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13. ABSTRACT (Maximum 200 words)

We have completed our Monte Carlo approach to impact ionization of electrons in GaAs, InP and InAs and most recently in $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$. We find that in all these materials the ionization mechanism is quantitatively different to what has been described in previous simplified models, such as Shockley's lucky electron theory. The dependence on the electric field is markedly different in $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$.

With regard to quantum transport, we have investigated the concepts of conductance and capacitance on a general basis and have developed criteria for the additivity of conductance in parallel mesoscopic channels.

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Thresholds of impact ionization in semiconductors

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Using a first-principles approach to the ionization rate, we re-examine some of the prejudices concerning impact ionization and offer a new view of the role of thresholds. We also discuss trends of ionization coefficients related to the energy band structure for silicon and a number of III-V compounds.

I. INTRODUCTION

Impact ionization (the exact inverse of the Auger process) in semiconductors has been studied extensively since the first theoretical investigations of hot carrier transport. It is now generally agreed that an accurate treatment of the ionization process itself requires a full band structure model and the associated complexities. In addition, the large phase space relevant for the two-particle inverse Auger process makes an analytic solution impossible, and only detailed numerical calculations can offer an idea of the magnitude of the matrix elements for the process. The earliest attempts to understand impact ionization have bypassed these difficulties and instead focused on simple "intuitive" concepts such as an electron temperature model, the lucky electron models of Shockley,¹ and others,^{2,3} and various models for important parameters of the theory or what has been perceived to be an important parameter. Prominent among these are the phonon mean-free path, the ionization threshold (the energy below which impact ionization can not occur), and the average energy of net emitted phonons. In addition, one needs various parameters of the energy band structure which, of course, influence both threshold and phonon scattering. It was shown subsequently by Shichijo and Hess⁴ that the energy dependence of phonon scattering is significant and its variations with energy influence the statistics of electrons enormously. One therefore must include a complete energy band structure or at least a strongly energy-dependent density of states to obtain the correct attempt frequency of electrons above the threshold to impact ionize. To obtain rates of impact ionization one needs to multiply this attempt frequency by the probability of the ionization event. This probability was virtually exclusively obtained from a formula derived by Keldysh.⁵ This formula cannot, unfortunately, account for the complexities introduced by the Bloch functions or an energy band structure with its minima at more than one symmetry point (typically at Γ , X , and L in the technologically important semiconductors). The problems of the Keldysh formula were first signaled by a numerical calculation of Kane⁶ which showed that the ionization rate of silicon increases above the threshold much more softly than predicted by Keldysh. Another set of difficulties becomes apparent from discussions by Capasso regarding the uncertainty principle.⁷ Since the electron system is in contact with a phonon bath, it does not form a Hamiltonian system, and therefore does not have a

strict threshold at all. This was quantitatively shown by Bude *et al.*⁸ who also showed that the high electric fields which are typically present when ionization becomes important have a significant influence on threshold and the softness of the rate. We show that as a consequence of these facts, many of the theoretical discussions in journals and textbooks⁹⁻¹¹ are misleading or even completely wrong.¹² A typical example is the calculation of threshold energy using the effective masses of the band edges.

Questions such as the dependence of ionization rates on the crystallographic direction need even more careful consideration. As an example, we will discuss the k -dependent ionization thresholds, revisiting the treatment of Anderson and Crowell.¹³

Our findings show that the concept of hard thresholds for the impact ionization rate needs to be abandoned for all materials which we have investigated. Our numerical simulations have instead shown effective thresholds which are significantly higher in the bands than the laws of energy and momentum conservation dictate. The existence of a threshold by itself cannot be deduced with physical rigor since the system of electrons is not Hamiltonian. The phonon bath plays an important role and broadens the threshold.⁸ Also, strong electric fields, usually present, exert a similar influence due to the intracollisional field effect.

An even more important factor for the effective threshold is the functional form of the density of states in the respective semiconductor. The minima of highest density of states (usually at X) play, therefore, a significant role for the location of the effective threshold. The density of states also deeply influences the magnitude of the average energy of the electrons. This magnitude in turn determines whether the ionization occurs due to electrons of the "bulk" or "center" of the distribution function or due to a few lucky ones as postulated by Shockley. The correlation of effective threshold and average energy to the density of states works against Shockley's lucky electron theory as far as the impact ionization coefficients (α and β) are concerned. The functional dependence of α and β on the field [$\exp(c/F)$ or $\exp(c/F^2)$] is also closely correlated to the rise of the density of states in the important energy range and not as much, as is claimed in most textbooks (including Ref. 14), on the question of whether lucky electrons are important for the ionization or not. We realize that our findings represent a very significant deviation from the conventional picture of impact ionization in semiconductors.

Our claims are not absolute in the sense that we can back them by mathematical proof. We can prove them only by computer experiments for a limited but important class of semiconductor materials. We believe that our computer experiments, which combine and optimize the numerical approaches of Kane,⁶ Baraff,¹⁵ and Hess and Shichijo,⁴ are the most complete hitherto preformed. They still are not based on exact band structures or scattering rates but on what one obtains within the framework of empirical pseudopotentials. This fact, however, should not influence the "bigger picture" that is discussed here.

