E_g$, or $x \ll x_0$, the threshold of the split-off hole is at the edge of the split-off band,

$$E_{th} = \Delta, \text{ and } k_{th} = 0. \tag{6}$$

For $\Delta < E_g$, or $x > x_0$, the threshold occurs higher than the edge of the split-off band.

From Fig. 2 we see that the hole threshold energy is just a little smaller at $x = x_0 = 0.049$, where $\Delta = E_g$, than at $x = 0$ where $\Delta > E_g$. That small change in threshold energy from $x = 0$ to $x = x_0$ is not significant enough to explain the large change in the hole ionization coefficient.

III. HOLE IMPACT IONIZATION SCATTERING RATE

For convenience in discussing hole-initiated impact ionization scattering, in Fig. 3 we represent the initiating hole and ionized electron with incoming arrows in the manner of a Feynman diagram. For an incident split-off hole of wave vector k_1 and spin s_1 which is scattered to state k_1' with spin s_2, and creates electron-hole pair with wave vectors k_2, k_2', and spins s_2, s_2', as shown in Fig. 1, the ionization rate $1/\tau$ is[13-15]

$$\frac{1}{\tau} = \left(\frac{2\pi}{\hbar}\right) \frac{1}{2} \sum_{s_1} \sum_{k_1' s_1'} \sum_{k_2 s_2} \sum_{k_2' s_2'} |\langle 2,2'|H_i|1,1'\rangle|^2$$
$$\times \delta(E_1 + E_1' - E_2 - E_2'), \tag{7}$$

where

$$H_i = \frac{1}{2} \int_V \int_V d^3 r \, d^3 r' \Psi^+(r) \Psi^+(r') \frac{e^2}{\epsilon} \frac{e^{-qr_{12}}}{r_{12}}$$
$$\times \Psi(r') \Psi(r), \tag{8}$$

and with

$$r_{12} = |r_1 - r_2|.$$

The dielectric constant is ϵ, the screening parameter is q,[16] V is the volume of the semiconductor, H_i is the Coulomb interaction Hamiltonian, and Ψ are the electron field operators. Ignoring the exchange term,

$$\langle 2,2'|H_i|1,1'\rangle = \int d^3 r_1 \, d^3 r_2 \phi_{k_1' s_1'}^*(r_1) \phi_{k_2' s_2'}^*(r_2) \frac{e^2}{\epsilon} \frac{e^{-qr_{12}}}{r_{12}} \phi_{k_1 s_1}(r_1) \phi_{k_2 s_2}(r_2)$$

$$= \int d^3 r_1 \, d^3 r_2 \phi_{k_1' s_1'}^*(r_1) \phi_{k_2' s_2'}^*(r_2) \sum_p \frac{1}{V} \frac{4\pi e^2}{\epsilon(p^2 + q^2)} e^{ip(r_1 - r_2)} \phi_{k_1 s_1}(r_1) \phi_{k_2 s_2}(r_2)$$

$$= \frac{4\pi e^2}{\epsilon V} \sum_p \frac{1}{p^2 + q^2} I_{oh}(k_1 s_1, k_1' s_1') I_{ch}(k_2 s_2, k_2' s_2') \delta_{k_1 + p, k_1'} \delta_{k_2 - p, k_2'}, \tag{9}$$

where c, o, h, and l represent the conduction band, orbit-spin split-off band, heavy-hole band, and light-hole band, respectively. Here φ_{ks} represent the electron states with momentum k and spin s, and

$$\phi_{k,s}(r) = e^{-ikr} u_{k,s}(r), \tag{10}$$

with periodic part u_{ks}.

$$I_{ij}(k s, k's') = \int_\Omega d^3 r u_{i,ks}^*(r) u_{j,k's'}(r). \tag{11}$$

Ω is the volume of a unit cell. If we define the overlap function as

$$G_{ij}(k,k') = \frac{1}{2} \sum_{s,s'} |I_{ij}(k s, k's')|^2, \tag{12}$$

then (7) becomes

$$\frac{1}{\tau} = 2\left(\frac{2\pi}{\hbar}\right)\int \frac{dk_2^3}{(2\pi)^3}\int \frac{dp^3}{(2\pi)^3}\left(\frac{4\pi e^2}{\epsilon}\right)^2\frac{1}{(p^2+q^2)^2}G_{oh}(\mathbf{k}_1,\mathbf{k}_1+\mathbf{p})G_{ch}(\mathbf{k}_2,\mathbf{k}_2-\mathbf{p})$$

$$\times \delta(E_1+E_1'-E_2-E_2'). \qquad (13)$$

Here we take V to the limit of infinity. Although the integrations in Eq. (13) appear to be over the entire momentum space, the actual integrations are limited by the δ function, which reflects the conservation of energy.

