Impact ionization rate and high-field transport in ZnS with nonlocal band structure

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The impact ionization rate in ZnS is calculated using a nonlocal empirical pseudopotential band structure and compared to previous results using a local calculation. The two resulting rates are then compared and simple fit formulas are presented. These are included in an ensemble Monte Carlo simulation of electron transport in bulk ZnS. The calculated impact ionization rate is then compared to experimental impact ionization coefficient data; reasonable agreement between the experimental data and the calculated impact ionization rate is obtained with an appropriate choice of optical deformation potentials. © 1996 American Institute of Physics.

I. INTRODUCTION

The study of transport phenomena in electronic materials has both theoretical interest and practical applications, particularly in semiconductor devices. The description of transient behavior of far-from-equilibrium systems and the evolution into a steady state is a challenging problem in nonequilibrium physics. Under the influence of strong driving forces such as an external electric field, linear response theory fails and new phenomena arise, which have been extensively studied for several decades (for a review, see Ref. 1). Practical interest arises in the simulation of small scale semiconductor devices where field strengths of up to 2–3 MV/cm may be reached.

Alternating-current thin-film electroluminescent (ACTFEL) devices are one particular technology in which high-field transport is of paramount importance in the device performance (see, for example Ref. 2). In such structures, a thin phosphor layer material such as ZnS is subject to a large electric field (typically 1–3 MV/cm) associated with an applied ac voltage. Due to field emission into the conduction band from trapped interface states at these field strengths, electrons accelerate to high enough energies to impact excite luminescent impurities such as Mn or Tb, giving off visible light useful for flat-panel display applications. The light emission process depends sensitively on the fraction of carriers above the threshold energy for impact excitation (≈2–2.6 eV) and, thus, on the details of the nonequilibrium electron distribution function. The impact excitation yield responsible for radiative transitions may be strongly affected by competing scattering mechanisms which dominate at high electric fields. In particular, band-to-band impact ionization also becomes important in these field ranges and may dominate scattering leading to carrier multiplication and field clamping. Therefore, obtaining an understanding of this mechanism and its dependence on electric field is critical for determination of the efficiency limitations in present day ACTFEL devices.

We have previously calculated the impact ionization rate for ZnS using a local empirical pseudopotential method (EPM) calculation for the band structure. However, the local EPM method suffers from the assumption of spherically symmetric atomic potentials. This problem is partially resolved in the nonlocal EPM by inclusion of nonlocal contributions to the pseudopotential arising from different angular momentum states. In the present article, we extend the previous local calculation by deriving a set of nonlocal pseudopotential form factors for ZnS and using the nonlocal EPM to calculate the impact ionization rate. These impact ionization rates are then used in a full-band Monte Carlo simulation of high-field transport for ZnS to calculate the impact ionization coefficient in order to compare calculated results to experimental data.

II. BAND STRUCTURE

Under high-field conditions in a semiconductor device, electrons are accelerated to high energies and, therefore, a realistic band structure has to be employed to correctly model the electron dynamics. One of the standard techniques of moderate computational effort for the calculation of realistic band structures is the empirical pseudopotential method (EPM) which describes the electrons in a crystal lattice by a one-electron Hamiltonian. The periodic potential \( V(\mathbf{r}) \) consists of the periodic crystal potential and electron–electron
Within the context of this expansion, the Schrödinger equation can be written as a set of homogeneous linear equations for the cell periodic part as

\[
\sum_{G'} \left[ \frac{\hbar^2}{2m} (\mathbf{k} + \mathbf{G})^2 - E_{n}(\mathbf{k}) \right] \delta_{\mathbf{G},\mathbf{G}'} + V(\mathbf{G} - \mathbf{G}') U_{n,\mathbf{k}}(\mathbf{G}') = 0,
\]