II. THE WAVE VECTOR DEPENDENT THRESHOLD ENERGY AND RESULTS FOR THE RATE IN SILICON

The first paper to carefully consider extending the threshold energy concept to realistic band structures suggested that because of the anisotropy and the multiplicity of bands in real crystals, the threshold energy should be defined as a function of direction in the crystal.¹³ An electron with a given initial wave vector, $\mathbf{k}_1$, could impact ionize only if its energy exceeded a minimum energy, $E_{th}(\hat{\mathbf{k}}_1)$, where $\hat{\mathbf{k}}_1$ is the unit normal in the $\mathbf{k}_1$ direction. Here, we review the approach used by Anderson and Crowell¹³ to calculate $E_{th}(\mathbf{k}_1)$, and demonstrate an inconsistency which exaggerates the importance of wave vector dependent thresholds of the wave vector anisotropy of the ionization rate.

First, we define the particles involved in the electron ionization process; considerations for the hole process follow in the same manner. Let $\mathbf{k}_1$ be the initial wave vectors for a conduction band electron which collides with a valence band electron of wave vector $\mathbf{k}_2$. The two final states are conduction band states of wave vector $\mathbf{k}_3$ and $\mathbf{k}_4$. In the semiclassical approximation, energy is conserved. Furthermore, the matrix element for the electron-electron interaction enforces crystal momentum conservation, and we can write

$$\mathbf{k}_1 = \mathbf{k}_3 + \mathbf{k}_4 - \mathbf{k}_2 + \mathbf{G}, \quad (1)$$

$$E_{n_1}(\mathbf{k}_1) = E_{n_3}(\mathbf{k}_3) + E_{n_4}(\mathbf{k}_4) - E_{n_2}(\mathbf{k}_2), \quad (2)$$

where $\mathbf{G}$ is a reciprocal lattice vector and $E_n(\mathbf{k})$ is the energy of an electron in band n with wave vector $\mathbf{k}$.

Given an initial $\mathbf{k}_1$, one can search all possible sets of $\mathbf{k}_3$, $\mathbf{k}_4$, $\mathbf{k}_2$, and $\mathbf{G}$ satisfying (1) and (2) to find the minimum energy that the incident particle *could* have, $E_m(\mathbf{k}_1)$. If the actual energy of the initial state $E_{n_1}(\mathbf{k}_1)$ is greater than $E_m(\mathbf{k}_1)$, then the impact ionization rate could be finite for this carrier. If $E_m(\mathbf{k}_1) > E_{n_1}(\mathbf{k}_1)$ for all n_1 , then impact ionization is impossible for a carrier with wave vector $\mathbf{k}_1$. $E_{th}(\hat{\mathbf{k}})$ is defined as follows: for a given direction in the Brillouin zone, $\hat{\mathbf{k}}$, E_m and E_{n_1} are compared. The possible values of $E_{th}(\hat{\mathbf{k}})$ are given by the energies where $E_m(\mathbf{k}) = E_{n_1}(\mathbf{k})$ as $\mathbf{k}$ varies along the direction $\hat{\mathbf{k}}$.¹³ Then,

$$E_{th}(\hat{\mathbf{k}}) \equiv \min_{\alpha, n_1} [E_m(\mathbf{k}) : E_m(\mathbf{k}) = E_{n_1}(\mathbf{k})],$$

$$\mathbf{k} = \alpha \hat{\mathbf{k}} \in BZ],$$

$$E_m(\mathbf{k}) = \min_{G, \mathbf{k}_3, n_3, \mathbf{k}_4, n_4} [E_{n_3}(\mathbf{k}_3) + E_{n_4}(\mathbf{k}_4) - E_{n_2}(\mathbf{k}_2)],$$

$$\mathbf{k}_3 + \mathbf{k}_4 - \mathbf{k}_2 + \mathbf{G} = \mathbf{k}. \quad (3)$$

An application of the Lagrange multiplier rule to the constrained minimum in (3) requires that the group velocities of states 2, 3, and 4 be equal.

$$\nabla E_{n_2}(\mathbf{k}_2) = \nabla E_{n_3}(\mathbf{k}_3) = \nabla E_{n_4}(\mathbf{k}_4). \quad (4)$$

This is a necessary condition for minimization. A minimum is guaranteed to exist since E_{n_3} and E_{n_4} are bounded from below and E_{n_2} is bounded from above. Of all the states 2, 3, and 4 for which the group velocities are equal, it is simple to choose the one which corresponds to the absolute minimum required in (3).

Although the above definition of $E_{th}(\hat{\mathbf{k}})$ describes whether or not an electron in a certain direction can impact ionize, the behavior of the rate beyond this threshold is unclear. If one assumes that it increases rapidly beyond the threshold, then this theory provides an extension of the energy-dependent thresholds of Keldysh and Shockley.

The problem as stated above has not been solved correctly in the original paper by Anderson and Crowell.¹³ They propose that in evaluating E_m for a given $\mathbf{k}$, the minimization over $\mathbf{k}_2$, $\mathbf{k}_3$, and $\mathbf{k}_4$ is achieved by states which are parallel:

$$\frac{\mathbf{k}_2}{|\mathbf{k}_2|} = \frac{\mathbf{k}_3}{|\mathbf{k}_3|} = \frac{\mathbf{k}_4}{|\mathbf{k}_4|} = \hat{\mathbf{k}}. \quad (5)$$

Consequently, their search for solutions of (4) extends only over the subset of states 2, 3, and 4 satisfying (5). Since their search range is drastically reduced, solutions for $E_{th}(\mathbf{k})$ were easily accomplished numerically. The actual solution of these equations requires considerably more effort.

