Implications of nonparabolicity, warping, and inelastic phonon scattering on hole transport in pure Si and Ge within the effective mass framework

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Hole mobility over a wide range of temperatures in pure Si and Ge is studied within the framework of effective mass theory using the Monte Carlo method. With this aim, we have implemented a three-band model (heavy, light, and split-off holes) introducing nonparabolicity even for the latter, which is usually considered parabolic in the literature. The warping in the heavy and light bands was taken into account, maintaining a spherical model for the split-off band. We also developed scattering rate expressions to be used in a Monte Carlo procedure with the nonparabolicity and warping effects included explicitly in the scattering rate expressions, an aspect neglected in the literature. In so doing, we calculated exactly the nonparabolicity functions for the valence band from the expressions provided by Kane [J. Phys. Chem. Solids 1, 82 (1956)]. Further, we modeled the acoustic phonons on an inelastic mechanism, generalizing previous work, and applying a temperature-dependent average to obtain typical values of the energy of the acoustic phonons involved in the scattering processes. We show that our treatment of hole transport provides results close to those reported experimentally and comparable to those obtained with more complex methods, but requiring much less computing time.


I. INTRODUCTION

The Monte Carlo simulation has been widely used to solve the Boltzmann equation for the study of electron mobility. The literature on this topic indicates the importance of taking the band structure into account as accurately as possible. In fact, there is an increasing interest in using full-band procedures such as the pseudopotential methods to calculate the dispersion relation. On the other hand, the effective mass theory has shown an amazing flexibility by continuing to obtain good results without involving excessive computing time. However, to retain its usefulness, the traditional parabolic description of the band structure must be improved. Indeed, it has been proved that nonparabolicity in the conduction band is an important factor in the behavior of electron dynamics.

To improve the behavior of the complementary devices used nowadays a good understanding of hole dynamics is essential. However, less research has been devoted to this area than to electron dynamics. The main reason is the complex structure of the valence band due to the degeneracy, warping, and pronounced nonparabolicity of the dispersion relation. In fact, the nonparabolicity of the valence band is more prominent than that of the conduction band even at low energies, so this effect should be more relevant in the modeling of hole dynamics. The strong anisotropy and degeneracy (heavy hole, light hole, split-off hole) of the valence band must also be incorporated in the analysis. The aim of this paper is to obtain a complete but simple model for phonon scattering rates, including nonparabolicity, warping, and the presence of different kinds of holes, within the framework of effective mass theory. In order to deal with this problem, we have developed a Monte Carlo simulator to evaluate hole velocity in intrinsic silicon and germanium, which highlights the importance of taking into account the above effects.

Previous papers dealt with this issue by using more complex models of the band structure, usually by the pseudopotential method. Addressing this topic, early Monte Carlo procedures based on effective mass theory took nonparabolicity into account to obtain the energy after a free flight by modeling the nonparabolicity functions with analytical piecewise energy-dependent expressions. However, the changes necessary in expressions of the scattering rates were not made explicit. The noninclusion of these modifications led to nonphysical results in the scattering rate calculations. Our objective is to avoid such meaningless behavior by elaborating a formalism that enables us to obtain simulated results comparable to the experimental ones, requiring less computing time without any loss of accuracy. This formalism will be derived from first principles, starting from Fermi’s golden rule and Kane’s description of the valence band. In addition, an interesting aspect of the presented band structure is the possibility of being the initial step towards the treatment of the modified Schrödinger equation for holes in future works in the same way it was done for electrons in previous papers, where the knowledge of the band structure is fundamental.

Furthermore, we incorporate an inelastic model of
acoustic phonon scattering, which has advantages for analyzing hole transport at low temperatures and fields. Since that our valence band model takes into account the three kinds of holes, we have extended the Bufler, Schenk, and Fichtner treatment to consider the whole set of scattering mechanisms, including interband processes so that a complete procedure is performed.

In Sec. II we introduce the formalism and obtain expressions of the scattering probabilities to be used when nonparabolicity of the valence band is taken into account. The determination of nonparabolicity functions is also analyzed in this section. These functions show the dependence of effective mass on energy. Section III is devoted to a discussion of the data obtained in our simulations. We apply our model to Si and Ge and compare the results with the experimental data detailed in the literature. Finally, in Sec. IV we draw our conclusions.

II. THEORETICAL FORMALISM

It is known that the probability per unit of time of changing a carrier state characterized by an initial wave vector \( \mathbf{k} \) to a final one \( \mathbf{k}' \) due to the interaction between hole and phonons is given by:

\[
P(\mathbf{k}, \mathbf{k}') = \frac{\pi}{\rho V \omega_q} \left( \frac{N_q}{N_q + 1} \right) G[\xi_{ij} q_j]^2 \delta(\epsilon' - \epsilon + \hbar \omega_q),
\]

where \( \rho \) is the crystal density, \( V \) its volume, \( \mathbf{q} \) the phonon wave vector and \( q_j \) its \( j \)-th component, \( N_q \) is the average number of phonons with wave vector \( q \), \( \omega_q \) the phonon frequency, obtained through the phonon dispersion relation, which we simplify by using a constant value for the optical phonons, and the simple relation \( \omega_q = \epsilon u \) for acoustic phonons, \( u \) being the average velocity of the sound, \( \xi_i \) is the \( i \)-th component of the phonon polarization vector \( \xi \), \( \Xi \) is the deformation potential tensor, and \( G \) is a function which takes into account the overlap between the Bloch functions of the states \( \mathbf{k} \) and \( \mathbf{k}' \); this function is \( 1/4(1 + 3 \cos^2 \theta) \) for intraband processes and \( 3/8 \sin^2 \theta \) for interband, which is the angle between \( \mathbf{k} \) and \( \mathbf{k}' \). In Eq. (1) upper and lower symbols refer to the phonon absorption and emission processes, respectively.

