# Reexamination of Electron Mobility Dependence on Dopants in GaAs

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## Abstract

The influence of dopant species on electron mobility in GaAs is investigated. Based on Thomas-Fermi theory to describe the charge density of the individual impurity ion we derive an analytical expression for the scattering rate. Employing these results in a Monte Carlo calculation we find a significant dependence of mobility on donor species for concentrations beyond $10^{18}$ cm$^{-3}$. With increasing concentration an increasing difference is observed, ions with larger atomic number lead to lower mobility values. In case of minority electron mobility no significant dopant dependence is predicted.

## 1. Introduction

The difference between majority and minority electron mobility is a well-known phenomenon caused by the different screening behavior of electrons and holes in semiconductors. In $n$-Si consistenly lower values for As-doping have been observed compared to P-doped samples in the high concentration range [1]. In compounds like GaAs, however, no such common trend has been found [2, 3]. Experimental data show broad scattering which is commonly attributed to compensation effects. The present study therefore is intended to clarify whether there is a general dependence on the dopant element apart from compensation. We show for the first time that consideration of the charge density of the valence electrons allows not only to distinguish the majority and minority case but also to differentiate between various acceptors and donors. The commonly used assumption of a delta-like impurity charge is unable to explain any influence of dopant species.

## 2. The Thomas-Fermi atomic model

Since the picture of the hydrogenic behavior of shallow impurities can well describe ionization and screening properties, we assume a hydrogen-like exponential electron

charge distribution consisting of $N$ electrons while retaining a point-like nucleus of total charge $Z$ (in units of the elementary charge $e$),

$$\rho_{\text{ion}}(r) = \rho_{\text{core}}(r) + \rho_{\text{el}}(r) = Z\,\delta(r) - \frac{N\,\alpha^3}{8\,\pi}\,\mathrm{e}^{-\alpha r}. \tag{1}$$

We minimize the Thomas-Fermi energy functional in the energy functional formulation [4, 5] to obtain the variational parameter $\alpha$ describing the spatial extent of $\rho_{\text{el}}(r)$ as function of the characteristic numbers $Z$ and $N$. The differential scattering cross section for impurity scattering can be formulated in the first Born approximation by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}(q) = \left(\frac{2\,e^2\,m^*}{\hbar^2\,\varepsilon}\,\frac{Z - F(q)}{q^2+\beta^2}\right)^2 \left(1 + \frac{\sin(q\,R)}{q\,R}\right). \tag{2}$$

The atomic form factor $F(q)$ (FF) is the Fourier transform of the electron charge distribution of the impurity atom,

$$F(q) = \int \rho_{\text{el}}(r)\,\mathrm{e}^{-i\,\mathbf{q}\cdot\mathbf{r}}\,\mathrm{d}V = \frac{N\,\alpha^4}{\left(q^2+\alpha^2\right)^2}. \tag{3}$$

The term containing $R$ in (2) accounts for the scattering on impurity pairs separated by the average distance $R$. $\beta$ denotes the inverse Thomas-Fermi screening length. The standard Brooks-Herring (BH) model is recovered by setting $F(q) = F(0) = N$ and $R \to \infty$.

## 3. Monte Carlo results

We calculate the electron mobility $\mu$ at 300 K employing the derived formulas in a single-particle Monte Carlo procedure using analytic band structure including phonon and plasmon interaction. The Pauli principle is accounted for by a rejection technique. The mostly overlooked concentration dependent change of the density of states is incorporated via an increase of the effective electron mass [6].

In Fig. 1 results for $n$-GaAs are shown in comparison with experimental data [2, 3, 7]. The simple (BH) model drastically overestimates $\mu$ for high concentrations, while the improved model for the example of Si-doping gives good agreement with experiments except in the very high doping range, where the remaining discrepancy may be explained by compensation and autocompensation, respectively. The influence of donor species is shown in Fig. 2. Inclusion of $F(q)$ generally reduces $\mu$ for donors which becomes clear from the behavior of the characteristic quantity $(Z - F(\theta))^2$ (Fig. 3). Since impurity scattering is elastic the scattering angle $\theta$ is given by $q = 2\,k\,\sin\left(\frac{\theta}{2}\right)$. Our results clearly indicate that ions with higher $Z$ result in lower values of $\mu$. The dependence on donor species is generally found negligible below $10^{18}$ cm$^{-3}$. The difference of $\mu$ between various donors increases with $n$ giving a maximum value of $\sim$20% at $10^{19}$ cm$^{-3}$ for Si and Sn-doping, respectively.

The minority mobility behavior is shown in Fig. 5. Depicted are results using BH and the improved model without the atomic form factor. The adjustment of plasmon cutoff as proposed in [8] is necessary for agreement with experiments. Finally the influence of $F(q)$ is shown in Fig. 6. Contrary to donors, $F(q)$ leads to a small increase of $\mu$ for acceptors. Furthermore, no significant dependence on the acceptor species is observed over the whole concentration range, which can be explained by the functional form of $F(q)$ for acceptors i.e. $Z < N$ (Fig. 4).

## 4. Conclusion

The present approach to our knowledge is the first physically based model to date which explains the dependence of the majority and minority electron mobility in GaAs on various species through the atomic number. While it predicts a noticeable influence in $n$-GaAs in the highly degenerate regime, we find no significant influence in $p$-material. Similar behavior is also expected in other compound semiconductors like InP [9] and Si as well [10].

