Ab-initio semi-classical electronic transport in ZnSe: The role of inelastic scattering mechanisms

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Abstract

We present a detailed ab-initio study of semi-classical transport in n-ZnSe using Rode’s iterative method. Inclusion of ionized impurity, piezoelectric, acoustic deformation and polar optical phonon scattering and their relative importance at low and room temperature for various n-ZnSe samples are discussed in depth. We have clearly noted that inelastic polar optical phonon scattering is the most dominant scattering mechanism over most of the temperature region. Our results are in good agreement with the experimental data obtained at different doping concentrations over a wider range of temperatures. Also we compare these results with the ones obtained with relaxation time approximation (RTA) which clearly demonstrate the superiority of the iterative method over RTA.

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I. INTRODUCTION

Semi-classical transport models [1–7] are still actively employed for transport calculations across various materials in the bulk form. Typically, they are employed to calculate the mobility, conductivity and eventually also the thermoelectric coefficients [1–7]. Most of the prevalent semi-classical simulation platforms employ the Boltzmann transport equation (BTE) within the relaxation time approximation (RTA) and well known packages have been employed. However, it is well known that the RTA cannot capture inelastic scattering mechanisms properly and one has to go beyond the RTA to capture these scattering mechanisms. This brings a serious issue when it comes to materials which possess strong optical phonon scattering mechanisms. The objective of this work is to use ZnSe as an example to elucidate the limitations of the RTA along while presenting a calculation that is based on the Rode iterative scheme solution of the BTE.

In the present work, the electron mobility and conductivity is investigated for n-type ZnSe at different doping concentrations and temperatures with ab-initio inputs. ZnSe is a wide band gap semiconductor, which is employed for making blue light emitting diode and lasers. For our theoretical analysis, all the parameters of band structure, density of states, wave function admixture, dielectric constants, piezoelectric constants, polar optical phonon (POP) frequencies, and acoustic deformation potentials are calculated by using the density functional theory (DFT). In ZnSe, POP scattering is the dominant scattering mechanism. Since POP scattering is inelastic, it modulates the electron energy making and therefore can not be treated within RTA in a proper way.

In this paper, we first compare the experimental data and RTA calculation, and establish that the RTA results underestimate the mobility by more than 50 percent at room temperature. In the process of presenting the results here, we also give a detailed insight about the various contributions of different scattering mechanism in ZnSe at different temperatures and doping concentrations. Since all required inputs are calculated by using density functional theory, our method can be further extended and used for mobility calculations of new materials for which many constants are not calculated experimentally.

This paper is organized as follows. In the following section, we first describe in detail the methodology by first elaborating on the Rode scheme for solving the Boltzmann transport equation. We specifically hint at how this method scores over the RTA in capturing inelastic scattering processes. We also detail the computational scheme of calculating various scattering rates starting from ab-initio simulations. In Sec. III, we describe the results in detail, where we first establish
using the calculated scattering rates that the inelastic POP scattering mechanism indeed dominates over a wide temperature range in the case of n-type ZnSe. We then describe our theoretical fits in comparison with relevant experimental works at different carrier concentrations. In Sec. IV, we conclude with an outlook from this work.

II. METHODOLOGY

A. The Boltzmann Transport Equation

The Boltzmann transport equation (BTE) describes the time-evolution of the state of charge carriers in both real and momentum co-ordinates via a distribution function given by [2–4]

\[ \frac{\partial f(k)}{\partial t} + v \cdot \nabla_r f + F \cdot \nabla_p f = \left. \frac{\partial f}{\partial t} \right|_{\text{coll}}, \]

where \( v \) is the carrier velocity, \( f \) describes the probability distribution function of carrier in real and momentum space as a function of time, \( F \) is the applied external force, \( \left. \frac{\partial f}{\partial t} \right|_{\text{coll}} \) represents the change in the distribution function with time due to collisions. The first term in (1) represents the rate of change of the carrier distribution \( f \) with time. The second term represents the diffusion due to a gradient in the carrier density and the third term represents the change in \( f \) due to all external forces. In the presence of an electric field \( E \), the external force \( F \) is given by \( eE \), and the BTE then becomes

\[ \frac{\partial f}{\partial t} + v \cdot \nabla_r f + \frac{eE}{\hbar} \cdot \nabla_k f = \left. \frac{\partial f}{\partial t} \right|_{\text{coll}}. \]  