In a Monte Carlo simulator it is important to know the probability per unit of time of the angles of a carrier state characterized by a wave vector \( \mathbf{k} \), \( (k, \theta, \phi) \) changing to \( (k', \theta', \phi') \). To obtain this probability, the integration of Eq. (1) over all the values of the modulus of \( \mathbf{k}' \) must be performed, with the angular dependence remaining unaffected, and multiplying by \( V/(2 \pi)^3 \), to account for the number of possible final states. At this point, it is essential to use the most accurate band model possible, but one that avoids excessive computing time. For the valence band, accuracy implies taking into account nonparabolicity and warping in the dispersion relation, because of their prominence.

The simplest model to take both these effects into account in the heavy and light bands is given by the relations:

\[
e_{HF}^\mathbf{k} = \frac{\hbar^2 k^2}{2m_0} |1 - g(\theta, \phi)| \chi_{HF}(\epsilon), \quad \epsilon \gg 0,
\]

\[
e_{L}^\mathbf{k} = \frac{\hbar^2 k^2}{2m_0} |1 + g(\theta, \phi)| \chi_{L}(\epsilon), \quad \epsilon \gg 0.
\]

Maintaining the same structure, we propose the following nonparabolic dispersion relation for the split-off holes:

\[
e_{S}^\mathbf{k} = \frac{\hbar^2 k^2}{2m_{so}} \chi_{S}(\epsilon) + \Delta_{so}, \quad \epsilon \gg \Delta_{so},
\]

with \( m_{so} \) an effective mass for the split-off holes (our method for estimating this will be explained later), \( m_0 \) being the rest electron mass, \( \chi(\epsilon) \) the nonparabolicity function of the corresponding band, which must be modeled correctly for all three kinds of holes, and \( g(\theta, \phi) \) the warping function used to describe variations in the energy relationship with \( \theta \) and \( \phi \). The most common form for this function is:

\[
g(\theta, \phi) = \sqrt{B^2 + C^2 q(\theta, \phi)}
\]

with

\[
q(\theta, \phi) = \sin^4 \theta \sin^2 \phi \cos^2 \phi + \cos^2 \theta \sin^2 \phi
\]

and \( A, B, \) and \( C \) representing the valence band parameters, characteristic of the material. The values utilized for silicon and germanium are shown in Table I. Finally \( \Delta_{so} \) is the split-off energy, which takes the value of 0.044 eV in Silicon and 0.295 eV in Germanium.

In the literature, a first approximation of the effective mass for nonparabolic and anisotropic bands is usually obtained by means of a comparison with a parabolic and

\[\text{TABLE I. Parameters used in our simulations.}\]

<table>
<thead>
<tr>
<th>Physical properties</th>
<th>Si</th>
<th>Ge</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m³)</td>
<td>(2.33 \times 10^3)</td>
<td>(5.32 \times 10^3)</td>
</tr>
<tr>
<td>Sound transversal velocity (m/s)</td>
<td>(5.3 \times 10^3)</td>
<td>(3.2 \times 10^3)</td>
</tr>
<tr>
<td>Sound longitudinal velocity (m/s)</td>
<td>(9.0 \times 10^3)</td>
<td>(5.4 \times 10^3)</td>
</tr>
<tr>
<td>Average sound velocity (m/s)</td>
<td>(6.5 \times 10^3)</td>
<td>(3.9 \times 10^3)</td>
</tr>
</tbody>
</table>

\[\text{Valence band parameters} \]

| \(|A|^2\) | \(|B|^2\) | \(|C|^2\) |
|----------|----------|----------|
| \(4.22\)  | \(0.78\)  | \(4.80\)  |
| \(13.38\) | \(8.48\)  | \(13.14\) |

\[\text{Heavy hole effective mass} \]

| \(m^*_{hh}\) | \(0.53\) | \(0.346\) |
| \(m^*_{lh}\) | \(0.156\) | \(0.042\) |
| \(m^*_{sh}\) | \(0.237\) | \(0.075\) |

\[\text{Scattering rates parameters} \]

| Equivalent temperature of optical phonon, \(\theta_{op}\) (K) | \(735\) | \(430\) |
| \(D^*(eV/m)\) | \(9.2 \times 10^10\) | \(1.02 \times 10^{11}\) |
| \(\Xi_0\) (eV) | | \(3.15\) |
| \(2.95\) | | |
spherical band structure. If we applied the same procedure to calculate energy and direction dependency for the effective masses in each band, we would obtain

\[
\begin{align*}
m_{H}(\epsilon, \theta, \phi) &= \frac{m_0}{|A[1 + g(\theta, \phi)]\chi_H(\epsilon)|}, \\
m_{L}(\epsilon, \theta, \phi) &= \frac{m_0}{|A[1 - g(\theta, \phi)]\chi_L(\epsilon)|}, \\
m_{S}(\epsilon) &= \frac{m_{so}}{\chi_S(\epsilon)}. 
\end{align*}
\]  

(6)

We will discuss the effect of nonparabolicity on these effective masses in Sec. III. With regard to warping, results show that for heavy holes the lower effective mass is in the [100] direction, while the higher value is in the [111] direction. The opposite behavior is true for light hole band, in both, Si and Ge. Previous studies have dealt with changes in direction of the effective masses for parabolic bands.

