Carrier Scattering Mechanisms: Identification via the Scaling Properties of the Boltzmann Transport Equation

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A method based on the scaling properties of the Boltzmann transport equation is proposed to identify the dominant scattering mechanisms that affect charge transport in a semiconductor. This method uses drift velocity data of mobile charges at different lattice temperatures and applied electric fields and takes into account the effect of carrier heating. By performing time-of-flight measurements on single-crystalline diamond, hole and electron drift velocities are measured under low-injection conditions within the temperature range 10–300 K. Evaluation of the data using the proposed method identifies acoustic phonon scattering as the dominant scattering mechanism across the measured temperature range. The exception is electrons at 100–200 K where conduction-band valley repopulation has a prominent effect. At temperatures below ≈80 K, where valley polarization is observed for electrons, transport dominated by acoustic phonon scattering is observed in different valleys separately. The scaling model is additionally tested on data from highly resistive gallium arsenide samples to demonstrate the versatility of the method. In this case, impurity scattering can be ruled out as the dominant scattering mechanism in the samples for the temperature range 80–120 K.

1. Introduction

The transport of charge in semiconductors has been studied intensely since the advent of the first semiconductor devices—rectifiers and transistors—in the mid-twentieth century. A detailed understanding of charge transport is imperative for the design of any electronic semiconductor devices. With the advent of a plethora of novel semiconductor materials, for example, silicon carbide, gallium nitride, diamond, and 2D materials such as graphene, charge transport in these materials has become an area of active research. Charge transport at the most fundamental level necessitates a full many-body quantum mechanical description, but such a model is often intractable and beyond present computational resources. Instead, a model with a suitable level of approximation is required for a useful description of transport phenomena.

For modeling charge transport in semiconductors, micro-scale semiconductor devices as well as semiconductor devices with larger dimensions, a semi-classical approach with the Boltzmann transport equation (BTE) often provides a suitable level of approximation.¹ The BTE is a kinetic equation that traces the time evolution of a distribution function of positions and momenta for the charge carriers. Interactions between carriers or between carriers and the lattice that cause energy dissipation (scattering) are treated through collision terms in the BTE. The mobile carriers are exposed to different scattering mechanisms while drifting within a host crystal. By studying transport phenomena, we can obtain information on the dominant scattering mechanisms. Through further approximations, moment expansions of the BTE lead to the hydrodynamic, drift-diffusion, and relaxation time approximation (RTA) approaches to charge transport.¹

In this work, we have measured drift velocity of charge carriers in an applied electric field by employing the time-of-flight (ToF) measurement technique. ToF has proved to be an extremely sensitive technique for measuring very low carrier concentrations in highly resistive semiconductors.²⁻¹ Drift velocity measurements on semi-insulating materials based on the ToF method have been previously reported for various types of radiation, for example, α and β-particles,⁴⁻⁵ pulsed electron beam,⁶ or Q-switched UV laser.⁷⁻⁸ By exploiting data from ToF measurements we show that the scaling properties of the BTE in the RTA approximation can be used to identify the dominant scattering mechanisms. This is demonstrated for two semiconductor materials—diamond and gallium arsenide (GaAs)—which exhibit different dominant scattering mechanisms. The analytical technique described here can provide significant insights for qualitative understanding and identification of the fundamental mechanisms affecting charge carrier transport.

2. Theoretical Model

The BTE evidently has limitations as it is a single particle description of a many particle system of carriers: correlations between carriers are not treated; the semi-classical treatment of
carriers as particles obeying Newton’s laws and the simple scattering assumes binary collisions that occur instantaneously in time and are localized in space. For the RTA to be valid, the relaxation time ($\tau_f$) is required to depend only on the scattering process itself and not on the distribution density function ($f$) or on the external force resulting from an applied electric field. In addition, the RTA is only valid under the condition of moderate applied electric fields. Despite these simplifying assumptions, the BTE-RTA description yields results for charge transport in semiconductors at micro-scale and larger dimensions that agree well with experiments.

