

USING THE RANDOM- k APPROXIMATION TO CONSISTENTLY INCORPORATE IMPACT IONIZATION INTO THE GENERALIZED EXPANSION METHOD FOR SOLVING THE MULTI-BAND BTE IN SILICON

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Abstract

We present here a consistent approach for determining impact ionization coefficients for a multi-band model in silicon. Using first-order perturbation theory and a random- k approximation, the impact ionization rate is determined to reflect the multi-band density of states in silicon. To account for the actual density of states, we have solved four coupled Boltzmann transport equations by combining a generalized Legendre polynomial expansion method with numerical techniques using finite differences and sparse matrices. Calculated values for the impact ionization coefficients agree very well with experiment for electrons in silicon, while being obtained in significantly less CPU time than required by analogous Monte Carlo calculations.

I. INTRODUCTION:

Fundamental analytical work on impact ionization was performed by Keldysh [1]. Since Keldysh presented his expression for impact ionization rate, several analytical or quasi-analytical investigations of impact ionizations have been performed which use Keldysh's results [2, 3]. These investigations have provided considerable insight into impact ionization, and the nature of Boltzmann equation in semiconductors. However, in the past, analytical formulations were usually constrained to an energy range which is limited to silicon's first conduction band, and therefore did not reflect silicon's true density of states. Furthermore, while agreement with experiment has been obtained, the use of Keldysh's formulation for silicon has not been fully justified since, from a theoretical point of view, Keldysh's expression was derived for a single parabolic conduction band, which is not strictly appropriate for silicon.

In this work, we extend these quasi-analytical investigations to a larger energy range which reflects silicon's actual density of states. Furthermore, instead of using the Keldysh expression, we derive an expression for impact ionization rate which is consistent with the actual density of states in silicon. The expression for impact-ionization is based on the random- k formalism, initially introduced by Kane [4]. Once an expression for impact ionization is obtained, we then use it, in conjunction with a quasi-analytical method of solving the Boltzmann transport equation, to calculate impact ionization coefficients.

II. ANALYTICAL FORMULATION:

A. Impact Ionization Rate:

To calculate impact ionization rates which accurately reflect the density of states in silicon, we begin with the random- k approximation presented by Kane [4]. With this formulation, Kane found that if he required energy to be conserved, but neglected conservation of crystal momentum, he obtained virtually the same results for impact ionization rates as when he required both energy and crystal momentum be conserved. In other words, Kane found that the energy dependent impact ionization rate could be expressed accurately in terms of the density of states. Mathematically, this energy-conserving, random- k approximation gives the following expression for impact ionization:

$$\frac{1}{\tau_{ii}(\varepsilon)} = A \sum_{n_2, n_3, n_4} \int \rho_{n_2}(\varepsilon_2) \rho_{n_3}(\varepsilon_3) \rho_{n_4}(\varepsilon_4) \delta(\varepsilon + \varepsilon_4 - \varepsilon_2 - \varepsilon_3) d\varepsilon_2 d\varepsilon_3 d\varepsilon_4 \quad (1)$$

where ε_4, n_4 refer to the energy and band containing the valence band electron; ε_2, n_2 and ε_3, n_3 are the energies and bands of the final electron states; $\rho_{n_i}(\varepsilon)$ is the density of states function in band n_i ; and A is an ionization coupling constant which can be determined empirically.

The sum over n_2, n_3 , and n_4 in equation (1) accounts for permutations of possible final energy bands allowed by energy conservation. The range of the summations is determined by the band structure and the conservation of energy. To evaluate equation (1), we take values for the density of states functions, $\rho_i(\varepsilon_i)$, from the effective, multi-band silicon dispersion relation given by Brunetti *et. al.* [5]. This band structure averages the actual dispersion relation over spheres, thereby providing the actual density of states. By accurately providing the density of states, this averaging is consistent with the use of the random- k approximation.