Clearly, the solution for E_m requires a minimization over all values of $\mathbf{k}_2$, $\mathbf{k}_3$, and $\mathbf{k}_4$ for a given $\mathbf{k}$. Only if the bands are isotropic is the solution for E_m achieved by parallel states. To demonstrate this we propose the following simple example. Instead of using spherical-parabolic bands, we take ellipsoidal-parabolic bands in two dimensions:

$$E_c = \alpha_x k_x^2 + \alpha_y k_y^2, \quad (6)$$

$$E_v = -E_g - \beta(k_x^2 + k_y^2), \quad (7)$$

where E_c and E_v correspond to the conduction and valence bands, respectively, and E_g to the band gap energy. Applying (4) and $\mathbf{k}_3 + \mathbf{k}_4 - \mathbf{k}_2 = \mathbf{k}$ to the bands defined in (6) requires that the minimum in $E_m(\mathbf{k})$ be achieved by states satisfying

$$k_{x_3} = k_{x_4} = \beta(\alpha_x + 2\beta)^{-1} k_x, \quad (8)$$

$$k_{y_3} = k_{y_4} = \beta(\alpha_y + 2\beta)^{-1} k_y, \quad (9)$$

$$k_{x_2} = [2\beta(\alpha_x + 2\beta)^{-1} - 1] k_x, \quad (10)$$

TABLE I. Wave vector dependent threshold in silicon.

Direction	Threshold (eV)	k_1	k_2	k_3	k_4
Anderson and Crowell					
$\langle 100 \rangle$	1.1	-0.40(1,0,0)	0.00(1,0,0)	0.80(1,0,0)	0.80(1,0,0)
$\langle 110 \rangle$	2.1	-0.47(1,1,0)	0.19(1,0,0)	0.86(1,1,0)	0.86(1,1,0)
$\langle 111 \rangle$	3.1	-0.02(1,1,1)	0.00(1,1,1)	0.99(1,1,1)	0.99(1,1,1)
Czajkowski <i>et al.</i>					
$\langle 100 \rangle$	1.18	-0.36(1,0,0)	0.01(1,0,0)	0.82(1,0,0)	0.82(1,0,0)
$\langle 110 \rangle$	2.10	-0.69(1,1,0)	0.31(1,0,0)	1.22(1,1,0)	1.22(1,1,0)
$\langle 111 \rangle$	3.39	-0.07(1,1,1)	0.01(1,1,1)	0.84(1,1,1)	0.84(1,1,1)

$$k_{y_2} = [2\beta(\alpha_y + 2\beta)^{-1} - 1]k_y. \quad (11)$$

These minimizing states are parallel to the initial state k only when $\alpha_x = \alpha_y$. Therefore, in general, for complicated band structures there is no simple relationship between the directions of the minimizing states and the initial state.

In silicon, in which the minimum of the conduction bands is at the X point, this error is particularly bad. Listed in Table I are typical results (Anderson and Crowell¹³ and Czajkowski *et al.*¹⁶) for the lowest thresholds in several symmetry directions in Si with wave vectors of the "threshold" states.

According to Table I, the threshold in the $\langle 111 \rangle$ direction in Si is greater than 3.0 eV, and therefore, the only initial states in the $\langle 111 \rangle$ direction which can impact ionize must have an energy of at least 3 eV. In Fig. 1 we show our results which demonstrate that it is clearly possible for electrons along the $\langle 111 \rangle$ direction with energies much less than 3 eV to impact ionize. Figure 2 shows the pseudopotential band structure in these crystallographic directions. The ionization rate is nonzero and large in the $\langle 111 \rangle$ direction even at electron energies as low as 2.2 eV. This directly contradicts the results shown in Table I which

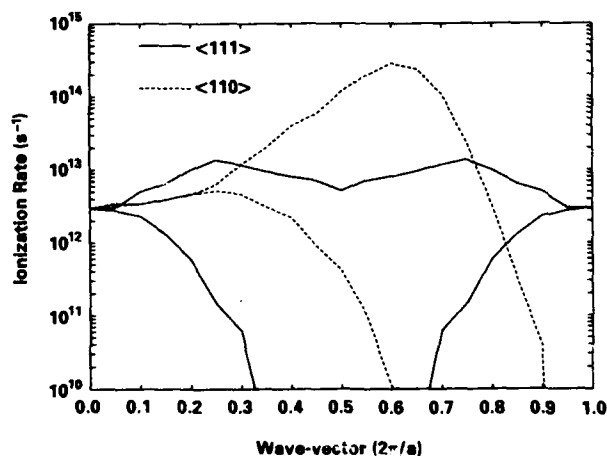


FIG. 1. Ionization rates in silicon for the two lowest conduction bands as a function of wave vector. Upper curves, second band; lower curves, first band. These results are obtained as described in Ref. 8 and are in agreement with Kane's theory (Ref. 6).