(2)

Under steady state and spatially homogeneous conditions, the above equation can be rewritten as:

\[ \frac{eE}{\hbar} \cdot \nabla_k f = \int [s(k,k')f(1-f) - s(k',k) f'(1-f)]dk', \]

(3)

where \( e \) is electronic charge, \( s(k,k') \) is the transition rate from state \( k \) to \( k' \) and \( s(k',k) \) is transition rate from state \( k' \) to \( k \). At low electric fields, the solution to the BTE is given by the distribution function

\[ f(k) = f_0[\varepsilon(k)] + g(k) \cos \theta \]

(4)

where \( f_0[\varepsilon(k)] \) is the equilibrium distribution function, and \( \cos \theta \) is the angle between applied electric field and \( k \). Here we have neglected the higher order terms, since we are calculating mobility under low electric field conditions. Now we have to calculate the perturbation in the distribution function \( g(k) \) for calculating the low-field transport properties. We are assuming that
\[
\cos \theta = 1, \text{ i.e., } k \text{ is aligned with the applied electric field. Now the perturbation } g(k) \text{ is given by } \]
\[
g_{k,i+1} = \frac{S_i(g_{k,i}) - v(k) \left( \frac{\partial f}{\partial \varepsilon} \right) - \frac{\varepsilon E}{\hbar} \left( \frac{\partial f}{\partial k} \right)}{S_o(k) + \frac{1}{\tau_{el}(k)}}. \quad (5)
\]

For the mobility and Seebeck coefficient calculations, this perturbation in distribution \( g(k) \) is used. The effect of inelastic polar optical phonon (POP) scattering is included through terms \( S_i(g) \) and \( S_o \) and the effect of elastic scattering is included through the relaxation time \( \frac{1}{\tau_{el}(k)} \) term. The second term in the numerator of (5) represents the thermal driving force and the third term in the numerator represents the electrical driving force. For mobility calculations, the thermal driving force is set to zero and only the electrical driving force is considered. The expression for \( S_i \) and \( S_o \) are given by
\[
S_o(k) = \int [s(k,k')(1-f') + s(k',k)f']dk' \quad (6)
\]
\[
S_i(g_k) = \int Xg_k'[s(k',k)(1-f) + s(k,k')f]dk' \quad (7)
\]

where \( X \) is the cosine of the angle between the initial and the final wave vectors, \( \frac{1}{\tau_{el}(k)} \) is the sum of the momentum relaxation rates of all elastic scattering process, which is given by
\[
\frac{1}{\tau_{el}(k)} = \frac{1}{\tau_{ii}(k)} + \frac{1}{\tau_{pz}(k)} + \frac{1}{\tau_{ac}(k)}, \quad (8)
\]

where the subscripts \( el, ii, pz \) and \( ac \) are used for elastic, ionized impurity, piezoelectric and acoustic deformation potential scattering processes respectively. The carrier mobility \( \mu \) is hence given by
\[
\mu = \frac{1}{3E} \int v(\varepsilon)D_s(\varepsilon)g(\varepsilon)d\varepsilon, \quad (9)
\]

where \( D_s(\varepsilon) \) represents density of states. The carrier velocity is calculated directly from the ab-initio band structure by using
\[
v(k) = \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial k}. \quad (10)
\]

From these, we can evaluate the electrical conductivity given as
\[
\sigma = ne\mu_e, \quad (11)
\]

where \( n \) is electron carrier concentration, and \( \mu_e \) is the electron mobility.
B. Computational method

The electronic structure calculations were performed using first-principles methods within the frame-work of Density Functional Theory (DFT) with Perdew-Burke Ernzerhof exchange correlation energy functional\[9\] based on a generalized gradient approximation. We used a projector augmented wave method as implemented in Vienna \textit{ab-initio} simulation package (VASP)\[8, 10, 11\]. Kohn-Sham wave functions of the valence electrons were expanded in plane wave basis with energy cut-off of 500 eV. Ionic relaxation was performed using conjugate-gradient method, until forces were reduced to within 0.01 eV/Angstrom. The Brillouin zone sampling was carried out using Monkhorst Pack grid of 11x11x11 k-points. The band structure is computed along the high-symmetry k-points in the Irreducible Brillouin zone, with 100 k-points between each pair of high-symmetry points and is shown in the Fig[11](a), while the self-consistent density of states (DOS) is shown in the Fig[3](b). Since as an input for the transport calculation within Rode’s method, only band structure for one valley is needed, we have performed non-selfconsistent calculation of the band energies in a special k-point mesh around the $\Gamma$ point with 8531 k-points. Using such dense mesh we have obtained very accurate group velocity and effective mass.

