

ELECTRON SCATTERING AT LOCALIZED
IMPURITY POTENTIALS IN GaAs

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Compensated GaAs suffers from depressed electron mobility, describable by a contribution proportional to $T^{-0.5}$, T being temperature. Previously suspected space charge scattering is contradicted by photo-Hall effect. Instead, we propose scattering at centers subtending a localized potential. We present data on carbon-compensated GaAs and explain them with an iterative solution to the Boltzmann equation without having to assume excessively high compensation ratios.

Magnitude and temperature dependence of electron mobility in compound semiconductors, such as GaAs, are reasonably well understood [1]. An exception is compensated GaAs showing a markedly depressed mobility, which can be well approximated by incorporating a contribution depending on temperature T as $T^{-0.5}$ [2].

Weisberg [3] suggested that dopant fluctuations cause space charge regions which contribute to additional carrier scattering. Such space charge scattering should be particularly strong in heavily compensated materials and would indeed display an inverse half-power temperature dependence of mobility [4].

In this paper we first summarize experimental evidence against the space charge scattering hypothesis in our GaAs samples. We then outline calculations utilizing an iterative solution to the Boltzmann equation, incorporating all the relevant scattering mechanisms in addition to a new mechanism: scattering at centers with a localized potential. We present results explaining the temperature dependence and the absolute magnitude of mobility in a number of samples of different origin. Finally, we address the problem of compensation of semiconductor samples.

Stringfellow and Künzel [2] measured the Hall coefficient in several compensated samples of GaAs during illumination by light of 800 nm wavelength. The illumination enhanced the low-temperature mobility as expected from screening of the ionized impurities by photo-generated carriers [5]; yet there was no enhancement at room temperature, which would, however, be expected for space charge (SC) scattering because of the reduction of the SC widths. These results must be considered as strong experimental evidence against

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the hypothesized mechanism of space charge scattering, at least for those samples [2].

An alternative explanation is based on a center with a localized scattering potential. Carbon is known to be a prevailing impurity for various methods of crystal growth. A correlation has been shown for the mobility and carbon content [2]. Similar to the treatment of scattering at isoelectronic impurities, a localized central-cell potential is assumed for these carbon-related impurity or impurity-complex scattering centers. The scattering cross section σ is given in terms of an energy parameter E_ℓ , which is related to the binding energy, by the relation [6]

$$\sigma = (4\pi/3)\hbar^2(2m^*E + 2m^*E_\ell)^{-1}, \quad (1)$$

where \hbar is Planck's constant divided by 2π , E is the electron energy, and m^* is the electron effective mass. Assuming that $E_\ell \gg E$, this relation for the cross section leads indeed to a mobility contribution varying inversely as the square root of temperature.

This suggestion requires, however, a careful and quantitative examination. A complete analysis of electron mobility is necessary, which not merely assumes this new scattering at localized potentials but also includes all other relevant scattering mechanisms as well as band structure details. It is further necessary to examine if data for various samples can be fitted with one and only one value for E_ℓ , satisfying the requirement that E_ℓ is much larger than the average electron energy over the temperature range concerned.

Polar optic, deformation potential acoustic, piezoelectric, ionized impurity (Brooks-Herring) and localized-potential modes of scattering are jointly considered in our analysis. Nonparabolicity of the conduction band and admixture of valence band p-type wave functions are also incorporated. All scattering except the polar optic mode are describable by relaxation times [6,7]. The complete scattering rate for polar optic interaction is considered [1]. Matthiessen's rule does not have to be assumed; in fact, all the scattering terms are directly included in the Boltzmann equation which reads

$$[\Sigma\tau^{-1}(E) + \lambda(E)]f_1(E) = \lambda_+(E)f_1(E+h\omega_0) + \lambda_-(E)f_1(E-h\omega_0) - \frac{e\hbar F}{m^*}(1+2\alpha E)^{-1}\frac{\partial f_0}{\partial E}. \quad (2)$$

Here $\Sigma\tau^{-1}$ denotes the sum of the reciprocal relaxation times for processes other than the polar mode scattering, $\lambda(E)$ is the scattering-out rate and $\lambda_\pm(E)$ are the scattering-in rates due to emission and absorption of polar optic phonons of energy $h\omega_0$, F is the applied electric field, e is the electron charge, α is the nonparabolicity parameter, and $f_0(E)$ and $f_1(E)$ are respectively the equilibrium and the functional perturbation in the carrier distribution function.

Equation (2) is solved for $f_1(E)$ by the numerical iterative method [1]. In the i^{th} step of iteration the values of $f_1(E)$ are obtained by using on the right-hand side the values of $f_1(E-h\omega_0)$ obtained in the $(i-1)^{\text{th}}$ step. For $i=1$, $f_1(E+h\omega_0)$ are put to zero. Four to five iterations are needed to give convergent results on mobility.