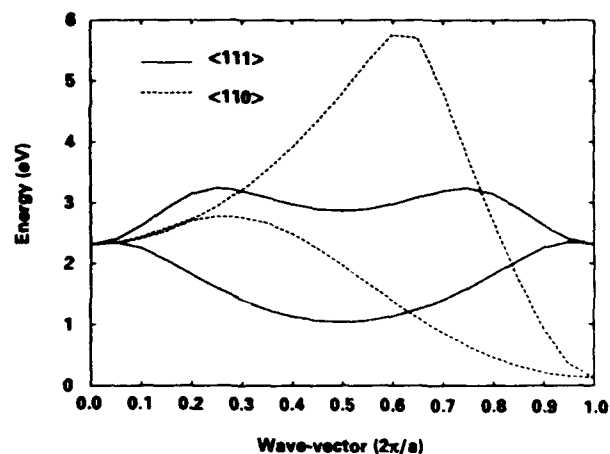


FIG. 2. Band structure of silicon for two lowest conduction bands as a function of wave vector. Upper curves, second band; lower curves, first band.

suggest that in the $\langle 111 \rangle$ direction, only electrons whose energy is greater than 3.1 eV can impact ionize. The same is true of the ionization rate in the $\langle 110 \rangle$ direction. The thresholds derived in the simplified manner of Anderson and Crowell are therefore inaccurate. Note that in all subsequent publications known to the authors, it was this simplified inaccurate model of thresholds that has been used. In addition, the wave vector dependent thresholds in Eq. (3) can tell little about the actual behavior of the ionization rate for energies above E_{th} since they distinguish only if a particular electron *can* ionize as a function of its direction and tell nothing about the actual behavior of the ionization rate for energies above $E_{th}(\hat{k})$.

We would also like to reiterate that a quantum treatment of the electrons and the phonon bath does not result in any absolute threshold at all due to collision broadening and the intracollisional field effect. In the following, we ignore this "smearing out" and show that the semiclassical inclusion of band structure and phonon scattering alone is sufficient to justify the concept of an effective threshold which is typically even higher than that of Anderson-Crowell and which shows, in the cases which we have considered in our computer experiments, very little anisotropy with respect to the crystallographic direction.

III. IMPACT IONIZATION IN POLAR SEMICONDUCTORS

In this section, we examine the average energy-dependent ionization rates of several important III-V compounds and the influence of these rates on bulk transport. We use the same theory as developed for silicon.^{6,8} Of special importance for our considerations is the average

ionization rate for electrons of a given energy which can be expressed as

$$R_{\text{ave}}(E) = \frac{\sum_n \int_{BZ} d^3k R_n(\mathbf{k}) \delta[E_n(\mathbf{k}) - E]}{\sum_n \int_{BZ} d^3k \delta[E_n(\mathbf{k}) - E]} = \frac{\sum_n \int_{BZ} d^3k R_n(\mathbf{k}) \delta[E_n(\mathbf{k}) - E]}{G(E)}, \quad (12)$$

where $R_n(\mathbf{k})$ is the ionization rate (transition probability per unit time) for an electron with wave vector $\mathbf{k}$ and band index n . The total density of states at energy E is $G(E)$, and $\int_{BZ} d^3k$ is an integration over the first Brillouin zone. Our theory for $R_n(\mathbf{k})$ is, as mentioned, very similar to the theory of Kane, and has been described in Refs. 6 and 8 extensively. Below, we review some of the salient features for this theory and present the results of our computer experiments.

A. Energy dependent ionization rates

Two quantities strongly influence the energy-dependent ionization rate: the threshold energy itself, and its hardness or softness (how impact ionization and phonon scattering compete). The Keldysh formula,⁵

$$R_{\text{Keld}}(E) = \frac{P}{\tau_{\text{ph}}(E_{\text{th}})} \left(\frac{E - E_{\text{th}}}{E_{\text{th}}} \right)^2, \quad E > E_{\text{th}} = 0, \quad E < E_{\text{th}} \quad (13)$$

has two adjustable parameters for a given phonon scattering rate $\tau_{\text{ph}} - E_{\text{th}}$, which is the threshold energy, and P which is a measure of the hardness of the threshold. (Actually, P is probably a better measure of the hardness of the threshold if the phonon energy relaxation rate is used in place of τ_{ph} .¹⁷) Monte Carlo (MC) calculations, which use the Keldysh formula, have deduced a relatively hard ionization threshold for most III-V semiconductors such as GaAs, and a soft threshold for Si.^{4,18-21} Although used in most high field transport simulations, the Keldysh formula applies only to materials with parabolic bands and a direct band gap. Real materials deviate significantly from this simple model band structure. It also does not represent a good parametrization of a general ionization rate since it allows only for a quadratic dependence on energy.

A direct calculation of (12) entails considerable computational effort, and has until now been carried out only for Si.⁶ Here, we present for the first time the energy dependent ionization rates for the III-V materials GaAs, InAs, InP, and the alloy $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$. The calculations have used a model similar to the Kane model for impact ionization⁶ for the semiclassical ionization rates in which local empirical pseudopotential methods were used to calculate the band structure and wave functions for each material.²³ Band structure fits were made to experimentally determined quantities as referenced in Refs. 21 and 24. Representative band structure parameters for these materials are shown in Table II. The density of states (DOS) for each material is plotted in Fig. 3.

