Resonant Electron Scattering Due to the Central Cells of Impurities Observed in AlGaAs under Hydrostatic Pressure

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In this paper we present results of electron mobility measurements on AlGaAs as a function of hydrostatic pressure which show the influence of resonant scattering by the central-cell potential of silicon. This is, we believe, the first direct observation of resonant impurity scattering in semiconductors.

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Impurity scattering in semiconductors is normally considered to be a result of the interaction of carriers with the long-range Coulomb potential of ionized impurities. This interaction, treated in one of several ways (e.g., Brooks-Herring,[1] Yanchev and co-workers[2,3]), can adequately describe mobility measurements in many cases but ignores the central-cell potential of the impurity.

The central-cell potential of a substitutional impurity in a III-V semiconductor can produce a deep level above the conduction-band edge. Here a deep level is referred to as one whose properties are defined by the impurity's central-cell potential rather than by interaction with band-edge states, as is the case for a shallow level.[4] Sankey, Dow, and Hess[5] point out that such a deep level is a sharp resonance having weak mixing with conduction-band states and that an electron at the energy of the resonance experiences strong scattering by the level. The scattering cross section is of the order of the square of the electron's de Broglie wavelength, λ_0^2, so that if the resonant level is very close to the conduction-band edge the cross section is very large, and scattering from the resonant level might dominate all other scattering mechanisms. Observation of such an effect is, however, difficult since the level must lie close to the band edge to influence the measured mobility, and even if a level does exist at an appropriate energy the reduction in mobility from that in similar samples without resonant deep levels is likely to be attributed to some more conventional scattering mechanism (e.g., a higher compensation ratio leading to more ionized-impurity scattering).

Common n-type dopants in $Al_xGa_{1-x}As$, such as Si and Sn, have been found to produce deep levels in the energy gap in addition to the desired shallow levels if x, the Al fraction, is greater than some critical amount.[6,7] The effect of increasing x is to change the band structure of the semiconductor, and the appearance of the deep level is interpreted as the raising of the energy of the conduction-band minimum past the position of a deep level which is degenerate with the conduction band at low Al fractions.

The application of hydrostatic pressure to AlGaAs increases the direct gap by $\simeq 11$ meV/kbar while the L point increases its energy with respect to the valence-band edge at Γ by $\simeq 4$ meV/kbar. The X point decreases its energy with respect to the valence band at Γ by $\simeq 1$ meV/kbar. Consequently, it is apparent that hydrostatic pressure has a similar effect on band structure to the increasing of the Al fraction, and Mizuta *et al.*[8] have observed the appearance of deep levels in AlGaAs for various Al fractions at high pressure. Therefore, alloying and the application of hydrostatic pressure both can tune the position of a deep level with respect to the conduction band and, in particular, as the level comes through the conduction-band minimum resonant electron scattering will occur. This therefore implies a critical AlGaAs composition such that the deep level is already resonant with the conduction-band edge at atmospheric pressure. However, it also implies that for alloy compositions with lower values of x, resonant scattering may be observed with use of hydrostatic pressure. As x decreases the pressure required increases. Application of hydrostatic pressure can thus be seen to be an ideal technique for observing resonant central-cell scattering as the relative position of the level can be varied in one sample, with all other parameters kept essentially constant.

Measurements were made on a sample of AlGaAs, with $x = 0.16$, doped with Si to give a Hall carrier concentration of 5.9×10^{17} cm^{-3}. The doped layer was 2.0 μm thick and had a 200-Å undoped GaAs cap. Below the doped layer was a 0.5-μm undoped $Al_{0.16}Ga_{0.84}As$ buffer layer and a 0.25-μm undoped GaAs layer grown on a semi-insulating substrate. It was designed to have no two-dimensional conduction at the heterojunction interfaces. The sample was grown by molecular-beam epitaxy at the Philips Laboratories Redhill at a substrate temperature of 600 °C and a growth rate of 2.5 μm/h.

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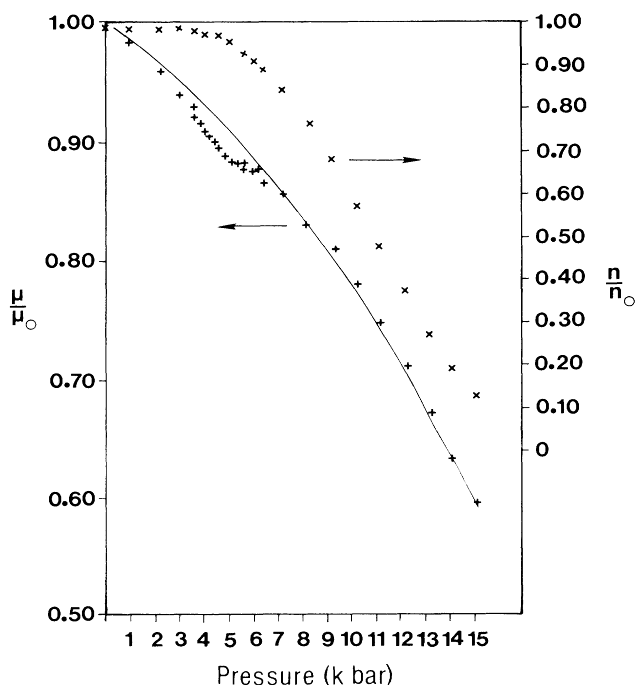

FIG. 1. Pressure dependence of Hall mobility and carrier concentration normalized to atmospheric-pressure values. Plusses are the experimental mobility values, crosses are the experimental carrier-concentration values. The solid line is the expected mobility variation obtained as described in the text.