As stated above, the accuracy of the calculation depends on correct modeling of the nonparabolicity functions, which in this case were calculated directly from Kane’s model for the valence band. If the nonspherical-nonparabolic dispersion relation for the valence band is represented by

\[
k^2 = \frac{2m_0}{\hbar^2} \gamma(\epsilon, \hat{k}),
\]

(7)

with \(\hat{k}\) being a unit vector in the direction of the wave vector \(\vec{k}\), the functions \(\gamma(\epsilon, \hat{k})\) are the roots of the Eq. (7)

\[
H_3\gamma^3 + H_2\gamma^2 + H_1\gamma + H_0 = 0,
\]

(8)

where

\[
egin{align*}
H_3 &= (A + 2B)(A - B)^2 - 3C^2(A - B)q(\theta, \phi) \\
&\quad - 54\left(\left(B^2 + \frac{C^2}{2}\right)^{3/2} + B\left(B^2 + \frac{C^2}{2}\right)\right)\rho(\theta, \phi), \\
H_2 &= (\Delta_{so} - 3\epsilon)[-A^2 + B^2 + C^2q(\theta, \phi)], \\
H_1 &= A\epsilon(3\epsilon - 2\Delta_{so}), \\
H_0 &= \epsilon^3(\epsilon - \Delta_{so}), \\
\rho(\theta, \phi) &= \sin^4 \theta \cos^2 \theta \sin^2 \phi \cos^2 \phi.
\end{align*}
\]

Equation (8) is solved exactly for the whole band, although this task can be much reduced using symmetry. Having estimated the band structure numerically, we then calculated the nonparabolicity functions. To obtain a non-angle-dependent \(\chi\), an angular average was taken. Two of the three solutions of Eq. (7) are unity at zero energy, the bottom of heavy and light bands. The third solution, related to the split-off band, was imposed on the unity at \(\Delta_{so}\), the bottom of the split-off band. To achieve this, we divided by a factor that can be identified with \(m_{so}\), obtaining a value (see Table I) in agreement with previous studies. The results of this procedure are shown in Fig. 1. In this figure we also represent a previous analytical approach for the silicon \(\chi\) functions, that appears in the bibliography. In that study, these functions were modeled by piecewise quadratic expressions.

We established a comparison between our valence band model for Si and Ge with the pseudopotential results given by Srivastava. We observed parallel behaviors up to 1 eV. Above this energy our model gives higher energies for the same wave vector.

We now specify expressions (1) for the different types of hole-phonon scattering to be taken into account in intrinsic silicon and germanium.

### A. Optical phonons

In a pure semiconductor, acoustic and optical scattering must be considered. Additionally, for each scattering mechanism, the hole may or may not remain in the same band (heavy, light, or split-off) after the scattering. To describe all the processes that take place, we have designated a capital letter for each band, \(H\) for heavy, \(L\) for light, and \(S\) for split-off holes. Thus we have three intraband mechanisms, designated \(HH\), \(LL\), and \(SS\) and six interband mechanisms referred to as \(HL\), \(HS\), \(LS\), \(SH\), and \(SL\). The first letter in the notation indicates the initial state, while the second relates to the final state.
For optical scattering, in order to obtain the probability function for the direction of the final wave vector, we must perform the integration of Eq. (1) over \( k' \). For this, the dispersion relation of the optical phonons is assumed to be constant \((=\hbar \omega_{\text{op}})\), and thus \( N_q \) can also be considered constant \((=N_{\text{op}})\), i.e., it remains independent of the phonon wave vector modulus and \( |\xi_q| \) \((=D^2)\), \( D \) is generally referred to as the optical deformation potential. \(^{21}\) By this process, the angular probability function gives us

\[
P(\mathbf{k}, \theta', \phi')_{\text{HH,LS}, \text{SH}} = \frac{D^2}{8\pi^2 \rho \omega_{\text{op}}} \left( \frac{N_{\text{op}}}{N_{\text{op}} + 1} \right) G_{\text{HH,LS}, \text{SH}}(\theta) \times \frac{\sqrt{e \pm \hbar \omega_{\text{op}}}}{2[a(1-g')^{3/2}J_H(e \pm \hbar \omega_{\text{op}})}
\]

\[
P(\mathbf{k}, \theta', \phi')_{\text{LL,LS}, \text{SH}} = \frac{D^2}{8\pi^2 \rho \omega_{\text{op}}} \left( \frac{N_{\text{op}}}{N_{\text{op}} + 1} \right) G_{\text{LL,LS}, \text{SH}}(\theta) \times \frac{\sqrt{e \pm \hbar \omega_{\text{op}}}}{2[a(1+g')^{3/2}J_L(e \pm \hbar \omega_{\text{op}})},
\]