There is one inconsistency in our $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$ band structure. While most parameters such as the band gap and the effective masses are easily fit, the Γ to L intervalley

TABLE II. Band structure parameters.

Material	E_{gap}	$E_{\Gamma-L}$	$E_{\Gamma-X}$	m_{Γ}^*
GaAs	1.4	0.25	0.32	0.067
InAs	0.32	1.10	1.75	0.032
InP	1.3	0.75	1.20	0.075
$\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$	0.75	0.78	1.10	0.041

separation $E_{\Gamma-L}$ turns out to be about 0.78 eV, a typical result for pseudopotential and kp theory,²¹ whereas some measurements have shown a separation of 0.55 eV.²⁵ In general, the pseudopotential minimum separation is not as precise as desirable (see the results for GaAs in Table II). Also, the split-off bands have not been accurately modeled using local pseudopotentials. However, they contribute very little to the ionization rate because of their relatively small density of states. Therefore, the local pseudopotentials without spin-orbit effects should give a fairly accurate estimation of the ionization rate, particularly, if one keeps in mind that the valley separation energy should be somewhat shifted.

In going from GaAs to InAs, the band gap shrinks from 1.4 to 0.32 eV while the $\Gamma-X$ and $\Gamma-L$ intervalley separations rise dramatically. This leads to a very small density of states for low energies in InAs and $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$ compared to that in GaAs. However, InP lies between these extremes in that it has a large band gap but the $\Gamma-X$ and $\Gamma-L$ intervalley separations are rather large. These band structure features lead to two very distinct behaviors for the bulk ionization coefficient as will be shown below.

Shown in Fig. 4 are the calculated results for the energy-dependent ionization rates for GaAs, InAs, InP, and $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$. Plotted along with each rate for comparison are Keldysh formula ionization rates, which are typical of those used in Monte Carlo simulations¹⁹ (parameters taken from Ref. 21).

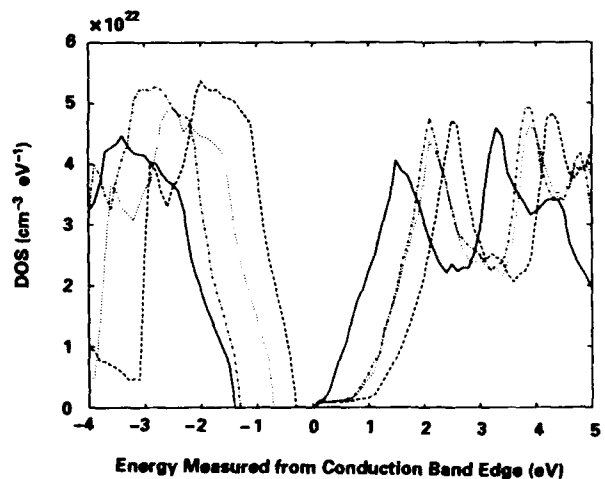


FIG. 3. DOS: solid line, GaAs; dashed line, InAs; dot-dashed line: InP, and dotted line: $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$.

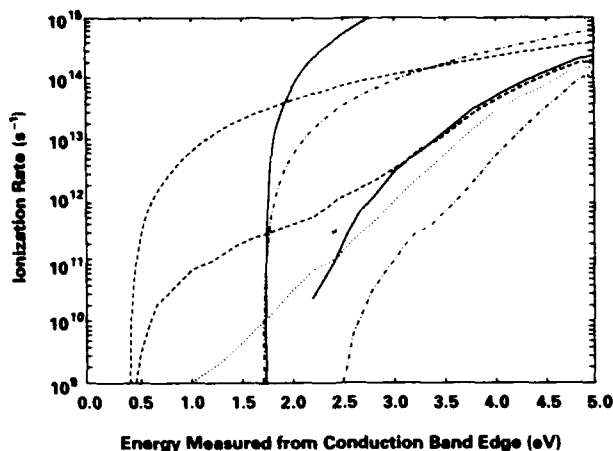


FIG. 4. Ionization rates: upper set of three curves, Keldysh formula; lower set of four curves, calculated ionization rates. Solid line: GaAs, dashed line: InAs, dot-dashed line: InP, and dotted line: $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$.

The semiclassical ionization rate thresholds for these materials are always larger than the band gap energy. In GaAs for instance, the ionization rate becomes nonzero for energies about 0.5 eV larger than the band gap, whereas in the InAs-like compounds, the threshold is closer to the band gap energy (0.1 eV larger than the band gap energy). The threshold in InP is almost 1 eV larger than the band gap energy. However, the actual energy at which the ionization rate becomes nonzero is difficult to determine when using a Monte Carlo integration algorithm as in Ref. 6. This mathematical threshold is also largely irrelevant as discussed above. A more practical measurement of an ionization threshold is to define the threshold as the minimum energy an electron must attain to contribute a large percentage to a macroscopic quantity such as the impact ionization coefficient α . This will be defined more clearly below in the discussion on bulk transport properties.