After making the approximation that holes are generated mostly at the top of the valence band, and inserting limits consistent with the spherical band model, equation (1) becomes

$$\frac{1}{\tau_{ii}(\varepsilon)} = A \int_0^{\varepsilon - \varepsilon_g - 1.75} \rho_1(\varepsilon_2) \rho_2(\varepsilon - \varepsilon_g - \varepsilon_2) d\varepsilon_2 + A \int_{\varepsilon - \varepsilon_g - 1.75}^{1.75} \rho_1(\varepsilon_2) \rho_1(\varepsilon - \varepsilon_g - \varepsilon_2) d\varepsilon_2 + A \int_{1.75}^{\varepsilon - \varepsilon_g} \rho_2(\varepsilon_2) \rho_1(\varepsilon - \varepsilon_g - \varepsilon_2) d\varepsilon_2 \quad \text{for } \varepsilon - \varepsilon_g \geq 1.75 \quad (2)$$

$$\frac{1}{\tau_{ii}(\varepsilon)} = A \int_0^{\varepsilon - \varepsilon_g} \rho_1(\varepsilon_2) \rho_1(\varepsilon - \varepsilon_g - \varepsilon_2) d\varepsilon_2 \quad \text{for } \varepsilon - \varepsilon_g < 1.75 \quad (3)$$

where $\varepsilon_g = 1.12eV$ is the energy gap for silicon.

B. Impact Ionization Coefficients:

To determine the impact ionization coefficients, we used the following expression which accounts for the density of states in higher bands:

$$\alpha_n = \sum_{i=1}^4 \frac{1}{v_d} \int_0^\infty \frac{1}{\tau_{ii}(\varepsilon)} f_0^{(i)}(\varepsilon) \rho^{(i)}(\varepsilon) d\varepsilon \quad (4)$$

where $f_0^{(i)}(\varepsilon)$ is the isotropic distribution function in band i ; $\rho^{(i)}(\varepsilon)$ is the density of states function in the i^{th} band; and v_d is the silicon saturation velocity.

Before we can calculate the impact ionization coefficients, we must first solve the Boltzmann transport equation (BTE) to find $f_0^{(i)}(\varepsilon)$.

C. Formulation of the BTE:

To obtain $f_0^{(i)}(\varepsilon)$, we use the Legendre polynomial (LP) expansion method for solving the BTE. Previously, investigators used a state of the art LP approach for impact-ionization studies which incorporated a first order LP expansion that accounted for one or two conduction bands in Si [6]. In this work, we use a generalized approach for obtaining the distribution function to arbitrarily-high LP order. We also include the effects of silicon's higher conduction bands.

To solve the BTE to arbitrarily high order and for densities of states which correspond to higher conduction bands, we first write a steady-state, homogeneous Boltzmann equation for each of the four bands of the spherically averaged silicon dispersion relation [5]. We also include the effects of acoustic, intervalley, interband phonon scattering, and impact ionization. The equation for a specific band is coupled to the other equations through impact ionization and interband scattering.

Next, with the LP approach, we expand the distribution function in each band, $f^{(i)}(\vec{k})$, in terms of Legendre polynomials to an arbitrarily high order:

$$f^{(i)}(\vec{k}) = \sum_{n=0}^{\infty} f_n^{(i)}(\varepsilon) P_n(\cos\theta) \quad (5)$$

where θ is the angle between \vec{k} and electric field \vec{E} ; $P_n(\cos\theta)$ are the Legendre polynomial basis functions which provide the angular dependence of the distribution function; and $f_n^{(i)}(\varepsilon)$ represent the unknown coefficients of the basis functions.

Once the distribution function has been expressed in terms of the LP expansion, the goal is to find the unknown coefficients $f_n^{(i)}(\varepsilon)$. We find the coefficients by using a variation of the generalized LP expansion approach [7]. With this method, LP orthogonality and recurrence relations are used to generate a system of equations for the unknown coefficients, $f_n^{(i)}(\varepsilon)$. The powerful aspect of this technique is that the equations for all the coefficients, $f_n^{(i)}(\varepsilon)$, have identical forms and are thus automatically generated to arbitrarily high order. In addition, in order to reduce the number of equations required for solution, and also improve upon numerical characteristics, we substituted odd-indexed LP equations into even-indexed LP equations and reformulated the Boltzmann equation into a system of second-order, linear, differential-difference equations. The analytical form of the generalized equation for even-indexed Legendre coefficients $f_n^{(i)}(\varepsilon)$ in band i , can be written as:

$$\begin{aligned}
& -\frac{2(eE)^2}{m_i^*} \left\{ \alpha_{n-1}\alpha_{n-2} \left[\frac{\tau_i\gamma_i}{\gamma_i'^2} \frac{\partial^2 f_{n-2}^{(i)}(\varepsilon)}{\partial \varepsilon^2} + \left(\frac{\tau_i'\gamma_i}{\gamma_i'^2} - \frac{\tau_i\gamma_i\gamma_i''}{\gamma_i'^3} - (n-2)\frac{\tau_i}{\gamma_i'} \right) \frac{\partial f_{n-2}^{(i)}(\varepsilon)}{\partial \varepsilon} \right. \right. \\
& \quad \left. \left. - \frac{n-2}{2} \left(\frac{\tau_i'}{\gamma_i'} - \frac{n\tau_i}{2\gamma_i} \right) f_{n-2}^{(i)}(\varepsilon) \right] + \left[\alpha_{n-1}\alpha_n \left(\frac{n}{n+1} \right) + \alpha_n\alpha_{n+1} \left(\frac{n+1}{n+2} \right) \right] \right. \\
& \quad \times \left[\frac{\tau_i\gamma_i}{\gamma_i'^2} \frac{\partial^2 f_n^{(i)}(\varepsilon)}{\partial \varepsilon^2} + \left(\frac{\tau_i'\gamma_i}{\gamma_i'^2} - \frac{\tau_i\gamma_i\gamma_i''}{\gamma_i'^3} + \frac{3\tau_i}{2\gamma_i'} \right) \frac{\partial f_n^{(i)}(\varepsilon)}{\partial \varepsilon} \right] \\
& \quad + \alpha_{n-1}\alpha_n \left(\frac{n}{2} \right) \left(\frac{\tau_i'}{\gamma_i'} - \frac{n\tau_i}{2\gamma_i} \right) f_n^{(i)}(\varepsilon) - \alpha_n\alpha_{n+1} \left(\frac{n+1}{n+2} \right) \frac{n}{2} \left(\frac{\tau_i'}{\gamma_i'} + \frac{n+1}{2} \frac{\tau_i}{\gamma_i} \right) f_n^{(i)}(\varepsilon) \\
& \quad + \alpha_{n+1}\alpha_{n+2} \left(\frac{n+1}{n+3} \right) \left[\frac{\tau_i\gamma_i}{\gamma_i'^2} \frac{\partial^2 f_{n+2}^{(i)}(\varepsilon)}{\partial \varepsilon^2} + \left(\frac{\tau_i'\gamma_i}{\gamma_i'^2} - \frac{\tau_i\gamma_i\gamma_i''}{\gamma_i'^3} + (n+3)\frac{\tau_i}{\gamma_i'} \right) \frac{\partial f_{n+2}^{(i)}(\varepsilon)}{\partial \varepsilon} \right. \\
& \quad \left. \left. + \frac{n+3}{2} \left(\frac{\tau_i'}{\gamma_i'} + \frac{n+1}{2} \frac{\tau_i}{\gamma_i} \right) f_{n+2}^{(i)}(\varepsilon) \right] \right\} \\
& = \begin{cases} \left[\frac{\partial f_0^{(i)}(\varepsilon)}{\partial \varepsilon} \right]_{coll} & \text{for } n = 0 \\ -\frac{f_n^{(i)}(\varepsilon)}{\tau_i(\varepsilon)} & \text{for } n = 2, 4, 6, 8, \dots, \infty \end{cases} \quad (6)
\end{aligned}$$

where $\alpha_n = \frac{n+1}{2n+1}$; γ_i' and γ_i'' are the 1st and 2nd derivatives of γ_i with respect to energy; $\tau_i(\varepsilon)$ is the total mean free time between collisions; and τ_i' is the 1st derivative of τ_i with respect to energy.

A similar system of equations is obtained for each band. To solve the system, we first truncate the expansion. Then, the entire system is discretized and then solved directly using Gaussian elimination for sparse matrices.

III. RESULTS:

In Fig. 1 we show the distribution function we obtained from solving the multi-band BTE. The solid line shows calculated values for the symmetrical part of the distribution function when 20 LP terms were used, while the dotted line shows the results of using only 2 LP terms; the diamonds give the results of Monte Carlo calculations which used the same Brunetti transport model. Solving the BTE to 20'th LP order required approximately 28 CPU seconds on a SUN4 workstation, while comparable Monte Carlo calculations took considerably longer.