\[
P(\mathbf{k}, \theta', \phi')_{\text{SS,LS}, \text{LS}} = \frac{D^2}{8\pi^2 \rho \omega_{\text{op}}} \left( \frac{N_{\text{op}}}{N_{\text{op}} + 1} \right) G_{\text{SS,LS}, \text{LS}}(\theta) \times \frac{\sqrt{2m_a^{3/2}}/h^3 e \pm \hbar \omega_{\text{op}} - \Delta_{\text{so}} J_S(e \pm \hbar \omega_{\text{op}})},
\]

where \( a = \hbar^2/2m_a\), \( G(\theta) \) is the above-mentioned overlap function for each transition, and

\[
J_H(e) = \left[ \frac{1}{\chi(e)_{\text{HH}, S}^{3/2}} - \frac{e}{\chi(e)_{\text{HH}, S}^{5/2}} \frac{d\chi_{\text{HH}, S}(e)}{e} \right],
\]

\[
J_L(e) = \left[ \frac{1}{\chi(e)_{\text{LL}, S}^{3/2}} - \frac{e - \Delta_{\text{so}}}{\chi(e)_{\text{LL}, S}^{5/2}} \frac{d\chi_{\text{LL}, S}(e)}{e} \right] .
\]

Note that once a particular scattering mechanism has been chosen, the direction taken by the hole after the scattering can be evaluated by means of the rejection technique, taking \( \cos \theta' \) in \([-1,1]\) and \( \phi' \) in the interval \([0,2\pi]\) randomly and using the following expressions:

\[
P(\mathbf{k}, \theta', \phi')_{\text{HH,LS}, \text{SH}} = G_{\text{HH,LS}, \text{SH}}(\theta)
\]

\[
P(\mathbf{k}, \theta', \phi')_{\text{LL,LS}, \text{SH}} = G_{\text{LL,LS}, \text{SH}}(\theta)
\]

\[
P(\mathbf{k}, \theta', \phi')_{\text{SS,LS}, \text{LS}} = G_{\text{SS,LS}, \text{LS}}(\theta),
\]

where the angle-independent factors in Eq. (14) have been removed.

The new functions defined in Eq. (15) are one of the main modifications that should be included in scattering rate expressions if nonparabolicity is being considered. In the parabolic case, the \( \mathcal{J} \) functions are in fact reduced to the unity. In addition, the importance of choosing the right \( \chi \) functions is now evident. Their role is now essential, not only to determine the state after a free flight but also to calculate scattering rate through the \( \mathcal{J} \) functions. Figure 2 shows these functions for silicon and germanium. We observed that for germanium, the scattering rate is enhanced considerably, especially for the light holes, where this increase is significant even at low energies. For silicon the variation is not so remarkable although it cannot be ignored, since the \( \mathcal{J} \) functions reach values greater than 2 and 3 for heavy and light holes, respectively, and are lower than 0.4 at energies close to 100 meV above \( \Delta_{\text{so}} \) for split-off holes. In the same figure, the \( \mathcal{J} \) functions obtained from the piecewise analytical expressions previously proposed (see Ref. 6) are shown. The results demonstrate that although certain approximations could be useful in the flight process, continuity, at least in the derivatives of \( \chi \), must be imposed in order to avoid meaningless results. A deeper discussion of these figures will be given in Sec. III.

Most of the approaches described in the literature obtain the energy of optical phonons from a typical temperature \( \theta_{\text{op}} \) by the relation \( e = \hbar \omega_{\text{op}} = k_B \theta_{\text{op}} \) with \( k_B \) being the Boltzmann constant. All the values used for the parameters defined above are shown in Table I.

From Eq. (14) we can calculate the probability per unit of time of changing the state of a hole of energy \( e \) by integrating over the whole solid angle, with the result...
\[ P(e)_{\text{LL,HL,SL}} = \frac{D^2}{\sqrt{2\pi \omega_{\text{op}}}} N_{\text{op}} \left( \frac{e \pm h \omega_{\text{op}}}{h^3} \right) \times \mathcal{J}_L(e \pm h \omega_{\text{op}}), \]

\[ P(e)_{\text{SS,HS,LS}} = \frac{D^2}{\sqrt{2\pi \omega_{\text{op}}}} N_{\text{op}} \left( \frac{e \pm h \omega_{\text{op}} - \Delta_{\text{op}}}{h^3} \right) \times \mathcal{J}_L(e \pm h \omega_{\text{op}}), \]

where \( D \) is the angular average of \( G \) multiplied by \( D^2 \). It can easily be demonstrated that the angular average of the \( G \) functions for interband and intraband scattering are equal, and so the \( D \) is a common value for all the optical scattering probabilities. Integration in the whole solid angle in Eq. (14) is commonly interpreted as an angular balance. In fact

\[ \langle m_H^L \rangle = \frac{m_0}{4\pi |A|^{3/2}} \int_0^{\pi} \int_0^{\pi} \frac{1}{[1 + g'((\theta, \phi))]^{3/2}} \sin \theta \sin \phi, \]

\[ \langle m_L^S \rangle = \frac{m_0}{4\pi |A|^{3/2}} \int_0^{\pi} \int_0^{\pi} \frac{1}{[1 + g'((\theta, \phi))]^{3/2}} \sin \theta \sin \phi, \]

The values \( \langle m_H^L \rangle, \langle m_L^S \rangle \) can be understood as angular averages of \( m_H^L(e=0, \theta, \phi) \) and \( m_L^S(e=0, \theta, \phi) \), the functions \( m_H(e, \theta, \phi) \) and \( m_L(e, \theta, \phi) \) being the effective masses depicted in Eq. (6). The average effective masses at the minima of the bands could be obtained from \( \langle m_H(e=0) \rangle = \langle m_H^L \rangle^{3/2} \) and \( \langle m_L(e=0) \rangle = \langle m_L^S \rangle^{3/2} \).