where \( V(\mathbf{G}) \) is the Fourier coefficient of the crystal potential. For the cubic zinc-blende lattice with a two-atom basis, this Fourier coefficient is usually written in the form of a symmetric and an antisymmetric contribution to the potential

\[
V(\mathbf{G}) = \cos \left( \frac{\mathbf{G} \cdot \mathbf{r}_B}{2} \right) V_s(\mathbf{G}) + i \sin \left( \frac{\mathbf{G} \cdot \mathbf{r}_A}{2} \right) V_a(\mathbf{G}),
\]

where \( \mathbf{r}_B \) is the basis vector connecting the cation and anion in the unit cell, \( V_s(\mathbf{G}) \) is the symmetric and \( V_a(\mathbf{G}) \) the antisymmetric pseudopotential form factor. In the local EPM, the pseudopotential is expanded with respect to angular momentum via

\[
V(r) = \sum_{l=0}^{\infty} P_l P_l V_l(r) P_l,
\]

where \( P_l \) are projection operators for the \( l \)th angular momentum component of the wave function. The nonlocal potentials \( V_l(r) \) are assumed to be spherical and are given by square wells of width \( R_l \) and depth \( A_l \). In the present work, only the contribution for \( l=2 \) is considered.

As a starting point, we used local pseudopotential form factors for ZnS,\(^6\) together with the nonlocal parameters reported for ZnSe.\(^5,7\) These values were then systematically varied to obtain a good fit to available experimental critical point and reflectivity spectrum data. Table 1 lists the local and nonlocal pseudopotential parameters derived from this procedure.

Figure 1 shows a comparison of the local and nonlocal band structures neglecting spin-orbit coupling. Significant differences are found around the \( K \) and \( \Gamma \) points which affect the calculated \( \mathbf{k} \)-dependent impact ionization rates, as dis-

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**TABLE I.** Form factors for generation of the ZnS band structure using the empirical pseudopotential method. For comparison, the local parameters for ZnS are also shown.\(^a\)

<table>
<thead>
<tr>
<th>Form factors (Ry)</th>
<th>( V_s^3 )</th>
<th>( V_s^4 )</th>
<th>( V_a^3 )</th>
<th>( V_a^4 )</th>
<th>( V_s^{11} )</th>
<th>( V_a^{11} )</th>
<th>( V_s^{12} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Local</td>
<td>-0.22</td>
<td>0.03</td>
<td>0.07</td>
<td>0.23</td>
<td>0.15</td>
<td>0.02</td>
<td>0.02</td>
</tr>
<tr>
<td>Local (present)</td>
<td>-0.218</td>
<td>0.046</td>
<td>0.072</td>
<td>0.181</td>
<td>0.104</td>
<td>0.015</td>
<td>0.015</td>
</tr>
</tbody>
</table>

**Nonlocal parameters**

<table>
<thead>
<tr>
<th>CAT</th>
<th>CAT</th>
<th>AN</th>
<th>AN</th>
<th>( \zeta )</th>
<th>( \mu )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A_2 )</td>
<td>( R_2 ) (Å)</td>
<td>( A_2 )</td>
<td>( R_2 ) (Å)</td>
<td>( \zeta )</td>
<td>( \mu )</td>
</tr>
<tr>
<td>-0.125</td>
<td>1.22</td>
<td>0.505</td>
<td>1.22</td>
<td>5.34</td>
<td>0.000165</td>
</tr>
</tbody>
</table>

\(^a\)See Ref. 6.

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**TABLE II.** Experimental and nonlocal EPM critical point transition energies with and without spin-orbit (SO) interaction.

