Carrier scattering by native defects in heavily doped semiconductors

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Calculations of the effect of charged native defects on carrier mobility in semiconductors are presented. The concentrations of native defects are calculated within the framework of the recently proposed amphoteric-native-defect model. The model provides a simple rule for identification of semiconductor systems in which defect scattering is important. It is shown that native-defect scattering is a dominant mechanism limiting electron mobilities in heavily doped n-type GaAs. It is also shown that native defects do not play any significant role in p-type GaAs.

In recent years considerable progress has been made in the understanding of carrier transport in semiconductors. Detailed models of standard scattering processes are now available and, in many instances, a good agreement between theoretical and experimental mobility data has been achieved.[1-3] An important, unresolved issue of the electron and hole transport concerns the contribution of charged naive defects to carrier scattering.

We show in this paper that scattering by naive defects can, under certain circumstances, be the most important scattering process limiting carrier mobilities in semiconductors. We use the recently developed amphoteric-native-defect model to calculate the concentration of native defects.[4,5] Incorporation of the carrier scattering by defects provides an explanation for an abrupt mobility reduction in heavily doped n-type GaAs.

It has been proposed that in GaAs relative abundances of vacancylike native defects are controlled by the defect reactions[5]

$$\mathrm{Ga_{Ga}}+V_{\mathrm{As}}\leftrightarrow(\mathrm{Ga_{As}}+V_{\mathrm{Ga}})\ , \tag{1a}$$

$$(\mathrm{As_{Ga}}+V_{\mathrm{As}})\leftrightarrow\mathrm{As_{As}}+V_{\mathrm{Ga}}\ . \tag{1b}$$

The defects exhibit a characteristic amphoteric behavior. In p-type GaAs with the Fermi level located close to the valence-band edge, the donorlike defects on the left-hand side of the reaction (1a) and (1b) are stable. On the other hand, the acceptorlike defects on the right-hand side are stable in n-type material. Also, because the defects have multiple charge states, their formation energy depends strongly on the Fermi-level position.[6] It has been shown that in n-type GaAs the acceptorlike defects V_{Ga} and $\mathrm{Ga_{As}}+V_{\mathrm{Ga}}$ can acquire a triple negative charge and therefore their formation energy is[5,6]

$$E_f=E_0-3E_F\ , \tag{2}$$

where E_F is the Fermi energy measured from defect-energy reference, E_{FS}, corresponding to the Fermi-level location at which the reactions (1a) and (1b) are in equilibrium. According to Ref. 7, $E_{\mathrm{FS}}=E_v+0.6$ eV for reaction (1b). In the following we confine ourselves to the case of electrons in GaAs. Since there is evidence[8] that V_{Ga} are dominant defects in heavily doped n-type GaAs, we consider reaction (1b) only. It should be noted, however, that qualitatively similar results are obtained for the defects given by reaction (1a).

From Eq. (2) one obtains the following expression for the concentration of triply ionized V_{Ga},

$$[V_{\mathrm{Ga}}]=C_0\exp[3(E_F-E_c)/kT]\ , \tag{3}$$

where E_c is the conduction-band edge, and C_0 is a constant. Both E_F and E_c are measured with respect to the Fermi-level stabilization energy E_{FS}.

In n-type GaAs doped with donors to the level N_{D^+} the concentration of free carriers is

$$n=N_{D^+}-3[V_{\mathrm{Ga}}]\ . \tag{4}$$

The Fermi energy is determined by the relationship

$$n=N_cF_{1/2}((E_F-E_c)/kT) \tag{5}$$

where $F_{1/2}(n)$ is the Fermi-Dirac integral and N_c is the conduction-band density of states. In heavily doped semiconductors, the location of the conduction-band edge, E_c, is modified by Coulomb interactions $E_c=E_c^0+\Delta E$. There are two contributions to the conduction-band-edge shift, ΔE:

(i) the shift of the conduction-band edge due to the electron-electron interaction[9]

$$\Delta E_1=-\frac{2e^2k_F}{\pi\epsilon_0}-\frac{e^2\lambda}{2\epsilon_0}\left[1-\frac{4}{\pi}\tan^{-1}\left[\frac{k_F}{\lambda}\right]\right]\ , \tag{6}$$

where the Fermi wave vector is given by the relation $k_F^3=3\pi^2n$, $\lambda=2e/\hbar(3n/\pi)^{1/6}(m^*/\epsilon_0)^{1/2}$ is the Thomas-Fermi screening parameter, m^* is the electron effective mass at the Fermi energy, and $\epsilon_0=12.9$ is the static dielectric constant.