**B. Acoustic phonons**

When dealing with acoustic scattering, the approximation \( \xi_{\beta} = \sum_{\gamma} \xi_{\beta \gamma}^2 \) is commonly employed in Eq. (1), where a constant \( \Xi_{\beta} \) is used to avoid the complexity of dealing with the deformation tensor \( \Xi \). Similarly, taking the relation of dispersion for acoustic phonons as a linear expression \( \omega_{\text{ac}} = \omega_{\text{ac}} \) has, as already stated, proved useful and sufficiently accurate. To obtain coupling constants for the scattering mechanisms (both acoustic and optical), the usual procedure is to fit the simulator results with the experimental data of drift velocity vs electric field. Our results, shown in Table I, are in the same order as those reported by other authors. 21

In general, hole-acoustic phonon scattering probabilities are dependent on the phonon wave vector, and the scattered phonon may have a wide range of energies, depending on the initial energy of the hole. When we studied the traditional formalism used to obtain them within the framework of effective mass theory, we took into account the conservation of momentum and energy in each scattering exactly, and although the results for mobility at high temperatures were similar to those found in the experimental data, at low temperatures the model failed. This persuaded us to treat acoustic scattering in a different way, working with an average of the acoustic phonon energies in a fashion similar to that proposed by Bufler, Schenk, and Fichtner, 11 but modifying it for use within the effective mass framework and extending it to interband scattering. In this way we were able to introduce the inelasticity of the hole-acoustic phonon process, thus providing more accurate results.

A hole in a state of energy \( e \) and wave vector \( \vec{k} \) could emit or absorb an acoustic phonon, changing its wave vector to \( \vec{k}' \). Considering the small warping approximation \( \hat{\delta} \) and supposing that the energy of the hole does not undergo a significant alteration in the momentum balance equation, we obtained the mean wave vector of the scattered phonon. For example, for intraband scattering, this value was \( \bar{q}=4/3k \). Using the density of states for holes and the occupation of the band, we can estimate an average of the mean wave vector of the scattered phonon \( \langle q \rangle \), and accordingly the mean energy of the scattered phonon through the dispersion relation, \( \langle e_{\text{ac}} \rangle = h\nu \langle q \rangle \). These averages are temperature dependent due to the occupation of the band and are influenced by the nonparabolicity of the bands through the \( \hat{\delta} \) functions, which appear in the density of states calculation. This leads to

\[ P(\vec{k}, \vec{k}') = \frac{\pi v^2}{\rho V u} G(\theta) \left( \frac{N(e_{\text{ac}})}{N(e_{\text{ac}}) + 1} \right) \delta(e' - e \mp \langle e_{\text{ac}} \rangle), \]

\[ = \frac{\pi v^2}{\rho V h u^2} G(\theta) \left( \frac{N(e_{\text{ac}})}{N(e_{\text{ac}}) + 1} \right) \delta(e' - e \mp \langle e_{\text{ac}} \rangle). \]

In fact, only \( \langle e_{\text{ac}} \rangle \) is needed. Applying the former approximations, we find that the average wave vector of the scattered phonon is given by

\[ q = k \sqrt{1 + s(e) - 2[s(e)]^{1/2} \cos \theta}, \]

where the \( s \) factor is a function of hole energy. It has different expressions depending on the type of scattering considered,

\[ s(e) = 1, \text{ for intraband scattering} \]

\[ s(e) = \frac{m_{\text{final}}X_{\text{final}}(e)}{m_{\text{initial}}X_{\text{final}}(e)}, \text{ for interband scattering } HL \text{ and } LH \]

\[ s(e) = \frac{m_{\text{so}}X_{\text{so}}(e)}{m_{\text{so}}X_{\text{so}}(e)}, \text{ for interband scattering } X, X \text{ being heavy or light} \]

\[ s(e) = \frac{m_{\text{so}}X_{\text{so}}(e)}{m_{\text{so}}X_{\text{so}}(e)} - 1, \text{ for interband scattering } SX, X \text{ being heavy or light} \]

(21)
These new expressions generalize the Bufler et al. procedure, and allow the treatment of interband scattering. To obtain the mean $q$ for a particular initial energy of the hole, we took an average in the whole solid angle

$$q(q) = \frac{1}{4\pi} \int q d\Omega$$

$$= \frac{1}{2} \int \left[ k \sqrt{1 + s(q) - 2\sqrt{s(q)} \cos \theta \sin \vartheta \cos \theta} \right] d\vartheta dt$$  \hspace{1cm}  \text{(22)}$$

Finally, we calculated a second average using the distribution function of holes

$$\langle q \rangle = \frac{\int_0^\infty q \bar{q}(q)e^{-\epsilon q^2}d\epsilon}{\int_0^\infty e^{-\epsilon q^2}d\epsilon} = \frac{\langle \epsilon_{\text{so}} \rangle}{\hbar u}.  \hspace{1cm}  \text{(23)}$$

Regarding Eqs. (19)–(23), and bearing in mind that the averages explained above eliminate the angular dependence of $q$, the only angle-dependent functions when the integral of Eq. (1) over the modulus $k'$ is performed are those obtained in the case of optical scattering. Therefore, for acoustic phonon scattering, the angular probabilities are the same as those shown in Eq. (16).