## References


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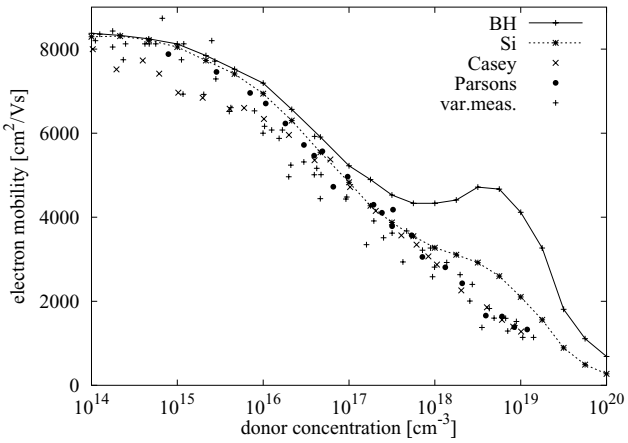


Figure 1: Majority electron mobility in GaAs

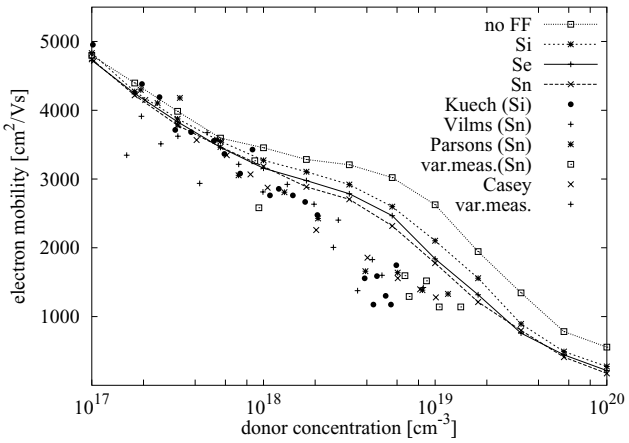


Figure 2: Majority electron mobility in GaAs for different donors

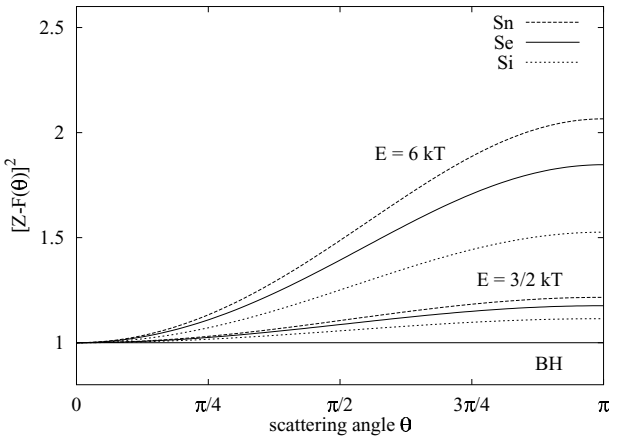


Figure 3: Characteristic scattering quantity $(Z - F(\theta))^2$ for different donors in GaAs

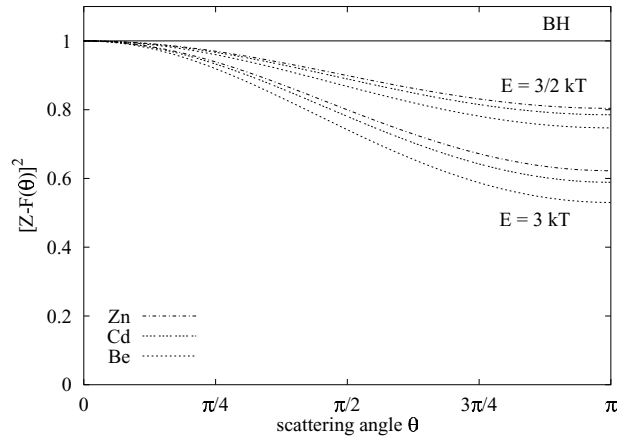


Figure 4: Characteristic scattering quantity $(Z - F(\theta))^2$ for different acceptors in GaAs

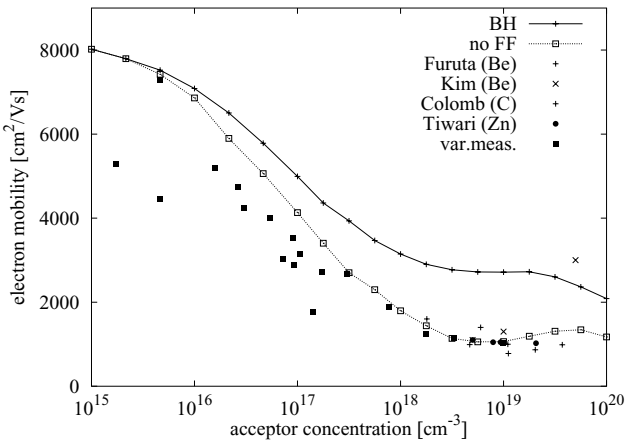


Figure 5: Minority electron mobility in GaAs

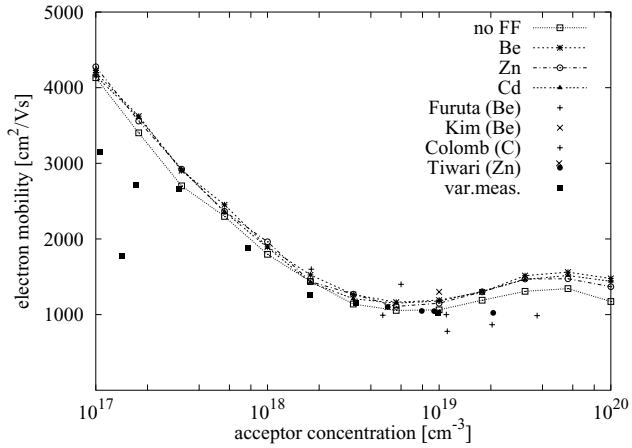


Figure 6: Minority electron mobility in GaAs for different acceptors