<table>
<thead>
<tr>
<th>Critical point transition</th>
<th>Experimental (in eV)</th>
<th>Nonlocal (SO)</th>
<th>Nonlocal (w/o SO)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Gamma_{15}-\Gamma_1 ) (0,0,0)</td>
<td>3.68</td>
<td>3.71</td>
<td>3.73</td>
</tr>
<tr>
<td>( L_3-L_1 ) (0.5,0.5,0.5)</td>
<td>5.73</td>
<td>5.58</td>
<td>5.60</td>
</tr>
<tr>
<td>( \Delta_3-\Delta_1 ) (0.5,0.0,0)</td>
<td>7.02</td>
<td>6.94</td>
<td>6.92</td>
</tr>
<tr>
<td>( \Delta_3-\Delta_1 ) (0.37,0,0)</td>
<td>7.50</td>
<td>7.58</td>
<td>7.60</td>
</tr>
<tr>
<td>Volume effect (0.57,0.36,0.14)</td>
<td>8.35</td>
<td>8.43</td>
<td>8.43</td>
</tr>
<tr>
<td>( \Lambda_3-\Lambda_2 ) (0.29,0.29,0.29)</td>
<td>9.0</td>
<td>8.89</td>
<td>8.87</td>
</tr>
</tbody>
</table>

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**FIG. 1.** Nonlocal pseudopotential band structure for ZnS (dashed line) compared to a band structure calculated using the local parameters given by Cohen and Chelikowsky (Ref. 6) (solid line).
The impact ionization rate is of fundamental interest for understanding the electron transport in semiconductors at high electric field strengths. Of particular interest are the orientation dependence and the threshold behavior which were studied for Si\(^{10-13}\) and GaAs\(^{12,14}\) recently, we have determined the impact ionization rate for ZnS\(^{4}\) following the scheme developed by Sano and Yoshii\(^{11}\) for Si using a very efficient deterministic numerical procedure. Their special integration scheme takes into account a rather large number of points in the Brillouin zone so that they were able to study effects of the anisotropy in \(k\) space as well as the threshold behavior for Si. Both were found to be direct consequences of the band structure.

In this article, we have included the nonlocal corrections of Section II in the band structure calculation for ZnS using the same calculation scheme.\(^{11,12}\) The impact ionization rate is determined from Fermi’s golden rule as

\[
r(k_1, \nu_1) = \frac{2\pi}{\hbar} \frac{\Omega^3}{(2\pi)^9} \sum_{\nu_2} \cdots \sum_{\nu_4} \int \cdots \int d^3k_2 \, d^3k_3 \, d^3k_4 \times |M_{\nu_1}(1,2;3,4)|^2 \delta(E_{\nu_1}(k_1) + E_{\nu_2}(k_2) - E_{\nu_3}(k_3) - E_{\nu_4}(k_4)),
\]

where \(\nu_1\) is the band index, \(M_{\nu_1}\) denotes the matrix element for ionization including direct (D), exchange (E), and umklapp processes,

\[
|M_{\nu_1}|^2 = 2|M_D|^2 + 2|M_E|^2 - |M_D^* M_E + M_D M_E^*|.
\]

Here the initial electron states correspond to an electron initially in the conduction band (1) and a second electron in the valence band (2). The final states are for both electrons in the conduction band [(3) and (4)]. The integrals are extended over the entire Brillouin zone. In order to obtain an energy-dependent impact ionization rate, the ionization rate (5) is integrated over all directions in \(k\) space to get

\[
R(E) = \frac{\sum_{\nu_1} \sum_{\nu_2} \int d^3k_1 \delta(E_{\nu_1}(k_1) - E) r(k_1, \nu_1)}{\sum_{\nu_1} \sum_{\nu_2} \int d^3k_1 \delta(E_{\nu_1}(k_1) - E)}.
\]

Analytical evaluation of the transition rate\(^{15,16}\) requires strong simplifying assumptions such as a parabolic band structure and free electron wave functions, which are not well founded for semiconductors with a direct (GaAs, ZnS) or even an indirect gap (Si, ZnS when omitting the first conduction band which does not contribute). Therefore, we numerically evaluate Eqs. (5) and (7) by means of the grid method of Sano and Yoshii\(^{11}\) in order to take into account a realistic, nonlocal band structure and corresponding wave functions in the entire Brillouin zone.