(ii) The second contribution to the conduction-band-edge shift comes from the electron-ionized impurity interaction[9]

$$\Delta E_2=-\frac{4\pi ne^2}{\epsilon_0a_0\lambda^3}=-\frac{e\hbar}{2}\left[\frac{\pi^3n}{\epsilon_0m^*}\right]^{1/2}\ , \tag{7}$$

where $a_0=\epsilon_0\hbar^2/m^*e^2$ is the effective Bohr radius.

It is now widely recognized that in GaAs the electrical activity of donor impurities is greatly reduced for doping levels exceeding $\sim 3\times 10^{18}$ cm^{-3} (Ref. 10). Also, an abrupt decrease of electron mobility has been reported for these high doping levels.[11,12] It has been proposed that the reduction of the concentration of electrically active donor impurities can be attributed to the formation of compensating amphoteric native defects.[10] Here we show that incorporation of the native defects as electron scattering centers explains the dependence of the electron mobility on donor concentration in heavily doped n-type GaAs.

In order to determine the concentration of the scattering centers, we use Eqs. (3)–(7) to calculate $[V_{Ga}]$ and n as functions of the donor doping level. The calculations were performed for $T=900$ K. It should be noted, however, that in a narrow temperature range, 700–900 K, typical for molecular-beam-epitaxy (MBE) growth of GaAs, $[V_{Ga}]$ is only very weakly dependent on temperature. The effect of the temperature on the equilibrium concentration of V_{Ga} is compensated by the temperature-dependent change of the Fermi energy and thus also the defect formation energy. The effectiveness of the V_{Ga} defect as an electron-scattering center depends on whether it acts as an isolated defect or forms a complex with positively charged donor impurities. Measurements of local-vibrational-mode spectra of heavily Si-doped GaAs have shown that a large portion of Si atoms form complexes with native defects, most likely V_{Ga}.[8] Also, in photoluminescence studies of heavily doped n-type GaAs the origin of so-called "self-activated"[13] centers has been attributed to (V_{Ga}-D) complexes. Here we assume that the mobility of V_{Ga} defects is high enough so that all the defects form $(V_{Ga}\text{-}D)^{2-}$ complexes. Accordingly, the effective concentration of charge scattering centers is

$$N_{cc}=N_{D^+}+3[V_{Ga}]\ . \tag{8}$$

Room-temperature electron mobility has been calculated using the standard approach.[1,2] At high doping levels the electron mobility is largely determined by charged center scattering with a small contribution from the phonon scattering. The inverse electron mobility is

$$\mu^{-1}=\mu_{cc}^{-1}+\mu_{ph}^{-1}\ ,$$

where μ_{ph} is the room-temperature phonon mobility limit[1] ~ 8500 cm^2/V s.

The mobility of electrons scattered by charged centers is[2]

$$\mu_{cc}=\frac{3\pi}{2}\frac{\epsilon_0^2\hbar^3}{e^3}\frac{n}{N_{cc}(m^*)^2F_{cc}}\ , \tag{9}$$

where $F_{cc}=\ln(\xi+1)-\xi/(\xi+1)$ and $\xi=(2k_F/\lambda)^2$.

The nonparabolicity of the conduction band has been incorporated in the calculation via an energy-dependent effective mass m^*.[14] Such an approach slightly overestimates the nonparabolicity effects by neglecting mixing of the valence- and conduction-band wave functions.[2] The calculations of the electron mobility μ were carried out using expression (8) for the concentration of charged scattering centers. The results of the calculations along with the experimental data on electron mobility in MBE-grown n-type GaAs (Refs. 11 and 12) are shown in Fig. 1. A rapid decrease of the electron mobility at high electron concentrations can be quantitatively explained assuming the value of $E_0=3.9$ eV for the V_{Ga} formation energy in Eq. (2). This value is very close to the formation energy of 4 eV determined from GaAs/Al$_x$Ga$_{1-x}$As superlattice intermixing experiments.[15] The calculations also show that, contrary to previous suggestion,[11] the nonparabolicity effects are not very significant, and cannot explain the abrupt decrease of the electron mobility. As is seen in Fig. 1, conductivity in n-type GaAs reaches a maximum value of about $2.4\times 10^3\ \Omega^{-1}$cm^{-1} at $n\sim 1\times 10^{19}$ cm^{-3}. This appears to be a basic limit of electrical conductivity achievable by doping in n-type GaAs. As was discussed previously,[10] the increased incorporation of compensating native defects in heavily doped n-type GaAs affects also the free-carrier concentration, leading to reduced activation of donor impurities at high doping levels.