C. Scattering Mechanisms

In this work, for calculating the mobility of ZnSe, four different types of scattering mechanisms are included (i) Ionized impurity scattering, (ii) Acoustic deformation potential scattering, (iii) Piezoelectric scattering and (iv) Polar optical phonon scattering. For ionized impurity scattering, the formulation provided by the Brooks-Herring approach is used. The ionized impurity is a significant scattering mechanism at low temperatures and high doping concentrations. The momentum relaxation rate for this mechanism with its \textit{ab initio} counterpart is given by following expression\[1, 7\]

$$\frac{1}{\tau_{ii}(k)} = \frac{e^4 N}{8\pi\varepsilon_0^2\hbar^2 k^2 v(k)} [D(k)\ln(1 + \frac{4k^2}{\beta^2}) - B(k)]$$

(12)

where $\varepsilon_0$ is the dielectric constant, $\hbar$ is the reduced Planck constant, and $\beta$ is the inverse screening length given by

$$\beta^2 = \frac{e^2}{\varepsilon_0 k_B T} \int D_s(\varepsilon) f(1 - f) d\varepsilon,$$

(13)

where $N$ is the concentration of ionized impurity and it is given by

$$N = N_A + N_D$$

(14)
where \( N_A \) and \( N_D \) is acceptor and donor concentrations respectively. The expressions for \( D(k) \) and \( B(k) \) is taken from Eq. (91) and (92) of reference [7].

Acoustic deformation occurs due to the coupling of electrons with non-polar acoustic phonons. The momentum relaxation rate for acoustic deformation potential scattering is given by [1, 7]

\[
\frac{1}{\tau_{ac}(k)} = \frac{e^2 k_B T E_D^2 k^2}{3\pi \hbar^2 c_{el} v(k)} \left[ 3 - 8c^2(k) + 6c^4(k) \right],
\]

where \( c(k) \) is the contribution of the p-type orbital to the wave function of the conduction band. For \textit{ab-initio} calculations, the wave function admixture \( c(k) \) is obtained through projecting the Kohn-Sham wavefunctions onto the spherical harmonics which are non-zero only within spheres centering the ions and is implemented in VASP package. Chemical bonds in compound semiconductors such as ZnSe are ionic in nature and the vibrations of atoms cause changes in the lattice constant. This perturbs the dipole moment between the atoms that eventually scatter the electrons. This kind of polar scattering due to acoustic phonons is called piezoelectric scattering and the polar scattering due to optical phonons is called polar optical phonon (POP) scattering. Piezoelectric scattering is important at low temperatures and at low doping densities in polar materials. Since ZnSe is polar, it necessary to include piezoelectric scattering to get a better fit for the mobility output at low temperature. The momentum relaxation rate for piezoelectric scattering with abinito parameters as input is given by [1, 7]

\[
\frac{1}{\tau_{pz}(k)} = \frac{e^2 k_B T P^2}{6\pi \varepsilon_0 \hbar^2 v(k)} \left[ 3 - 6c^2(k) + 4c^4(k) \right]
\]