In addition to the BTE-RTA we will make two further assumptions: i) the carrier energy function ($\mathcal{E}$) is homogeneous of second degree in momenta, that is, it is a quadratic function. ii) The scattering rate has a power law dependence on both the lattice temperature and the carrier energy. The first assumption means that the energy function satisfies 

$$\mathcal{E}(\vec{p}) = \lambda \vec{p}^2 \mathcal{E}(\vec{p}),$$

where the momenta are taken along the principal directions of the valley and relative to the band minimum. Here $m_x$, $m_y$, $m_z$ are the effective masses in the principal directions.

The second assumption holds for several common scattering mechanisms. For acoustic deformation potential scattering the scattering rate $\tau^{-1}_{ac}$ is given by

$$\frac{1}{\tau_{ac}} = \frac{m_{dos}^{1/2} \sqrt{2D_{ac} kT}}{\pi \hbar^2 v_l^2 \rho^2 l^2 \sqrt{\mathcal{E}}}$$

where $D_{ac}$ is the band edge energy shift per unit strain, $\rho$ the density, $v_l$ the longitudinal acoustic phonon velocity, and $m_{dos}$ the density-of-states effective mass. Thus we have a power law dependence $1/\tau_{ac} \propto \mathcal{E}^{r/s}$, with exponents $r = 1$, $s = 1/2$.

Many other scattering mechanisms approximately obey a power law. For example for ionized impurity scattering, the scattering rate can be described by the Brooks–Herring (B–H) expression

$$\frac{1}{\tau_{BH}} = \frac{Z^2 q^2 N^\pm}{16 \sqrt{2m_{dos} \pi \epsilon_0^2 \epsilon_0^2}} \ln(1 + b) - b/(1 + b) \mathcal{E}^{5/2}$$

with

$$b = 8m_{dos} L_D^2 \mathcal{E}/\hbar^2,$$

$$L_D^2 = \frac{\epsilon_1 \epsilon_0 kT}{q^2 N^\pm}$$

We can write:

$$b = 8m_{dos} \frac{\epsilon_1 \epsilon_0 kT}{q^2 h^2 N^\pm} \approx 8m_{dos} \frac{\epsilon_1 \epsilon_0 kT}{q^2 h^2 N^\pm} = 6.5 \cdot 10^{15} \text{cm}^{-3} \epsilon_1 \epsilon_0 T_{N^\pm}^2$$

where the positive sign is taken for heavy holes and the negative sign for light holes. The $\gamma$'s are Luttinger parameters. Likewise, in both direct and indirect bandgap materials such as GaAs and diamond (see Figure 1), the electron energy near a conduction band minimum (a valley) can to first non-vanishing order be written

$$\mathcal{E} = \frac{p_x^2}{2m_x} + \frac{p_y^2}{2m_y} + \frac{p_z^2}{2m_z}$$

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Figure 1. Comparison of the band structure for a) direct bandgap GaAs and b) indirect bandgap diamond (with its six equivalent conduction band minima).
and therefore $b \gg 1$ if, for example, $T > 10$ K and $N_i^< < 10^{20}$ cm$^{-3}$. Consequently the factor $\ln(1 + b) - b/(1 + b)$ is dominated by the logarithmic term. For the identification of scattering mechanisms, this slowly varying factor can be ignored which still yields an excellent approximation, and we find

$$r \propto T^s E^a$$

assuming that the ionized impurity concentration $N_i^>$ is independent of the temperature. Approximate power law dependencies for several common scattering mechanisms are summarized in Table 1.