Numerical calculations are performed with parameter values given in [8]. Experimental results for doping densities below 10^{17}cm^{-3} are considered. In this range all the compensating acceptor atoms

are here assumed to produce localized potentials [2]. The electron concentration, n , is taken to be the same as that quoted for each sample. Good agreement between the calculated and the experimental mobilities is obtained for all the samples over the temperature range 77-300 K with a single value of E_ℓ , namely 95 meV.

The nature of the agreement is illustrated for two samples in Fig. (1).

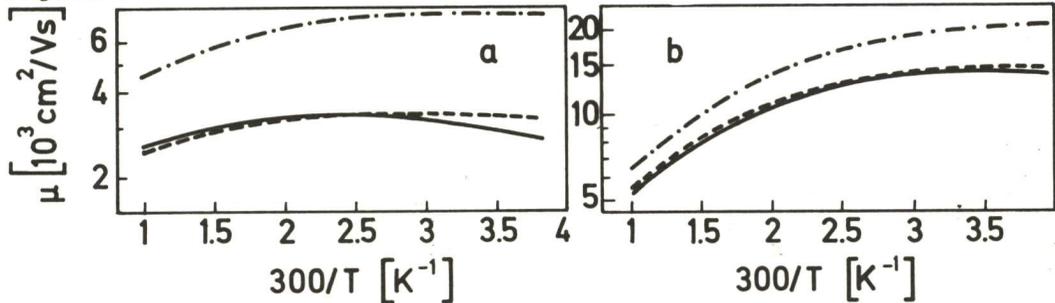


Fig.1. Variation of Hall mobility with temperature: The solid lines indicate the experimental results of Stringfellow and Künzel (a) and of Pödör et al. (b). The dashed and the dash-dotted lines give respectively the calculated values including and excluding localized potential scattering.

Here the localized potential scattering is found to be more important in the sample of Stringfellow and Künzel [2] than in the sample of Pödör et al.[10]. This is expected from the larger acceptor concentration in the former case.

The values of the ionized impurity concentration required to fit the calculations to the experiments when localized potential scattering is considered using the single value of 95 meV for E_ℓ are denoted by N in Table I. The quantities N' in Table I give the

Table I. Impurity concentrations required to fit various experimental results

Sample No.	Source	$10^{-15}n$ (cm^{-3})	$10^{-15}N$ (cm^{-3})	$10^{-15}N'$ (cm^{-3})
236	[9]	1.4	30.8	58.8
85/2	[10]	22	28.6	44
3TZ-HB/XS	[11]	16	51.2	128
GA-2	[12]	1.3	6.5	9.75
AL-1	[12]	27.4	41.1	68.5
1033A	[2]	14.6	73	189.8
III	[13]	4	20	40
II	[13]	1	3	5

values of ionized impurity concentration needed for a fit with experiments excluding localized potential scattering. The required compensation ratio (N'/n) is found to be significantly larger than that needed when localized potential scattering is incorporated (namely, N/n).

Compensation by minority dopants, e.g. acceptors in n-type materials, is a quantity of great practical significance, because it describes the purity of a semiconductor and directly affects transport properties. An exact experimental determination of compensation is, however, still a difficult task. Only estimates can usually be derived from Hall mobility data, especially from values in ranges of temperature where ionized impurities dominate the scattering. Such methods in essence lump all mobility-depressing mechanisms, thus ascribe the total exclusively to compensation, which is therefore usually overestimated. Very large compensation ratios are thus often quoted for compound semiconductors.

Other methods of measuring the compensation have involved a detailed analysis of temperature-dependent photoluminescence from donor-acceptor pairs [14]. A substantially lower compensation was found than from Hall effect. Chemical analysis of Sn-doped GaAs by secondary ion mass spectroscopy [15] showed that the amphoteric Sn could not be made responsible for the very high compensation which would follow from Hall data.

This conflicting evidence is bothersome both for a proper materials analysis and for a thorough understanding of carrier mobilities. One solution to this dilemma is the assumption that for those cases the predominant compensation is not caused by the usual shallow donors but rather by some deeper level, which escaped detection in the photoluminescence analysis [14]. Our data and mobility analysis support such an explanation and also indicate that the previously derived, unrealistically high degrees of compensation do not follow as inevitable conclusion. The lowered mobility is thus not caused by excessive shallow acceptors but rather by a comparatively smaller concentration of more strongly scattering acceptor centers with localized potentials. The chemical nature of these centers is not clarified at present. A carbon-related complex seems to be the most probable candidate, for example in the form of an isoelectronic carbon-carbon pair on adjacent Ga and As sites.

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