Polar optical phonon scattering is the most dominant scattering mechanism near room temperature and in the higher temperature regime. Since POP scattering is inelastic and anisotropic, the Rode iterative scheme is used to directly evaluate the scattering rates so that the momentum relaxation rate is given by [5, 7]

\[
S_o = (N_{po} + 1 - f^-)\lambda_0^- + (N_{po} + f^+)\lambda_0^+
\]

\[
\lambda_o^+ = \beta^+ [(A^+)^2 \ln \left| \frac{k^+ + k}{k^+ - k} \right| - A^{+cc^+} - A^{+cc^+}]
\]

\[
\beta^+ = \frac{e^2 \omega_{po} k^+}{4\pi \hbar v(k^+) \left( \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0} \right)}
\]

\[
A^+ = aa^+ + \frac{(k^+)^2 + k^2}{2k^+} cc^+.
\]
where subscript plus denotes scattering out by absorption so it is to be evaluated at an energy $\varepsilon + \hbar \omega_{po}$ and the subscript minus denotes scattering out by emission so that it is to be evaluated at energy $\varepsilon - \hbar \omega_{po}$. If energy is less than $\hbar \omega_{po}$, then the emission of phonons is not possible and hence $\lambda_0^-$ is to be considered to be zero, $N_{po}$ is the number of phonons and is given by

$$N_{po} = \frac{1}{\exp(\hbar \omega_{po}/k_B T) - 1}. \tag{21}$$

The in scattering operator for POP is given by [5, 7]

$$S_i = (N_{po} + f) \lambda_i^- g^- + (N_{po} + 1 - f) \lambda_i^+ g^+, \tag{22}$$

$$\lambda_i^+(k) = \beta^+ \left[ \frac{(k^+)^2 + k^2}{2k^+k} (A^+)^2 \ln \left| \frac{k^+ + k}{k^+ - k} \right| - (A^+)^2 - \frac{c^2(e^+)^2}{3} \right] \tag{23}$$

**D. Ab-initio Inputs**

The computed band structure and density of states for ZnSe is shown in Fig. 1. As already mentioned, we have calculated the band structure using the density functional theory using a three dimensional $k$ mesh around the conduction band minimum (CBM). The conduction band is expressed as the average energy of the electrons as function of $k$ from the CBM. In order to evaluate the group velocities, we have first calculated the derivatives of the conduction band energy with respect to $k$, performed an analytical fitting of the conduction band with a six degree polynomial and divided the conduction band into four segments [1, 12] to obtain a smooth curve for both mobility and conductivity. The Fermi level is obtained by calculating the carrier concentration using [24] and matching it to the given concentration:

$$n = \frac{1}{V_0} \int_{\epsilon_c}^{\infty} D_S(\epsilon) f(\epsilon) d\epsilon, \tag{24}$$

where $D_S(\epsilon)$ represents density of states at energy $\epsilon$, where $\epsilon_c$ represents the bottom of conduction band and $V_0$ represents the volume of the cell. We have calculated the low and high frequency dielectric constants [13, 14], polar optical phonon frequencies $\omega_{po}$ [15], the elastic constant and the piezoelectric constant by using the density functional perturbation theory as implemented in VASP. The acoustic deformation potential is obtained by mimicking a uniform lattice deformation due to acoustic phonons which results a shift of the conduction band minimum. The deformation potential is given by

$$E_D = -V \left( \frac{\partial E_{CBM}}{\partial V} \right)_{V=V_0}. \tag{25}$$
Where $E_{CBM}$ is the conduction band minimum and $V_0$ is the equilibrium volume. All the calculated \textit{ab-initio} parameters and experimental values are shown in table I.

E. Simulation Flowchart

The flowchart for our mobility and conductivity calculations using the Rode method with the \textit{ab-initio} inputs is shown in Fig. 2. First, we have to calculate all required inputs using the first principles methods detailed in the previous section. Then we have to perform the analytical fitting of the band structure, to obtain smooth curves in order to calculate the group velocities of the carriers with $k$. Then the smoothed band structure is used to calculate the Fermi level using (24). The calculations are sensitive with respect to the calculated Fermi level and hence must be done carefully with good precision. Next we have to calculate various scattering rates for different scattering mechanisms by using (12), (15), (16), and (17). These scattering rates are then used to calculate the perturbation in the distribution function using (5), keeping the scattering in the term $S_1^{(1)}(g(k)) = 0$ for the first iteration. Since the scattering in the term is also dependent on $g(k)$, the perturbation in the distribution function cannot be calculated directly. This calculated perturbation $g^{(1)}(k)$ is used to calculate $S_1^{(2)}(g(k))$, and then using this $S_1^{(2)}(g(k))$, $g^{(2)}(k)$ is calculated. This procedure is repeated until the perturbation calculation of $g(k)$ converges. This convergence is exponential [7], so normally it requires a few iteration for convergence. Now the obtained $g(k)$ is used to calculate the desired transport coefficients. If $g(k)$ is obtained right after the first order iterate, it will replicate the RTA results of the transport coefficients.