A. Scattering rate without composition disorder enhancement

From Kane's model,[17] the Bloch functions can be expressed in terms of an s-like atomic state $[S]$ and p-like atomic states $[X]$, $[Y]$, and $[Z]$. Using the same symbols that Kane uses, with the arrows representing the spins,

$$u_{h,\alpha} = [(X+iY)\uparrow]/\sqrt{2}, \quad u_{h,\beta} = [(X-iY)\downarrow]/\sqrt{2},$$

$$u_{i,\alpha} = a_i[iS\downarrow] + b_i[(X-iY)\uparrow]/\sqrt{2} + c_i[Z\downarrow], \quad (14)$$

$$u_{i,\beta} = a_i[iS\uparrow] + b_i[-(X+iY)\downarrow]/\sqrt{2} + c_i[Z\uparrow],$$

where $i = c, l, o$, and

$$a_i = kP(E_i'+2\Delta/3)/N,$$

$$b_i = (\sqrt{2}\Delta/3)(E_i'-E_g)/N, \quad (15)$$

$$c_i = (E_i'+2\Delta/3)(E_i'-E_g)/N,$$

where P is the value of the momentum matrix element, and E_i' are the roots of

$$E'(E'-E_g)(E'+\Delta)-(kP)^2(E'+2\Delta/3)=0. \quad (16)$$

Therefore,

$$I_{ih}(\mathbf{k}\alpha,\mathbf{k}'\alpha) = -\left(\frac{b_i(k)}{2}+\frac{c_i(k)}{\sqrt{2}}\right)\sin\theta\sin\frac{\theta}{2}, \quad (17)$$

$$I_{ih}(\mathbf{k}\alpha,\mathbf{k}'\beta) = -\left(\frac{b_i(k)}{2}+\frac{c_i(k)}{\sqrt{2}}\right)\sin\theta\cos\frac{\theta}{2}, \quad (18)$$

and the overlap functions

$$G_{ih}(\mathbf{k},\mathbf{k}') = \tfrac{1}{2}\left[b_i(k)/\sqrt{2}+c_i(k)\right]^2\sin^2\theta, \quad (19)$$

$$G_{ij}(\mathbf{k},\mathbf{k}') = [a_i^*a_j+(b_i^*b_j+c_i^*c_j)\cos\theta]^2$$

$$+\frac{1}{2}\left(\frac{1}{\sqrt{2}}b_i^*b_j-b_i^*c_j-c_i^*b_j\right)^2\sin^2\theta, \quad (20)$$

where θ is the angle between k and k'.

Without simplification, it is difficult to calculate the sixth order integration in Eq. (13). If we assume that the bands are parabolic, we can analytically carry out all but one of the angular integrations in Eq. (13) and obtain an expression with a triple integral, which can be calculated numerically. Because the assumption of parabolic bands is only satisfactory for states near the band edges we can calculate, with acceptable accuracy, only the scattering rates involving states near the band edges. The calculation for x, when it lies between 0 and just over x_0, is within this limitation. The result is shown in Fig. 4.