Taking the above into account, the acoustic scattering probability for all these different processes is given by

$$P_{1,F}(\epsilon) = \frac{1}{2\pi} \left( \frac{\Xi^2 \sqrt{3} \epsilon_{\text{so}}}{\hbar u} \right)^{3/2} \left( \frac{N_{\epsilon_{\text{so}}}}{N_{\epsilon_{\text{so}}}} \right) \left( \frac{N_{\epsilon_{\text{so}}}}{N_{\epsilon_{\text{so}}} + 1} \right)$$

$$\times \sqrt{\epsilon \pm \langle \epsilon_{\text{so}} \rangle_{1,F} \epsilon \pm \langle \epsilon_{\text{so}} \rangle_{1,F}}$$  \hspace{1cm}  \text{(24)}$$

or

$$P_{1,S}(\epsilon) = \frac{1}{2\pi} \left( \frac{\Xi^2 \sqrt{3} \epsilon_{\text{so}}}{\hbar u} \right)^{3/2} \left( \frac{N_{\epsilon_{\text{so}}}}{N_{\epsilon_{\text{so}}}} \right) \left( \frac{N_{\epsilon_{\text{so}}}}{N_{\epsilon_{\text{so}}} + 1} \right)$$

$$\times \sqrt{\epsilon \pm \langle \epsilon_{\text{so}} \rangle_{1,S} - \Delta_{\text{so}} \epsilon \pm \langle \epsilon_{\text{so}} \rangle_{1,S}}.$$  \hspace{1cm}  \text{(25)}$$

In the equations above, the $I$ and $F$ subscripts signify the initial and final types of hole in the scattering. The latter expression is valid for scattering only where the final state is a split-off hole, while the former is valid for the remaining mechanisms. The upper symbols relate to absorption, while the lower are used for emission.

### III. RESULTS

We begin this section with a deeper commentary on the nonparabolicity functions and their implications for the remainder of the results through the functions $\mathcal{S}$, presented in this paper. As explained in Sec. II, the nonparabolicity functions $\chi(q)$ were obtained numerically from the Kane formalism. They depend on the type of hole, and of course, they will be different for Si and Ge. For Si, we also compared our results with the piecewise continuous function approximations given by Dewey and Osman.\(^6\) In addition, we show the nonparabolicity function for the split-off band $\chi_s$. Up to $\Delta_{\text{so}}$, this function is meaningless, starting at the bottom of the split-off band. This function behaves in the opposite manner to the others, showing an increase in the whole range of energies, although reaching an asymptotic trend at high energies.

Equation (6) indicates the dependence of the effective mass on $\epsilon$ for whatever direction. As a consequence of the $\chi$ functions calculated, this relation implies that heavy and light hole effective masses increase when energy grows, becoming approximately twice as great for high energies as for low ones. However, we observed the opposite behavior with the split-off band. This band has usually been treated as parabolic in the literature, neglecting the change in effective mass.

For Ge, we observe a lesser nonparabolicity effect for the heavy band, while for the light band, on the other hand, a significant increase in effective mass is revealed when energy increases, this being caused by the strong nonparabolicity, which is four times greater at high energies than at the bottom of the band. The split-hole band starts at 295 meV and the behavior of the nonparabolicity function occurs all the way round, a common feature with Si. Thus we find a decrease in the effective mass of split-off holes when the energy rises, reaching less than half the value of the effective mass at the bottom of the band.

Figure 2 shows the $\mathcal{S}$ functions derived from our $\chi$ functions. We have also plotted the $\mathcal{S}$ functions obtained from previous parameterizations. The use of approaches to nonparabolicity without continuous derivatives results in discontinuities in the $\mathcal{S}$ functions, and consequently to meaningless scattering probabilities. It is worth noting that although some analytical approximations may be accurate enough to explain certain kinds of phenomena, careful modeling is necessary in order to take into account nonparabolicity in hole transport.

In this paper we have chosen to use the exact solution because our purpose is to study hole transport rather than to simplify the calculation process by means of analytical expressions. Additionally, we show the $\mathcal{S}$ function for the split-off band, demonstrating that the scattering rates related to this kind of hole are reduced, due to the behavior of the nonparabolicity function.

For Ge there is a highly significant change in this function for light holes, while for heavy and split-off holes the behavior is similar to Si. This implies very significant differences in the scattering probability values respect to those calculated, as usual, with a parabolic model using effective mass at the bottom of the band. We have indicated in the figure the values at 1 eV for each $\mathcal{S}$ function. These values will change less for higher energies.