III. RESULTS

A. Scattering Rate vs Energy

For a comparison between the different scattering mechanisms in n-ZnSe, the scattering rate as a function of energy is plotted in Fig. 3 and Fig. 4 for different doping concentrations $N_D = 1 \times 10^{10} cm^{-3}$ and $N_D = 1 \times 10^{15} cm^{-3}$ at temperatures 30 K and 300 K. At low doping and lower temperatures, the piezoelectric scattering is considered the most dominant scattering mechanism for low energy carriers. At a temperature of 30 K, the average energy of carriers is
$\frac{3}{2} k_B T = 0.0038 eV$, and hence most of the carriers are in the low energy region. At low temperatures, around the average energy of carriers, both piezoelectric and acoustic deformation potential scattering mechanisms are approximately equal. So at lower doping and at lower temperatures, piezoelectric scattering and acoustic deformation potential scattering are the most dominant scattering mechanisms.

At higher doping ($1 \times 10^{15}$) for low temperatures, ionized impurity scattering is most dominant for low energy carriers. At 300 K, POP scattering is the most dominant scattering mechanism for all electron energies for both higher and lower doping. So POP scattering is the most important scattering mechanism at temperatures ranging from room temperature to higher. Since all working devices operate in this temperature region, it is necessary to properly include POP scattering for a good theoretical mobility calculation. Since RTA is not valid for inelastic scattering mechanisms, other abinitio RTA based codes such as the BoltzTrap [21] code may not produce the desired results in the case of n-ZnSe.

**B. Electron Mobility**

By using the Rode iterative method based on the flowchart detailed above, the electron mobility is calculated for three different experimentally characterized n-ZnSe samples for different doping concentrations over a wide temperature range. The donor and acceptor concentrations for different experimentally characterized n-ZnSe samples taken from different references is shown in Tab. II. Figure 5 shows a comparison between the experimentally measured and theoretically calculated mobilities using our Rode scheme as well as the RTA method. Overall there is good agreement between the theoretical and experimental curves when considering the Rode scheme results and score much better than RTA results. The calculated mobility for sample (a), (b) and (c) using the Rode method has an average relative error of 18.44% and 20.56% and 4.08% respectively. While mobilities calculated using the RTA have average errors of 113.46%, 54.67% and 42.77% for sample (a), (b) and (c) respectively.

For sample (a), the Rode calculation shows an error of $-15.03\%$ and $-7.27\%$ at 200 K and 300 K respectively, while the RTA shows an error of $-133.45\%$ and $-117.88\%$ at 200 K and 300 K respectively. The Rode method shows an error of $-4.67\%$ at 300 K for sample (b), while the RTA shows an error of $-53.88\%$ at 300 K with respect to the experimental curve. For sample (c), the Rode calculation shows an error of $-3.86\%$ and $-1.05\%$ at 200 K and 300 K respectively, while
the RTA shows an error of $-51.49\%$ and $-57.85\%$ at 200 K and 300 K respectively. Therefore, all in all the RTA results are quite inappropriate for mobility calculations of polar materials.

Figure 6 shows the calculated conductivity with respect to the experimental one for sample (b). The conductivity calculated by the Rode iterative method is again much better that conductivity calculated by using the RTA method. The calculated conductivity shows a very good qualitative and quantitative agreement with respect to the experimental data. Figure 7 shows the overall mobility and the mobility by considering only one type of scattering mechanism at a time for sample (c). The lower mobility is most dominant in deciding the overall mobility. From this figure it is clear that POP is the most dominant scattering mechanism, from 70 K to higher temperatures. Figures 8 and 9 show the mobility for different doping concentrations at 77 K and 300 K by assuming a compensation ratio of 1. With increasing doping concentration, the curves show a decrease in mobility due to an increase in the number of ionized centers.