Using the above method, we were able to obtain values for ionization coefficients with the use of only one unknown adjustable parameter, the ionization coupling factor A . The value of A has

been determined to be 45000 when an expansion of 20 LP terms was employed; and 55000 when only 2 LP terms were used. Fig. 2 demonstrates the agreement between the values obtained from our calculations and the experimental data of Lee *et. al.* [8] for impact ionization coefficients.

IV. CONCLUSION:

We have developed an efficient and physics-based method in obtaining impact ionization coefficients for the multi-band model in silicon. The impact ionization rate is derived from basic principles with a suitable random- k approximation for the multi-band model considered. A generalized Legendre polynomial expansion method is combined with numerical techniques to solve the system of four coupled multi-band Boltzmann equations. Excellent agreement has been obtained between our calculations and the results of both Monte Carlo method and experiment. The efficiency of this method makes it well suited for studying impact ionization and hot-electron phenomena in semiconductor devices.

V. ACKNOWLEDGMENT:

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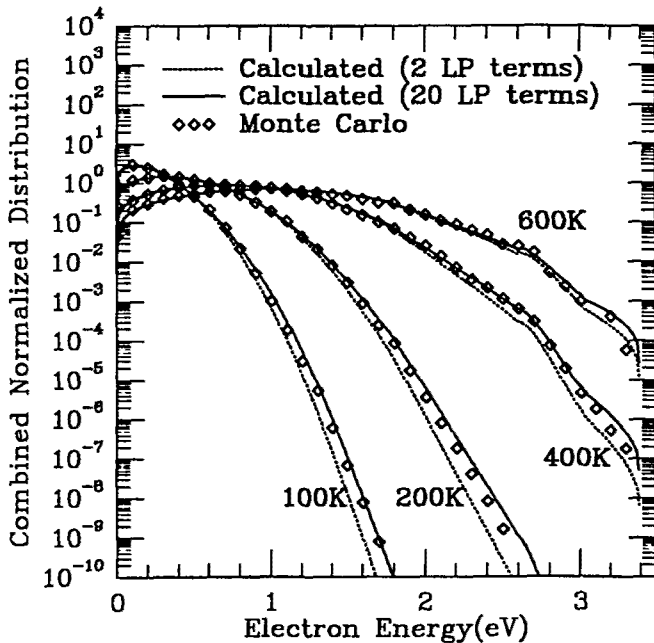


Fig. 1. The isotropic distribution function f_0 plotted for different electric fields are compared with results of MC calculations.

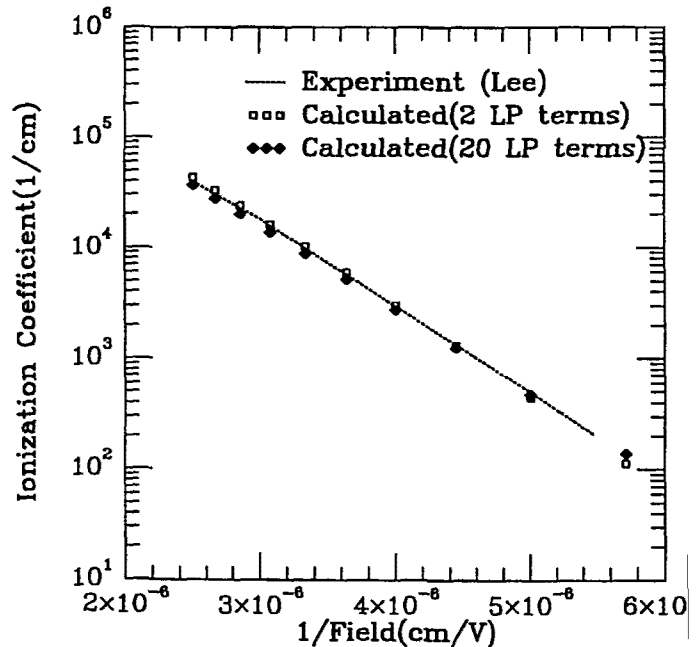


Fig. 2. Impact ionization coefficient is plotted versus the reciprocal electric field and compared with experimental values.