For realistic band structures, there is a complicated interplay between the threshold energy and hardness of the threshold. It is possible, however, to make the following rough classifications pertaining to direct gap materials. For small band gap materials with large $E_{\Gamma-X}$ and $E_{\Gamma-L}$, the threshold energy is close to the band gap energy and the threshold is soft. In this case, electrons with an energy slightly greater than the band gap energy above the conduction band minimum are located in the Γ minimum. The final states are also located in the Γ minimum where the density of states is very small. In these cases, the ionization rate will be roughly proportional to the product $G_c(E_3)G_c(E_4)$, where E_3 and E_4 are the final state energies. Therefore, the ionization rate near threshold will increase slowly until it is possible for the intervalley states to become final states. We have numerically shown that this is the case for InAs and $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$.

For larger band gap materials with small $E_{\Gamma-X}$ and $E_{\Gamma-L}$, the threshold energy will be slightly larger than the band gap and the threshold will be harder. If $E_{\Gamma-X}$ and $E_{\Gamma-L}$ are small, the low energy DOS will be large and will in-

crease rapidly with energy; hence, the available final states for impact ionization increase rapidly with initial electron energy. Although electrons near threshold will lie high in the band structure and will have a wide range of wave vector magnitudes, the low-energy final states have a large wave vector spread, and energy and momentum conservation raises the threshold energy only a little above the band gap energy. This is true for GaAs.

If the band gap is large and $E_{\Gamma-X}$ and $E_{\Gamma-L}$ are large, the energy and momentum conservation requirement can force the threshold energy to be substantially larger than the band gap energy. Since the final states are restricted to the Γ valley until high initial particle energies are reached, it may be impossible to conserve both energy and momentum unless the initial state electron energy is much larger than the band gap energy. This condition pertains to InP with a 1.3 eV band gap and a valley separation of more than 0.7 eV.

In addition, the Coulomb matrix element responsible for the electron-electron interaction can play an important role in determining the ionization rate in III-V's, especially for energies near threshold. Since the matrix element has a rough $1/q^2$ dependence (see Refs. 6 and 8), the ionization rate for initial state energies for which the average q exchanged is small are enhanced by factors of 10 to 100 compared to ones for which q is a substantial fraction of the BZ . Because the average q exchanged is much smaller for energies near threshold, the average matrix elements for these states are larger than those of higher energy. This effect is most pronounced for smaller band gap materials such as InAs.

B. Bulk transport and ionization coefficient α

In all four materials which we have considered here, the ionization rates calculated are much smaller than those obtained by the empirical Keldysh formula which has been used in past Monte Carlo simulations (see Fig. 4). However, it is possible to obtain Monte Carlo fits using the new Kane-type results to experimentally obtained values of the impact ionization coefficient α without appreciably changing the total phonon scattering rate. We have approximated the impact ionization coefficients α for electrons and β for holes as

$$\alpha = \frac{\sum_{n_c} \int_{BZ} d^3k f_{n_c}(\mathbf{k}) R_{ave}[E_{n_c}(\mathbf{k})]}{\sum_{n_c} \int_{BZ} d^3k f_{n_c}(\mathbf{k}) v_d}, \quad (14)$$

$$\beta = \frac{\sum_{n_v} \int_{BZ} d^3k [1 - f_{n_v}(\mathbf{k})] R_{ave}[E_{n_v}(\mathbf{k})]}{\sum_{n_v} \int_{BZ} d^3k [1 - f_{n_v}(\mathbf{k})] v_d}, \quad (15)$$

where $v_n(\mathbf{k})$ is the group velocity, $f_n(\mathbf{k})$ is the distribution function, and n_c and n_v are the conduction and valence band indices, respectively. The fact that one can virtually obtain the same result for α using two totally different sets of ionization rates has been noticed by Tang for the case of silicon,¹⁸ and represents a general property of the Boltzmann equation and scattering mechanisms that involve some form of threshold (see, for instance Ref. 26).

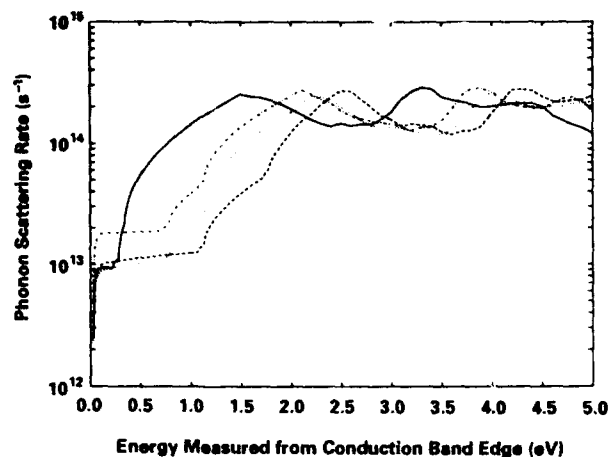


FIG. 5. Phonon scattering rates used in MC simulations. Solid line: GaAs, dashed line: InAs, dot-dashed line: InP, and dotted line: $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$.