In the amphoteric native defect model, the concentration of compensating defects critically depends on the location of the band edges with respect to E_{FS}. In GaAs, E_{FS} is located in the lower half of the band gap at $\sim E_v+0.6$ eV.[10] Hence, in n-type material, the formation energy of compensating acceptors is greatly reduced. This mechanism of defect formation is not operational in p-type GaAs, since much higher doping levels are required to achieve the same reduction of the defect formation energy in this case. Therefore, even for doping levels

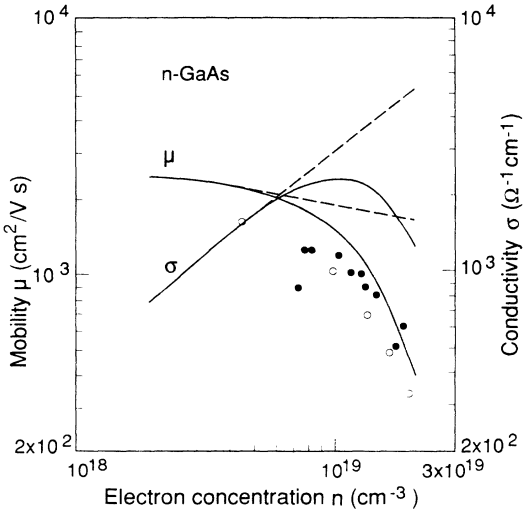

FIG. 1. Room-temperature electron mobility and conductivity in heavily doped n-type GaAs. The solid lines represent the calculations in which effects of native defects were included. The broken curves correspond to the standard case in which the concentration of charged scattering centers is equal to the carrier concentration. The experimental points represent the data of Ref. 11 (○) and Ref. 12 (●).

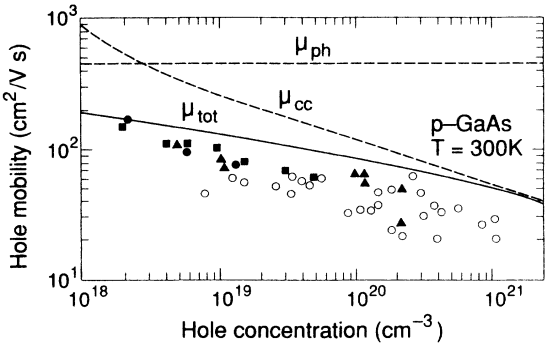

FIG. 2. Room-temperature electron mobility in heavily doped p-type GaAs. μ_{ph} and μ_{cc} are the mobilities due to phonon and charged-center scattering, respectively. The combined Hall mobility is represented by μ_{tot}. The experimental data for C- (○, Ref. 17) and Be- (●, Ref. 17; □, Ref. 18; ▲, Ref. 19) doped GaAs is also shown.

exceeding 10^{20} cm^{-3}, amphoteric native defects do not play any significant role in limiting free-hole concentration.[15] Also, one expects that in p-type GaAs, scattering by native defects will be much less pronounced than in n-type GaAs.

We have calculated the hole mobility in GaAs using a model of partially coupled valence bands.[16] In the model, the interband scattering is treated in an approximate manner. The heavy- and light-hole mobilities are determined separately and then their contribution to the Hall mobility is calculated using the standard procedure for two-band transports. As is shown in Fig. 2, the room-temperature hole mobility is determined by the optical-phonon deformation potential and charged impurity scatterings. The total mobility is very weakly dependent on the hole concentration. Assuming that the concentration of the charged centers is equal to the hole concentration, we find that the calculated mobility is in reasonable agreement with available experimental data on carbon-[17] and beryllium-[17–19] doped GaAs. This confirms our expectations that native defects do not play any significant role in hole scattering in p-type GaAs.

In conclusion, we have demonstrated that, using the concept of amphoteric native defects, one can calculate the contribution of native defects to the carrier scattering. In particular, the calculations show that an abrupt reduction of electron mobility in heavily doped n-type GaAs results from the Fermi-level-induced formation of ionized gallium vacancies. It is also found that there is a distinct asymmetry in the defect formation in n- and p-type GaAs. Even in very heavily doped p-GaAs, the reduction of the defect formation energy and thus also an enhacement of the defect concentration is small and does not produce any of the effects observed in n-type GaAs.

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