If carrier heating can be completely ignored, that is, $T = T_{lattice} = T_{carrier}$, carrier transport is ohmic $\nu_{ohm} = \mu E$, and with the assumptions 1 and 2 from above, the mobility $\mu$ obeys

$$\mu \propto T^{−s}$$

(see Supporting Information). This dependence of the mobility on the temperature is often used to identify the dominant scattering mechanism when accurate drift mobility data can be obtained as a function of temperature. However, in many cases it may be impossible or impractical to measure drift velocity in the ohmic region because it is necessary to use higher electric fields, with resulting carrier heating, so that $T_{carrier} > T_{lattice}$.

This, more general, case can be analyzed by studying the scaling properties of the BTE-RTA. In the Supporting Information it is shown that under the stated assumptions the drift velocity $\nu_{carrier}$ can be written $\nu_{carrier} = \sqrt{T^s h(T^s E)}$, where $h$ is a function of a single argument with $\alpha = -r - s - \frac{1}{2}$. It is therefore possible to test a given hypothesis of what the dominant scattering mechanism is under given conditions by plotting $\nu_{carrier}$ versus $T^s E$ from a set of experimental data of the drift velocity $\nu_i = [\nu_i]$ at different lattice temperatures $T_i$ and electric fields $E_i = [E_i]$, (i = 1, ..., n). If the hypothesis is correct, the data points will fall on one universal curve.

A more systematic method for determining $\alpha$ is to employ a statistical measure for the correlation between two datasets. For a set $S$ of paired sample points $S = \{(x_1,y_1),...,\{x_n,y_n\}\}$ assume that $r = \text{corr}(S)$ is a measure of the correlation between $(x_i,y_i)$ pairs. We can then form $r(\alpha)$ by taking $S$ to be the set of pairs $(T^s E, \nu_i)$. The value of $\alpha$ that maximizes $r(\alpha)$, that is, the value that gives the highest degree of correlation, is then used to identify the dominant scattering mechanism. A useful correlation measure in this context is Spearman's rank correlation coefficient,[18] usually denoted $r_S$. Spearman's correlation is a measure of the strength of a possibly non-linear but necessarily monotonic association between two sets of variables. Examples are given in Section 4 where we present drift velocity data for diamond and GaAs together with $\nu_i$ versus $T^s E$ plots and calculations of Spearman's correlation coefficient.

### 3. Experimental Section

To acquire drift velocities for charge carriers, a conventional ToF technique was used. The technique is ideally suited for drift velocity measurements at very low carrier concentrations and for highly resistive materials. In this case, electron–hole pairs were created by external means using a pulsed UV laser.[2,8,19] In the ToF technique, the motion of free carriers in an electric field induced a current that could be measured at contacts on the sample surface by an external circuit. The induced current was related to the electron motion according to the Shockley–Ramo theorem.[20,21] The transit time was obtained from the full-width half-maximum (FWHM) of the ToF current transit, and the carrier velocity was thus given by the sample thickness divided by the transit time. The largest source of error in the measured carrier velocity originated from possible inhomogeneity in the electric field, due to trapped charge in the sample. The inhomogeneity in the field could however be estimated from the shape of the current pulse.[22] A maximum error in the measured drift velocities of $\pm 5\%$ was estimated for all samples. The schematic of the ToF setup is illustrated in Figure 2.