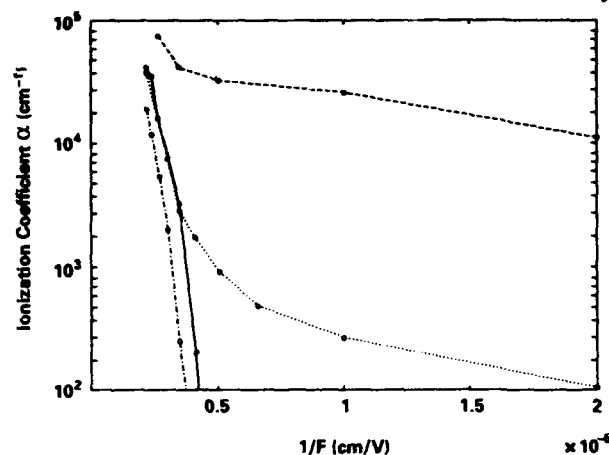


FIG. 6. Calculated impact ionization coefficient α as a function of inverse field, $1/F$. Solid line: GaAs, dashed line: InAs, dot-dashed line: InP, and dotted line: $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$.

We have performed full band structure bulk Monte Carlo simulations and have calculated distribution functions and macroscopic quantities such as α and drift velocity as a function of field for four III-V compounds. Our Monte Carlo simulation uses two pseudopotential conduction bands for drift due to the field, and includes several scattering mechanisms such as polar-optical phonon scattering and intervalley scattering (see Ref. 14). The optical phonon energies we have used are similar to those of Refs. 19–21. In addition, the impact ionization rates shown here were also included as energy-dependent scattering mechanisms. The phonon scattering rates at high fields are taken to be proportional to the total density of states in the conduction band, which is a good approximation for deformation potential scattering.¹⁸

Figure 5 shows the total phonon scattering rates used in these MC simulations. These scattering rates were adjusted to roughly match bulk measurements of α for GaAs,²⁷ InP,^{28,29} and $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$,³⁰ but because there is little data available on the InAs ionization coefficient, phonon scattering rates comparable to $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$ were used in this case. Figure 6 shows the values of α corresponding to these phonon scattering rates.

Although bulk transport parameters can be roughly matched using both the Keldysh-type and our new Kane-type results, the distribution functions which result are quite different and therefore, a different interpretation of the ionization threshold is in order. For instance, in GaAs, typically used phonon coupling constants predict total phonon scattering rates which peak at $3 \times 10^{14} \text{ s}^{-1}$ near 1.5 and 3.3 eV, have an average high energy value of about $2 \times 10^{14} \text{ s}^{-1}$ (see Ref. 21), and an ionization rate from the Keldysh formula as shown in Fig. 4. In these models, the ionization rate quickly surpasses the total phonon scattering rate near 2 eV. Because both the energy lost in impact ionization and the ionization rate are large, almost no electrons can achieve energies greater than 2.25–2.5 eV. Therefore, in these GaAs simulations, the distribution functions

have truncated high-energy tails, and α is determined primarily by how many electrons can reach an effective threshold (near 2.0 eV). This number is critically determined by the phonon scattering rate and qualitatively behaves corresponding to the Shockley "lucky electron" model. The same behavior is seen in other III-V materials when simulated in this manner.¹⁹ Notice, however, that in order to fit experiment, the Keldysh parameters for each material vary by orders of magnitude from material to material (see Fig. 4), and phonon rates can vary by factors of 3 to 4.

In contrast, a different picture of ionization thresholds is obtained from the ionization rates calculated here in the Kane-type approach. For example, in GaAs, the total phonon scattering rate is roughly 20% lower than that of Ref. 21, but the ionization rates are a factor of 1000 lower. In our simulations, the ionization rate plays little role in determining the distribution function up to very high fields, since it is several orders of magnitude smaller than the phonon scattering rate. The ionization coefficient α is instead determined by the high-energy tail of the distribution function above 2.0 eV integrated with the ionization rate. In this model, the ionization rate samples the high-energy tail without disturbing it very much. Figures 7 and 8 show the distribution function in GaAs and $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$ as a function of energy for various values of electric field. In GaAs, as the field is increased and the distribution heats up, however, there are electrons which reach 3.5 eV where the ionization rate is between 10^{12} and 10^{13} s^{-1} . At these energies, the energy loss rate due to impact ionization exceeds that due to phonons, and the part of the high-energy tail above these energies is truncated by impact ionization. However, impact ionization has little effect on the distribution function for energies less than the extremely high value of 3.5 eV. The same picture of impact ionization holds for the other materials which we have investigated here. Notice that our results contradict another common prejudice in the theory of impact ionization. It often has

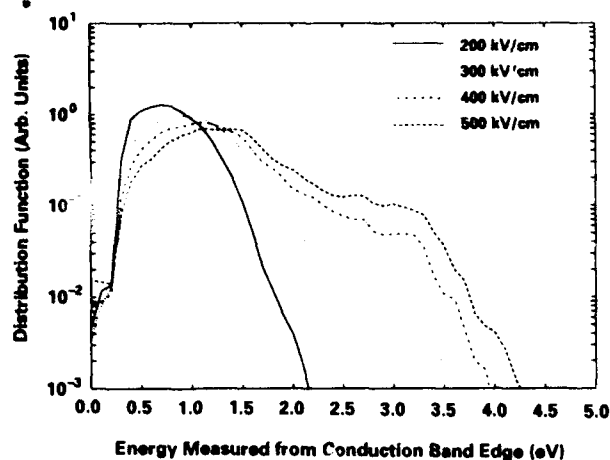


FIG. 7. Normalized electron distribution function in GaAs including DOS.

been assumed that the ionization rate cannot be much smaller than the phonon scattering rate to give significant values of α . Moll³¹ considered the effect of several phonon collisions in between ionizing events, but his arguments are based on assumptions which do not account for the complicated form of the energy distribution of the electrons.