Our model allows us to study the population in each band in several conditions, see Fig. 3. For Si, we simulated at 77 and 300 K with electric fields parallel to [100] and [111]. For low fields, no influence on the direction of the field is noticeable in any band at the temperatures considered. This is consistent with the idea that when the electric field is null,
the direction of application is meaningless, and so the field will not affect the population. At 77 K, when the field increases, some differences arise, depending on the direction of the field. Over 0.2 kV/cm, the heavy hole population is more important when the field is in the [111] direction. A maximum is observed at fields near 7 kV/cm in the heavy hole population, in parallel with a minimum in the light hole population. For higher fields, the number of heavy holes decreases, while the number of light and split-off holes starts to rise slightly. It is worth noting that for high fields, the difference between the populations of heavy and light holes is almost constant, whether the field is [100] or [111], being around 1.5% for both kinds of hole. At 300 K, the differences in the populations of the bands for applied fields in different directions arise at over 10 kV/cm, and are not as significant as at 77 K. Moreover, a slow rise in the heavy hole population is observed, related to a slow decrease in the light hole population when the magnitude of the field increases. The split-off band is almost unaffected, remaining at around 1.5% of the total hole population.

For Ge, we repeated the study at 40 and 220 K. At 40 K, the difference between the heavy hole populations when the field is applied in the directions indicated is around 0.5% at high fields, while at very low fields it remains very low. The difference between [100] and [111] is slightly enhanced over 0.02 kV/cm. In the same manner as for Si, the heavy hole population is enhanced when the field is [111]. At 220 K, the difference between [100] and [111] is almost negligible up to 10 kV/cm. The differences at lower fields are a consequence of statistical dispersion. At high fields the difference in the heavy hole population is around 0.25%, being enhanced when the field is applied parallel to the [111] direction. Over 6 kV/cm, the heavy hole population starts to decrease, while the light hole population increases its value to exceed 10% of the total population. This value in the electric field is also related to a slight rise in the split-off hole population, however the rise is not sufficient to affirm that split-off holes will start to play an important role, because in the higher field studied, the population was lower than 0.5%. In fact, the high value of $\Delta_m$ in Germanium makes the contribution of the split-off band to the whole behavior negligible; note that this split-off figure is the only one with a logarithmic $Y$ axis.

Our results for drift velocity versus external electric field are plotted in Fig. 4. For Si we obtained a good level of agreement at a wide range of temperatures. We compared our data with the experimental data at 77, 160, and 300 K, considering applied fields parallel to the [100] and [111] directions. For Ge, we studied the relation between drift velocity and applied electric field at 40, 130, and 220 K, parallel to [100] and also to [111]. We found a good level of agreement between the simulations and the experimental data. One of the main advantages of the presented model is the low computation time to provide results. Table II shows running times and the respective uncertainty of the obtained drift velocities using a laptop computer with a Pentium 4, 3.06 Ghz microprocessor and 512 MB DDR RAM.

At high fields, drift velocity is in all cases lower when the direction of the field is [111]. Referring back to our earlier comments on the population of the bands, we found a clear relation between these and drift velocity. At low fields the populations are the same, regardless of the direction to the applied field. However, when the field increases, the heavy hole population is higher in the [111] case, both in Si and Ge, and at the whole set of temperatures studied, and this causes a lower drift velocity in this direction. This is confirmed by the fact that the differences caused by the direction of the field, both in drift velocity and in the population of holes, start at around the same values of the field, as shown in the Fig. 5. Moreover, in the [111] direction, the heavy holes in the semiconductors studied exhibit the highest effective mass, due to warping, while in the [100] direction, they exhibit the lowest, which leads us to conclude that the difference between drift velocity in the [111] and [100] cases is a combination of both effects: different effective masses due to warping and different hole populations in the bands.

Another interesting aspect of hole dynamics is mean energy and its relation to electric field. When the field increases, the mean energy of holes also rises. This relationship has already been investigated with pseudopotential-based algorithms. Using our model, we evaluated mean energy vs electric field, obtaining similar results to those for Ge and...
Si. The results are particularly accurate for Ge at a wide range of temperatures 77, 130, 190, and 300 K. In silicon, the temperatures studied were 77, 300, and 430 K. For this semiconductor, although a general agreement in behavior could be established, a higher slope for the 77 K plot can be seen in electric fields between 0.04 and 0.4 kV/cm. In this range we found mean energies higher than those predicted by full band close to 0.1 kV/cm. This fact has been investigated, and is due to the values of the deformation potentials needed to fit drift velocity vs electric field. Previous studies\textsuperscript{12} showed that this behavior arises when optical phonon scattering becomes as important as acoustic. It is for this reason that the effect appears only at 77 K, since at 160 and 300 K optical phonon scattering is significant at low fields. It also

![Si results](image)

![Ge results](image)

**FIG. 4.** Comparison between the experimental data and the Monte Carlo calculations of velocity as a function of the applied field for Si (a) and Ge (b). Symbols refer to experimental data (see Refs. 14 and 23), while curves are for MC results. A good agreement is shown at a wide range of temperatures.

**FIG. 5.** Comparison between our model (EM) and previous work (see Ref. 5) based on the full band framework (FB) for mean energy of the holes vs electric field for Si and Ge at various temperatures. We observed a more significant heating at 77 K for fields near 0.1 kV/cm. For Ge our model predicts almost the same values given by Nguyen et al. at the whole range of fields and temperatures studied.