The value of q is very small, almost zero, in this case. For $0 \leqslant x \leqslant x_0$, the threshold is at the split-off band edge, and $\Delta k = 0$, and the denominator $[(\Delta k)^2+q^2]^2$ of the integrand in Eq. (13) is at the minimum and is almost zero at the threshold. However, if no other factors are involved, the integrand is zero nevertheless because the overlap function is zero at $\Delta k = 0$. That leads to a scattering rate of zero at threshold. This means that most of the hole impact ionizations are not initiated near the threshold. This may also be described in terms of the effective threshold energy being higher than the threshold energy determined by energy and momentum conservation.[7]

Beside the overlap function being zero, the density of the final states of scattering by an initiating hole near the threshold in $Al_xGa_{1-x}Sb$ with $x = 0$ is larger than that with $x = x_0$. In other words, the integration volume for the integral of Eq. (13) is larger for $x = 0$ than for $x = x_0$. That is why the scattering rate decreases as x increases from $x = 0$ to $x = x_0$ in Fig. 4. This result conflicts with the experimental hole ionization coefficient enhancement. Thus, the band-structure feature $\Delta = E_g$ cannot by itself explain the enhancement. It is clear that the fact that $\Delta k = 0$ for composition $\Delta \geqslant E_g$ cannot alone explain the enhancement of the scattering rate.

For compositions where $x > x_0$, $E_g > \Delta$ and the scattering rate is small and increases with E_1 slowly, because $\Delta k = 0$ no longer holds at threshold.
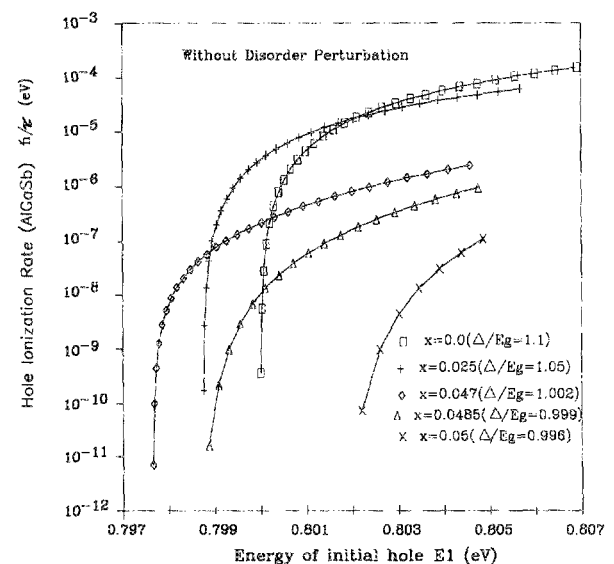

FIG. 4. Hole initiated impact-ionization scattering rate without composition disorder-induced enhancement.

B. Scattering rate with composition disorder enhancement

In the study of the lasing properties of III-V compound semiconductors for long wavelength lasers, AlGaSb has been found to have a very large Auger recombination rate. In explaining the enhancement of the Auger recombination in ternary compounds, Takeshima[18] pointed out that the enhancement is caused by the composition disorder induced mixing of an s-like state into the valence-band state. Because impact ionization is the reverse process of Auger recombination, it should also be enhanced by the same mechanism.

To some degree, this order destroys the orthogonality of the wave functions of the original system. In fiber optics, this order induces mode mixing. In semiconductors, this order induces mixing among electron energy bands.

A detailed discussion of composition disorder induced band mixing can be found in Chadi's work.[19] In a ternary compound $A_x B_{1-x} C$, A atoms and B atoms are distributed randomly over the anion (cation) sites; therefore, the electrons in the crystal see random variation of the potential at the anion (cation) sites over the average periodic potential. The variation in the potential, which is a perturbation to the periodic potential,[18] induces the mixing of an s-like state with the valence state. Assuming that the perturbation potential is $U(r)$, with l and n representing the band index, we have

$$\langle l \mathbf{k}' | U | n \mathbf{k} \rangle = U_{ln} \delta_{\mathbf{k}', \mathbf{k}}, \tag{21}$$

to first order,

$$\phi_{n\mathbf{k}}^{(1)} = \phi_{n\mathbf{k}}^{(0)} + \sum_{l \neq n} \phi_{l\mathbf{k}}^{(0)} \frac{U_{ln}}{E_n(\mathbf{k}) - E_l(\mathbf{k})}, \tag{22}$$

$$u_{n\mathbf{k}}^{(1)} = u_{n\mathbf{k}}^{(0)} + \sum_{l \neq n} u_{l\mathbf{k}}^{(0)} \frac{U_{ln}}{E_n(\mathbf{k}) - E_l(\mathbf{k})}, \tag{23}$$

$$I_{ch}^{(1)}(\mathbf{k}, \mathbf{k}') = I_{ch}^{(0)}(\mathbf{k}, \mathbf{k}'), \tag{24}$$