The free charge carriers in the setup were generated using a short UV pulse of 800 ps (FWHM) from a quintupled Nd:YAG laser with a 313 Hz repetition frequency and a wavelength of 213 nm. This wavelength corresponded to a photon energy of 5.82 eV (above the diamond band gap of 5.47 eV) with an absorption length in diamond of 3 \(\mu\)m. Several interference filters blocked lower harmonics and neutral density filters allowed reducing the intensity to any desired level. As electron–hole pairs were generated very close to one of the sample surfaces it was possible to transport either holes or electrons (depending on the applied bias polarity) through the sample and extract them at a receiving electrode. To detect the induced current, a low-noise broadband current amplifier was used, with a bandwidth of 1 GHz and a gain of 24 dB, together with a digital storage oscilloscope (DSO). The bias on the contacts was applied using a 50 \(\mu\)s pulse via a bias-tee. The short pulsed bias ensured capacitive voltage distribution across the sample and avoided undesirable sample charging. For the study, one intrinsic single-crystalline diamond sample synthesized by Element Six Ltd. and a highly resistive (>10$^9$ \(\Omega\) cm$^{-1}$) commercially available GaAs sample were chosen. The sample thicknesses were 490 \(\mu\)m (diamond) and 625 \(\mu\)m (GaAs). Semitransparent contacts were deposited on the two opposite [100] faces of the samples. The sample preparation, ToF setup, and data evaluation is described in more detail in refs.[23,24]. The semitransparent contacts made it possible to both apply a homogeneous electric field and to create electron–hole pairs in the vicinity (to a depth of a few micrometers) of the illuminated surface of the sample, due to the strong absorption of 213 nm light. The samples were mounted in a ceramic chip carrier, wire bonded, and placed in a liquid helium cooled Janis ST-300MS vacuum cryostat with UV optical access. The temperature was monitored using a LakeShore 331 temperature controller with...
Figure 2. Left: schematic of the time-of-flight setup and sample configuration used for the measurements. The electric field is applied in parallel with the [100] direction. The system enables separate measurements of the hole and electron drift velocity by changing the applied field polarity. Right: typical ToF current traces for electrons and holes in diamond at 300 K for two different voltages of both polarities.

Figure 3. Measured hole drift velocity in diamond at different bias fields and temperatures. Inset: hole drift velocity as function of applied electric field below 80 K. The error in the velocity is estimated to be less than ±5% for all data points, which approximately correspond to the size of the symbols.

4. Results and Discussions

4.1. Determination of Dominant Scattering Mechanisms in Diamond

For the diamond sample, the drift velocity was measured at temperatures in the interval 10–300 K with steps of 20 K and for applied electric fields in the interval 90–4200 V cm\(^{-1}\). The drift velocities of electrons and holes could be measured independently by switching the bias polarity. The measured hole drift velocity versus applied electric field is plotted in Figure 3 for the temperature range 10–300 K. It is known from drift mobility measurements\(^1,2,5,26\) and Hall measurements\(^27,28\) that in diamond below 300 K carrier scattering tends to be dominated by acoustic deformation potential (ADP) scattering together with impurity scattering.

To investigate the scattering mechanisms in our sample, the velocity data from Figure 3 are presented in \(\frac{v}{\sqrt{T}}\) versus \(T^\alpha E\) plots in Figure 4, for \(\alpha = -2, 1, \text{ and } -0.5\), corresponding to ADP,
ionized impurity, and neutral impurity scattering, respectively. It is clear that while in Figure 4a the data points all lie on a single curve with little deviation, this is not at all the case in Figure 4b,c. A plot of Spearman’s correlation coefficient \( r_\alpha \) for the full dataset with \( T = 10–300 \text{ K} \) exhibits a maximum at \( \alpha = -2 \) with \( r_\alpha(-2) = 0.9986 \), a very high degree of correlation (see inset in Figure 4a). Consequently the data are consistent with ADP scattering but clearly inconsistent with neutral or ionized impurity scattering. This can be explained by the low impurity concentration in this sample, which is known from electron paramagnetic resonance to have an impurity concentration below \( 10^{14} \text{ cm}^{-3} \). The small deviation from the curve seen in Figure 4a for temperatures 280 and 300 K can be attributed to the onset of optical phonon scattering which becomes significant near and above room temperature.\(^3,25\) At very low temperatures, well below 80 K, some deviation from ADP scattering behavior can be observed, see inset to Figure 4a. This is most likely due to some influence of impurity scattering, especially so at the lowest temperature, 10 K.