**TABLE II.** Examples of running times and data uncertainties.

<table>
<thead>
<tr>
<th></th>
<th>Si</th>
<th>Ge</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>77 (K)</td>
<td>300 (K)</td>
</tr>
<tr>
<td></td>
<td>Electrical field (kV/cm)</td>
<td>Simulation time (s)</td>
</tr>
<tr>
<td>0.3</td>
<td>160</td>
<td>0.0070</td>
</tr>
<tr>
<td>3</td>
<td>90</td>
<td>0.0037</td>
</tr>
<tr>
<td>30</td>
<td>39</td>
<td>0.0026</td>
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</table>
TABLE III. Comparison of the mobility calculated in this paper, the experimental data, and that provided by the pseudopotential method (Ref. 5).

<table>
<thead>
<tr>
<th>Hole mobility (cm²/V s)</th>
<th>Si</th>
<th>Ge</th>
</tr>
</thead>
<tbody>
<tr>
<td>T (K)</td>
<td>Present work</td>
<td>Pseudopotential</td>
</tr>
<tr>
<td>77</td>
<td>11 108±1095</td>
<td>12 100±1090</td>
</tr>
<tr>
<td>130</td>
<td>17 027±454</td>
<td>6 610±379</td>
</tr>
<tr>
<td>190</td>
<td>16 420±936</td>
<td>6 010±480</td>
</tr>
<tr>
<td>300</td>
<td>527±36</td>
<td>479±30</td>
</tr>
</tbody>
</table>

8See Ref. 24.
9See Ref. 14.
10See Ref. 25.
11See Ref. 26.

justifies the nonexistence of this behavior in Ge, due to the lower energy of its optical phonons, which makes them relevant even at low temperatures. We can affirm that our model gives results comparable to those obtained by full band methods, thus offering evidence that our model also provides a useful view of valence band for the semiconductors studied.

Finally, we calculated drift velocity for very low fields (lower than plotted in Fig. 3, in fact) to evaluate ohmic mobility for both Silicon and Germanium. The comparison of our results with the experimental data and with those obtained by the pseudopotential method is shown in Table III. This table makes evident the high level of agreement with the experimental results, obtained by our simulation at the whole range of temperatures. Interestingly, the worst datum provided by our method (Ge at 77 K), is close to the pseudopotential result. Regarding Si at 300 K, we observe that our model provide a mobility higher that the last reported measurements, although considering the value of the error, it remains close to the two quoted experimental data.

The simple procedure shown in this paper is therefore able to produce reasonable hole mobilities, thus providing an attractive alternative for studying hole transport. These results confirm the value of effective mass framework if appropriate precautions are taken with scattering rate expressions and with nonparabolicity modeling.

IV. CONCLUSIONS

Our paper introduces a model designed to study hole transport in pure Silicon and Germanium. With this model we obtained the drift velocity versus the applied electric field, and consequently the mobility, at a wide range of temperatures.

To develop our model we implemented a Monte Carlo simulator and used effective mass theory to calculate the band structure. In so doing, we evaluated exactly the nonparabolicity of the valence band for the three kinds of holes (heavy, light, and split-off) described in Kane’s work, obtaining the χ functions. Once these functions had been calculated, we modified the scattering rate expressions to take nonparabolicity into account, which resulted in multiplica-

tion of the parabolic scattering rates by new functions, named ϑ. Their calculation indicates the importance of using adequate analytical approaches for χ.

Our results show a significant increase in heavy and light scattering rates, while a decrease is observed in the case of split-off holes. The increment is particularly marked for the light hole band.

We also took into account that scattering with acoustic phonons should be modeled as an inelastic process. We extended one model presented in the bibliography in order to introduce this effect in the three types of hole, calculating the mean energy for each process.

With the simulator described above, we obtained the population in each band at different temperatures and directions of the applied field. The results show that at low fields the effects of direction are not noticeable. However, at high fields, a greater contribution of the heavy holes is observed at [111] than at [100]. The split-off holes do not play a significant role in Germanium due to the high value of Δsso, while in Silicon their contribution is greater.

We found a clear relation between the drift velocity and the occupation of each band. The data indicate greater velocities in the [100] direction, not only because of the smaller effective mass of heavy holes in this direction but also due to the lower number of heavy holes when the field is applied in the [100] direction.

Our method confirms the main features of hole transport calculated by full-band algorithms. In fact, we evaluated the mean energy of the holes provided by our model and compared them with those calculated by the pseudopotential method. The figure shows an excellent level of agreement between the two procedures. This is more noticeable when the variety of electric fields and temperatures used in the comparison is taken into account. The similarity is particularly evident in the case of Ge. In Si the main differences were located at 77 K and in an applied field between 0.04 and 0.4 kV/cm. In that range, our data are explained by the fact that optical phonon scattering becomes as important as acoustic at that field and temperature. At higher temperatures this phenomenon has already produced, so this behavior is not expected.

Finally we calculated the low field mobility for Si and Ge at a wide range of temperatures. The data we obtained
agree with the experimental data and with those calculated by the pseudopotential method. This indicates that the effective mass framework might continue to be a useful tool, within its limits, as long as the appropriate expressions are used in the calculation of nonparabolicity functions and in modeling of the scattering rates.

ACKNOWLEDGMENTS

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2 See http://www.research.ibm.com/DAMOCLES/