Soft thresholds have also been recently included in the "Ridley lucky electron model." These models incorporate Keldysh-type ionization rates whose magnitudes are much closer to those calculated here.^{17,22} These models can successfully predict many features pertaining to the ionization coefficients α and β ; however, because they are phenomenological models they do not give an accurate representation of the ionization process and thus cannot predict some important aspects of the distribution function.

A more practical definition of thresholds pertaining to these very low ionization rates is to define an effective threshold energy. If we define a "significant" ionization rate as $\alpha > 1$ and look to see which portions of the ionization rate versus energy curve contribute to $\alpha > 1$, we find

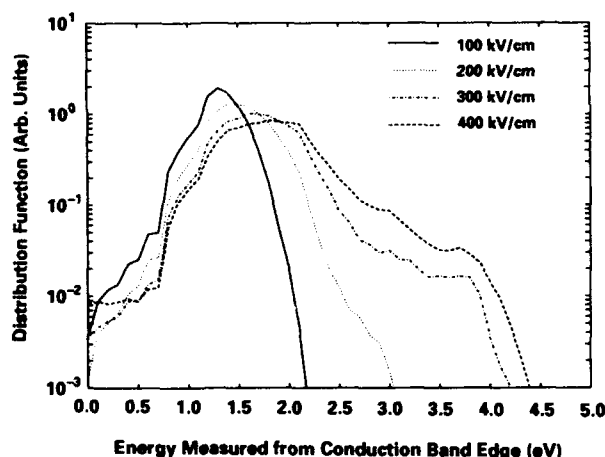


FIG. 8. Normalized electron distribution function in $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$ including DOS.

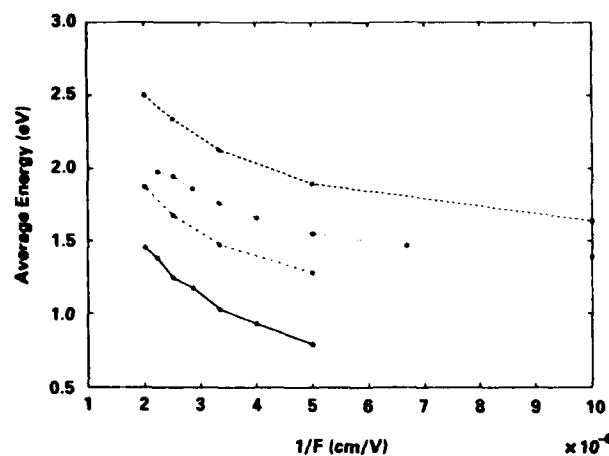


FIG. 9. Average electron energy as a function of inverse field. Solid line: GaAs, dashed line: InAs, dot-dashed line: InP, and dotted line: $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$.

that for these materials there is no "significant" contribution to α for values of the ionization rate less than 10^9 s^{-1} . The effective ionization threshold is then the lowest energy for which the ionization rate is greater than 10^9 s^{-1} .

As a result of the small ionization rates, the average energy of the distribution function is much higher in our simulation. Figure 9 shows the average energies for the four materials calculated here. These plots demonstrate an important trend. The higher the intervalley energies, the higher the average energy. For example, InAs, which has the highest intervalley energy separations exhibits the highest average energy, whereas GaAs, which has the lowest intervalley energy separations exhibits the lowest average energies. This situation is expected to occur because there is little energy loss due to impact ionization compared to phonon scattering. It is this fact which leads to two very dissimilar behaviors in α vs $1/F$ plots. In GaAs and InP, α behaves as $e^{-F_0/F}$ where F_0 is some large constant. For these materials, α drops quickly to zero for fields less than 200 kV/cm. This is a result of high effective threshold energies, particularly in InP, and low average energies in GaAs. In contrast, in InAs and $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$, α deviates significantly from the $e^{-F_0/F}$ form due to relatively low threshold energies and high average energies.

IV. CONCLUSIONS

We have reviewed the role of thresholds in impact ionization considering the $\mathbf{k}$ dependence and energy dependence of the ionization cross section as well as the notion of "effective" ionization thresholds for bulk transport. In our discussion of the $\mathbf{k}$ anisotropy, we have shown that earlier theories of ionization rate anisotropy have been calculated in error, and we have presented a more rigorous calculation of the ionization rate in silicon as a function of $\mathbf{k}$. This more rigorous result demonstrates that these earlier theories have overestimated the anisotropy of the ionization rate. We have also calculated from first principles the ionization rates in GaAs, InAs, InP, and $\text{Ga}_{0.43}\text{In}_{0.57}\text{As}$ which

are found to be much smaller than the phonon scattering rates and exhibit soft threshold behavior. These rates differ markedly from the established Keldysh formula ionization rates. The differences imply much "hotter" electron energy distribution functions and much higher "effective" threshold energies leading to the conclusion that the "lucky electron" picture of impact ionization is inadequate in these important semiconductors.

ACKNOWLEDGMENTS

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