For electrons the measured drift velocity is shown in Figure 5 for 10–300 K. Here the situation is more complicated than for holes because of the repopulation effects between the different conduction band valleys.\(^3,22\) At temperatures above approximately 200 K, intervalley scattering is rapid, resulting in equally populated conduction-band valleys, while at temperatures below approximately 100 K intervalley scattering is negligible, which results in electron states with a fixed valley polarization. In this case two modes of transport with fast and slow electrons can be observed in the current trace\(^30\) (see inset in Figure 5). The slow electrons are resident in the two valleys on the axis parallel to the applied field, while the fast electrons reside in the other four orthogonal valleys. The drift of the slow and the fast electrons give rise to two square current pulses. The measured current is the sum of these currents, and the drift velocities are determined from the durations of the two pulses. At intermediate temperatures, negative differential resistance (NDM) can be observed due to a field-dependent degree of repopulation.\(^28\)

The drift velocity data are presented in \( \frac{v}{\sqrt{T}} \) versus \( T^\alpha E \) plots for \( \alpha = -2, 1, \) and \( -0.5 \) in Figure 6a–c. For temperatures above 200 K, where repopulation effects can be ignored, the data points can be seen to fall on one curve in (a) but not in (b) or (c) just as in the case of holes. A plot of Spearman’s correlation coefficient \( r_\alpha \) restricted to temperatures in the interval 200–300 K, exhibits a maximum at \( \alpha = -2 \) with \( r_\alpha(-2) = 0.9985 \) (see inset in Figure 6a). The data points for \( T < 80 \text{ K} \) can be seen to follow two curves (see inset) depending on the state of the valley polarization of the electrons. The drift mobility measurements were conducted with the electric field along the [100] direction. In this electric field the degeneracy between the two conduction band electrons (‘valleys’) on the \( \Delta \) lines between the \( \Gamma \) and \( X \) points is lifted (see Figure 1b). Because of the anisotropic energy dispersion in the valleys, electron states in the two valleys on the (100) axis in \( k \)-space have a lower drift velocity in the field than the electron states in the four valleys on the orthogonal axes.\(^10,31\) The transit times of the two different species can be measured individually in the ToF experiment, which explains the presence of two curves in the inset to Figure 6a. The Spearman correlation coefficients at \( \alpha = -2 \) for these two sets of data are \( r_\alpha(-2) = 0.9943 \) and 0.9923, for fast and slow electrons, respectively.

We conclude that even though the dominant scattering mechanism cannot be determined for 100 K < \( T < 200 \text{ K} \) due to the repopulation effect, it is still possible to identify ADP scattering as the dominant scattering effect for \( T > 200 \text{ K} \), and also for valley polarized electrons at \( T < 100 \text{ K} \).

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Figure 4. Hole transport in diamond. Plots based on the data of Figure 3, presented as \( \frac{v}{\sqrt{T}} \) versus \( T^\alpha E \) for three cases: a) \( \alpha = -2 \), b) \( \alpha = 1 \), and c) \( \alpha = -0.5 \), corresponding to acoustic deformation potential scattering, ionized impurity scattering, and neutral impurity scattering, respectively. Insets in (a) show: (right) the hole transport under 80 K with the same scaling factor and (left) a plot of Spearman’s correlation coefficient \( r_\alpha \) for the full dataset with \( T = 10–300 \text{ K} \).
Figure 5. Measured electron drift velocity in diamond at different applied electric fields and temperatures. Inset: shows drift velocity for the valley polarized electrons as function of applied electric field below 80 K where two types of electron transport (fast and slow) are experimentally distinguishable from the current trace. The NDM region is indicated by the dotted ellipse.