$$I_{oh}^{(1)}(\mathbf{k}, \mathbf{k}') = I_{oh}^{(0)}(\mathbf{k}, \mathbf{k}') + \frac{U_{oc} U_{ch}}{E_G(E_G + \Delta)} I_{cc}^{(0)}(\mathbf{k}, \mathbf{k}'), \tag{25}$$

where the unperturbed terms are those given in last section. The overlap functions

$$G_{ch}^{(1)}(\mathbf{k}, \mathbf{k}') = G_{ch}^{(0)}(\mathbf{k}, \mathbf{k}'), \tag{26}$$

$$G_{oh}^{(1)}(\mathbf{k}, \mathbf{k}') = G_{oh}^{(0)}(\mathbf{k}, \mathbf{k}') + \gamma G_{cc}^{(0)}(\mathbf{k}, \mathbf{k}'), \tag{27}$$

where

$$\gamma = \left(\frac{U_{oc} U_{ch}}{E_G(E_G + \Delta)} \right)^2. \tag{28}$$

The quantity γ can be calculated as in Refs. 18 and 19.

Because of the composition disorder, the overlap function is no longer zero at $\Delta k = 0$. Thus, together with the fact that $\Delta k = 0$ at threshold for $x \leqslant x_0$, greatly enhances the scattering rate.

The calculated result is shown in Fig. 5. It is clear that the impact ionization scattering rate near threshold for $0 < x \leqslant x_0$ is greatly enhanced. The enhancement decreases as x approaches zero and the $\Delta = E_g$ composition. For $x = 0$ the mixing is zero, and the overlap function is zero at $\Delta k = 0$ and the integral of Eq. (13) is small. As x increases, the
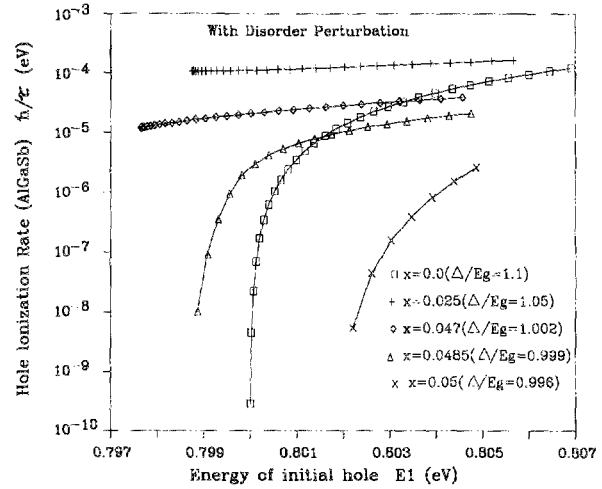

FIG. 5. Hole initiated impact-ionization scattering rate with composition disorder-induced enhancement.

overlap function increases at $\Delta k = 0$. Because the denominator of the integrand is nearly zero at $\Delta k = 0$, the integrand is very large and nearly infinity, although x is small and there is just a small amount of band mixing. This leads to large enhancement of the scattering rate as x increases from 0. As shown in Fig. 5, the scattering rate $\hbar/\tau$ at threshold for $x = 0.25$ is about 10^{-4} eV comparing to 0 of the result in last section. However as x increases to x_0 the density of the final states of the impact ionization with $\Delta k = 0$ decreases, as we discussed in the last section, so that the scattering rate decreases, despite the overlap function increases. This means that the maximum hole ionization coefficient will occur for x between 0 and x_0, but not at x_0 as suggested in Ref. 2.

IV. CONCLUSION

The enhancement of the hole impact ionization coefficient near the $\Delta = E_g$ composition can be explained by the enhancement of the ionization scattering rate, as is shown in the Monte Carlo simulation.[8] The enhancement of the scattering rate is obtained by virtue of the fact that $\Delta k = 0$ at threshold and the mixing of the s-like state into the valence state induced by the composition disorder in ternary compounds. The calculated result indicates that the maximum hole ionization coefficient should occur for x between zero and the $\Delta = E_g$ composition. Our result is consistent with the conclusions drawn from the Monte Carlo simulation.

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