The interaction between electrons in the bands is described by a statically screened Coulomb potential. Inclusion of the wave-vector dependence of the dielectric function \(\epsilon(q)\) is of importance for the calculation of the matrix elements in semiconductors, as pointed out by Laks et al.\(^{17}\) For the interaction between conduction and valence electrons, we apply a \(q\)-dependent dielectric function derived by Levine and Louie.\(^{18}\) This model incorporates the correct long-range and short-range properties of the dielectric function and, in addition, effects due to the presence of the semiconductor energy gap in the excitation spectrum.

The interaction between electrons in the conduction band is described by a Debye potential with an inverse screening length \(\kappa = [n_0 e^2/(\epsilon_0 k_B T)]^{1/2}\) for a temperature of \(T = 300\) K and a corresponding electron density of \(n_0 = 10^{16}\) cm\(^{-3}\). The choice of \(n_0\) and, thus, also of \(\kappa\) is of minor importance for the numerical results.

The \(k\) vectors are restricted to the first Brillouin zone. For umklapp processes we have to consider terms which go up to 113 \(G\) vectors of the pseudopotential band-structure calculation. The respective expansion coefficients, i.e., those belonging to reciprocal lattice vectors with \(|G| > \sqrt{20}/(2\pi/a)\), were calculated by means of perturbation theory.\(^{12,19}\)
For the numerical treatment of Eqs. (5) and (7), the δ function is replaced here by rectangles of unit area with a height of 1/δE and a corresponding width of δE. A value of δE=0.1 eV was found to be small enough to ensure good convergence. This was proved by test calculations with a finer grid as well as with a value of δE=0.2 eV. The broadening above is related in a sense to effects such as collision broadening and intracollisional field effect. However, explicit consideration of such effects is not included in the present work.

An important feature of the grid method used in our previous article and in Ref. 11 is that storage of energy values and wave functions can be restricted to the irreducible wedge (IW) if the symmetry properties of the Brillouin zone are fully exploited. We take a mesh of 152 points in the IW [Δk_i=1/12(2π/a)]. For the study of the average ionization rate R(E) the summations over the conduction band indices were restricted to the four lowest bands, whereas all four valence bands were taken into account.

In order to investigate the influence of the band structure (see Fig. 1) on the ionization rate, we examine r(k_1,v_1) [Eq. (5)] along three symmetry lines. For both the local and the nonlocal band structures in the first conduction band, there are no points at all satisfying the threshold condition and, therefore, the total rate is due to electrons in the higher—mainly the third and fourth—conduction bands. The anisotropy of the ionization rate of ZnS for electrons initiating impact ionization from the second, third and fourth bands is shown in Fig. 3. Comparing these results with the band-structure data, a coincidence of the qualitative behavior of the impact ionization rate for the three directions and the third and fourth conduction bands can be stated. The pronounced differences between the local and nonlocal impact ionization rates at the L and K points exactly correspond to differences in the band structures. However, as for the local band structure, the attempt to manifest this correlation by applying a power-law fit formula for r(k_1,v_1) did not lead to a satisfactory result. This problem is caused by the strong anisotropy of the matrix element. Furthermore, the necessity to consider the region of large energies above the second conduction band, where band degeneracies and multiple level crossings occur, complicates the correlation of impact ionization to the band structure. For such large energies, the quality of the EPM band structure becomes questionable as well.