Figure 6. Electron transport in diamond. Plots based on the data of Figure 5, presented as \( v \sqrt{T} \) versus \( T \) for three cases: a) \( \alpha = -2 \), b) \( \alpha = 1 \), and c) \( \alpha = -0.5 \), corresponding to acoustic deformation potential scattering, ionized impurity scattering, and neutral impurity scattering, respectively. Insets in (a) show: (right) data below 80 K for electrons in different valleys parallel and orthogonal to the applied electric field direction and (left) a plot of Spearman’s correlation coefficient \( r_s(\alpha) \) for data in the temperature interval \( T = 200–300 \) K.
4.2. Determination of Dominant Scattering Mechanisms in GaAs

To further demonstrate the versatility and also the limitations of the scaling method, we performed ToF drift velocity measurements on highly resistive GaAs samples. These measurements concern only electron transport, while we were not able to observe any time-resolved transport for holes. The inset in Figure 7a (left) shows drift velocity data from electron transport in GaAs for 80 K < T < 120 K. For this temperature interval it was possible to obtain reliable drift velocity data from our GaAs samples. At temperatures outside this range trapping and detrapping of mobile charges causes polarization effects which complicate the interpretation. As can be seen from the plots in Figure 7, the data points can be seen to fall on one curve in (a) for α = 0, but not in (b), for α = 1 or (c), for α = −1/2. Therefore it is possible to rule out impurity scattering (ionized and neutral impurity) as the dominant scattering mechanism in this high purity sample. In addition, a plot of Spearman’s correlation coefficient $r_s(\alpha)$ exhibits a maximum at $\alpha = 0$ with $r_s(0) = 0.9958$ (see inset in Figure 7). As can be seen in Table 1, there is no scattering mechanism with $\alpha = 0$, and it is clear that we have to look elsewhere for a candidate. It is well known that polar optical phonon (POP) scattering is a very strong scattering mechanism in compound semiconductors such as GaAs. POP scattering as the dominant scattering mechanism in GaAs for T = 80–120 K has been observed previously in Hall measurements on high-resistivity n-type GaAs\(^{[12]}\) and is predicted by theoretical mobility calculations on pure GaAs.\(^{[13]}\) However, POP scattering is neither elastic nor isotropic and the relaxation time approximation in the BTE is invalid even under low-field conditions, and therefore cannot be easily included in our scaling approach. Instead other methods to calculate the low field drift velocity are necessary such as Rode’s iterative solution method to the BTE or Monte Carlo simulations.

5. Conclusions

In order to identify the dominant scattering mechanisms in a semiconductor, we have proposed a method that uses drift velocity data of mobile charges at different lattice temperatures and applied electric fields. This technique takes into account the effect of carrier heating, and is based on the scaling properties of the Boltzmann transport equation. The usefulness of this approach was demonstrated on diamond and GaAs samples. For diamond, hole and electron drift velocities within the temperature range 10–300 K were measured. Evaluation of the data identifies acoustic phonon scattering as the dominant scattering mechanism across the whole measured temperature range, except for electrons at 100–200 K where conduction-band valley repopulation complicates the interpretation. At temperatures below 80 K, transport dominated by acoustic phonon scattering was observed in different conduction-band valleys. For electrons in GaAs, impurity scattering could be ruled out as the dominant scattering mechanism in the temperature range 80–120 K and the limitations in treating polar optical phonon scattering were also discussed. In addition, Spearman’s rank correlation coefficient has been used as a statistical method to systematically determine the exponent $\alpha$. We anticipate that our technique will prove to be an important tool to study and identify scattering processes in many highly resistive semiconductor materials, for example, intended for detector applications.
Supporting Information
Supporting Information is available from the Wiley Online Library or from the author.

Acknowledgements
The authors would like to thank the Swedish Research Council (VR, Grant No. 2018-04154) and the Olle Engkvist Foundation (Grant No. 198-0384) for their financial support. In addition, the Swedish Energy Agency (Grant No. 2018-04154) and the Olle Engkvist Foundation (Grant No. 18:246) are gratefully acknowledged by the authors.

Conflict of Interest
The authors declare no conflict of interest.

Keywords
Boltzmann equation, charge transport, diamond, GaAs, scattering, Spearman correlation