IV. CONCLUSION

We presented an *ab-inito* semi-classical transport calculation for the mobility and conductivity of n-ZnSe by using Rode iterative method in order to conclusively illustrate the role of inelastic scattering processes. We recognized that inelastic polar optical phonon scattering is the most dominant scattering mechanism over most of the temperature region. A good agreement with various experiments was observed for different doping concentrations over a wider range of temperatures. In comparing our results against that obtained using the relaxation time approximation method, we clearly noted the discrepancy in explaining experimental results, thereby pointing out the need to advance semi-classical transport calculations beyond the relaxation time approximation. Further work will be extended p-type semiconductor and multivalley transport.

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TABLE I: Abinito calculated inputs compared to experimentally measured values

| Parameters          | Ab-initio | Experimental |
|---------------------|-----------|--------------|
| \( a \) (nm)        | 0.574     | 0.566[16]    |
| \( \varepsilon_0 \) | 7.45      | 9.31[17]     |
| \( \varepsilon_\infty \) | 3.44 | 6.11[17]     |
| \( m^* \)           | 0.091     | 0.17[18]     |
| \( \varepsilon_g \) (eV) | 1.17 | 2.78[7]      |
| \( E_D \) (eV)      | 12        | –            |
| \( \omega_{po} \) (THz) | 5.88 | 7.50[6]      |
| \( c_{11}(10^{10}N/m^2) \) | 7.99 | 8.72[19]     |
| \( c_{12}(10^{10}N/m^2) \) | 4.54 | 5.24[19]     |
| \( c_{44}(10^{10}N/m^2) \) | 3.71 | 3.92[19]     |
| \( e_{14}(C/m^2) \) | -0.08162  | 0.044[20]    |
| \( P \)             | 0.0392    | 0.0224       |

\( a \) : Parameters are \( a \) (lattice constant), \( \varepsilon_0 \) (low frequency dielectric constant), \( \varepsilon_\infty \) (high frequency dielectric constant), \( m^* \) (effective mass), \( \varepsilon_g \) (band gap), \( E_D \) (acoustic deformation potential), \( \omega_{po} \) (POP frequency), \( c_{11}, c_{12}, c_{44} \) (elastic constants), \( e_{14} \) (Piezoelectric constant) and \( P \) (Piezoelectric coefficient).

FIG. 1: Band structure and density of states for ZnSe, Fermi level is set to zero at valence band maximum.
Calculate Input Parameters and Band Structure by Using First Principles

Analytical Fitting of Band Structure

Calculate Fermi Level

Scattering Rates

$S_i(g(k)) = 0$

Perturbation $g(k)$

$g(k) = \frac{S_i(g(k)) - eE \frac{\partial f}{\partial k}}{S_o(k) + \nu_{el}(k)}$

$S_i(g(k))$

$g(k)$ Converges

Yes

No

Transport Coefficients

FIG. 2: Flowchart for transport coefficient calculation from ab-initio inputs
FIG. 3: Scattering Rates vs Energy for $N_D = 1 \times 10^{10} cm^{-3}$

FIG. 4: Scattering Rates vs Energy for $N_D = 1 \times 10^{15} cm^{-3}$

TABLE II: Doping of different experimentally fabricated n-ZnSe Samples

| Sample | $N_D - N_A (cm^{-3})$ | Donor, $N_D (cm^{-3})$ | Acceptor, $N_A (cm^{-3})$ |
|--------|------------------------|------------------------|--------------------------|
| a [22] | $1 \times 10^{15}$    | $2.9 \times 10^{15}$   | $1.9 \times 10^{15}$    |
| b [23] | $1.1 \times 10^{16}$  | $6 \times 10^{16}$     | $4.9 \times 10^{16}$    |
| c [24] | $6.3 \times 10^{15}$  | $7.5 \times 10^{15}$   | $1.2 \times 10^{15}$    |
FIG. 5: Calculated and experimental measured mobility with temperature variation for ZnSe at Different Doping. More detail about donor and acceptor concentration is shown in table II.

FIG. 6: Calculated and experimental measured conductivity with temperature variation for sample b.
FIG. 7: Contribution of mobility from different scattering mechanisms for Sample (c)

FIG. 8: Calculated mobility for different doping concentration at 77 K

FIG. 9: Calculated mobility for different doping concentration at 300 K