The average energy-dependent ionization rate R(E) given by Eq. (7) can, however, be approximated by a simple fit formula, given by

$$\tilde{R}(E) = P(E - E_{th})^a.$$  \hspace{1cm} (8)

The parameters are P = 5.14 x 10^{10} s^{-1} (eV)^{-a}, E_{th} = 3.8 eV, and a = 5.183 for the local, and P = 18.2 x 10^{10} s^{-1} (eV)^{-a}, E_{th} = 4.0 eV, and a = 4.556 for the nonlocal band structure, respectively. Figure 4 shows the energy-dependent ionization rates for the local and nonlocal band structures. Even though the band structure is known to have an important influence on the impact ionization, the two fit curves do not differ too much. The primary difference between the local and nonlocal EPM impact ionization rates is a slight hardening of the threshold for the nonlocal band structure; the threshold energy E_{th} is raised by about 0.2 eV and the initial slope increases slightly. Beyond 8 eV the two curves merge into the Born approximation.

We have neglected phonon-assisted impact ionization processes as well as deep level ionization in our present calculations. These effects may be important at high fields. Furthermore, other high-field effects such as collision broadening or the intracollisional field effect also must be considered for a more comprehensive description of the transport process of hot electrons in semiconductors similar to that in Refs. 20 and 21.

The aim of further studies may be related to assessment of the influence of the obtained anisotropy effects on the ionization coefficient, a, where an additional effect of the band structure is expected. Furthermore, the influence of dynamic screening, which was found to be substantial for Si, has to be studied also for ZnS.
IV. IMPACT IONIZATION COEFFICIENT AND HIGH-FIELD TRANSPORT

We have included the nonlocal band structure of Sec. II and the impact ionization rate results of Sec. III into a full-band Monte Carlo simulation of high-field transport in ZnS. In the Monte Carlo method for electron transport in semiconductors (see, for example, Ref. 24), the motion of particles through a solid is assumed to be described by semiclassical free trajectories interrupted by instantaneous, random scattering events. The scattering rates and scattering cross sections for the relevant mechanisms are calculated using time-dependent perturbation theory, and the computer random number generator used to generate the stochastic free flight times and angles after scattering. We have previously reported a Monte Carlo simulation of high-field transport of ZnS using a simplified, three-valley, nonparabolic band model.

The extension to a full-band Monte Carlo model basically follows that used by the Illinois group and described in detail elsewhere. Full-band Monte Carlo simulation of ZnS and ZnSe using this approach with a local EPM calculation has previously been reported by Brennan and later by Pennathur et al. Essentially, we use a density-of-states model in which the scattering rates calculated using the nonparabolic band model are renormalized by the actual density of states calculated directly from the nonlocal EPM of Sec. II at energies in excess of the $\Gamma - L$ energy. The justification for this approach is that at high energies, the scattering rate is dominated by optical deformation potential scattering which is isotropic and dependent only on the coupling constant and the final density of states.

The relevant scattering mechanisms for ZnS used in the present work have already been discussed in Ref. 25. They include polar optical phonons, acoustic phonons, ionized impurities, and neutral impurities at low energies, and optical deformation potential scattering at high energies (which includes intra- and intervalley scattering). Collision broadening and effects due to the intracollisional field effect are neglected in the present work apart from a constant broadening factor used in selecting the final state after scattering, and in calculating the impact ionization scattering rates (see Sec. III). The dynamics of particles between flights, and the states after scattering, are determined using the actual nonlocal band structure. Here we include electron transport in the first four conduction bands, and ignore the dynamics of holes in the valence band generated during the impact-ionization process. The anisotropic wave-vector dependence of the impact ionization rate discussed in the previous section is not evaluated, in accordance with the assumptions of the full-band model of isotropic scattering at high energies. Instead, the energy averaged impact ionization rate (see Fig. 4) given by Eq. (8) is utilized with the parameters derived from the fit to the nonlocal rate as discussed in the previous section.

We calculate the electron impact ionization coefficient $\alpha$ as a function of electric field in ZnS by finding the number of impact ionization events per unit time from the steady-state Monte Carlo simulation for a given field. The results are shown in Fig. 5 and compared with the experimental data reported by Thompson and Allen which are the only known results to date of this quantity for ZnS. The impact ionization coefficient is determined from carrier multiplication in reversed biased Schottky diodes assuming equal electron and hole ionization coefficients. While the assumption of equal electron and hole coefficients is poor in smaller band-gap materials such as Si, larger band-gap materials such as SiC have approximately equal rates. The main uncertainty in comparing the present transport model to the experiment are the precise deformation potentials to be used for the conduction band of ZnS. To our knowledge, there are no reported measurements of the optical deformation potentials for inter- and intravalley scattering. Brennan used optical deformation potential values similar to those reported for GaAs in his work.

To bring our ZnS Monte Carlo simulation into agreement with the experimental results, we have treated the deformation potentials as adjustable parameters, and attempted to fit the impact ionization data of Thompson and Allen, as shown in Fig. 5. We have used two adjustable parameters, one the deformation potential in the lowest conduction band, and a second deformation potential characterizing the upper bands. These deformation potentials are indicated as a pair of markers in Fig. 5 for $D_1$, $D_II$, and $D_{III}$ which represent three fitting attempts to the experimental data. The deformation order potential optical scattering rate associated with these three parameter sets is plotted in Fig. 6 for the first and upper conduction bands. Fig. 6(a) shows the scattering rate in the first band which ends at approximately 3.6 eV. The zeroth-order deformation potential scattering rate below 1 eV is zero in the $\Gamma$ valley due to the usual symmetry arguments. The second band in ZnS based on the nonlocal calculation presented here begins at approximately 1.6 eV as shown in Fig. 6(b).
from the data of Thompson and Allen\textsuperscript{29} at lower fields. One
level impurities. Such effects have already been deduced
served for other materials such as Si and GaAs, and may
curvature in the $1/E$ plot is somewhat stronger than that ob-
erved for other materials such as Si and GaAs, and may
represent additional contributions to the multiplication
current at high fields such as field or impact ionization of deep
level impurities. Such effects have already been deduced
from the data of Thompson and Allen\textsuperscript{29} at lower fields. One
problem in comparing between experiment and theory is the
role of secondary electrons. In the Monte Carlo simulation,
the impact-ionized electron–hole pair is not considered, just
the primary electron before and after impact ionization. The
effect of these secondary carriers may result in a reduction in
the impact ionization rate derived experimentally at high
fields which is not accounted for in the theoretical model.
Alternately, the discrepancies between the experimental and
calculated impact ionization rates shown in Fig. 5 may be
evidence for the necessity of calculating the full energy- and
wave-vector-dependent deformation potential across the en-
tire Brillouin zone, such as that reported for Si.\textsuperscript{30} A similar
calculation for ZnS will be the subject of future work.

V. CONCLUSIONS

Recent calculations of the impact ionization rate\textsuperscript{4} and
electron transport of ZnS (Refs. 7 and 28) have shown the
band structure to be of importance in determining the high-
field transport properties of ZnS. Therefore, we have per-
formed a nonlocal EPM calculation for the ZnS band struc-
ture to go beyond the standard local EPM scheme. This
nonlocal band structure is the basis for a recalculation of the
impact ionization rate. Although differences in the local and
nonlocal ionization rates are apparent when the ionization
rates are examined along specific symmetry directions, the
local and nonlocal directionally averaged ionization rates are
virtually identical.

An ensemble Monte Carlo simulation of high-field elec-
tron transport in bulk ZnS is performed which employs the
nonlocal, directionally averaged impact ionization rate. All
relevant scattering mechanisms of the conduction electrons
are included. Treating deformation potentials as adjustable
parameters, the calculated ionization coefficient is fit to ex-
erimental data,\textsuperscript{29} and reasonable agreement of the ionization
coefficient as function of the inverse field is obtained. How-
ever, distinct differences in the curvature of the ionization
curves indicate that further effects such as deep level ioniza-
tion, secondary carrier generation, or wave-vector-dependent
deflection potentials have to be accounted for in order to
obtain a more detailed picture of high-field transport in bulk
ZnS.

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