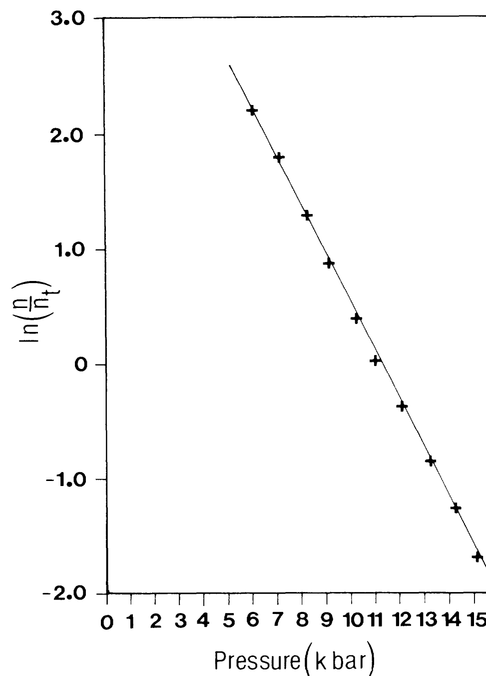

FIG. 2. Plot of $\ln(n/n_t)$ vs pressure to obtain the rate of deepening of the deep level with respect to the Fermi energy. Plusses are the experimental points. The solid line is the least-squares fit.

Resistivity and Hall-effect measurements were made on a standard van der Pauw cloverleaf specimen at room temperature in a piston-and-cylinder system for the generation of hydrostatic pressure to 15 kbar. A 50:50 mixture of castor oil and amyl alcohol was used as the pressure-transmitting medium, and pressure was measured with a Manganin resistance manometer.

The carrier concentration and mobility as functions of hydrostatic pressure normalized to atmospheric-pressure values are shown in Fig. 1. Consider first the carrier concentration. The sample begins trapping out electrons at $\simeq$4.5 kbar, corresponding to the deep impurity level moving through the Fermi level.

The deep-level occupancy, n_t, can be written as

$$n_t = \frac{N_t}{1+\delta\exp[(E_D - E_F)/kT]},$$

where N_t, E_D, and δ are the density, energy, and degeneracy of the deep level, respectively, and E_F is the Fermi energy. Taking $n_t = N_t - n$, where n is the carrier concentration in the band, we obtain

$$n/n_t = \delta\exp[(E_D - E_F)/kT].$$

In Fig. 2 we plot $\ln(n/n_t)$ vs P. The data are well described by a straight line, which corresponds to a rate of pressure-induced deepening of the trap with respect to the Fermi energy of 10.7 ± 0.5 meV/kbar. This pressure coefficient is in good agreement with the work of Robert *et al.*[9] who needed to invoke a deep level in a Si-doped $Al_{0.3}Ga_{0.7}As$ heterojunction, with a pressure coefficient of 11 meV/kbar, to account for their change in 2D electron concentration with pressure. It is not possible from our analysis to determine an exact value for the degeneracy, δ, but it indicates that δ lies between 6 and 8, consistent with the impurity level being associated with either the X minima or the L minima of the conduction band, respectively. From the rate of movement of the level with pressure, we estimate it to be approximately 90 meV above the bottom of the conduction band at atmospheric pressure.

Turning now to the pressure dependence of the mobility in Fig. 1, it is immediately striking that there is a decrease in the mobility from the general trend centered around 4.5 kbar, the pressure at which trapout starts. The solid curve in this figure is an expected Hall-mobility variation, obtained by our taking into account carrier transfer to higher minima and fitting to the pressure dependence of the mobility in the Γ minimum. Results of this fit are in good agreement with work on other heavily doped AlGaAs samples (to be published elsewhere) and on heavily doped GaAs,[10] and are primarily due to the pressure-induced increase of the electron effective mass. The difference between this line and the experimental points we ascribe to resonant central-cell

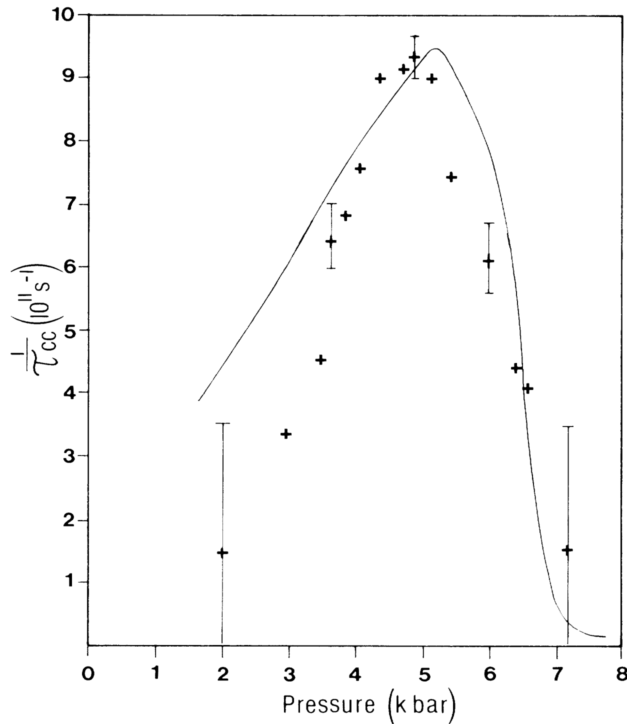

FIG. 3. Electron scattering rate associated with resonant central-cell scattering plotted as a function of pressure, which corresponds to variation of the position of the resonance in energy. Plusses are the experimental values obtained from the mobility data in Fig. 1. Typical error bars are indicated. The solid line is the theoretical curve based on the analysis of Sankey, Dow, and Hess (see Ref. 5).

scattering as the Si deep level moves through the conduction-band edge under the influence of pressure.

Since the dip in mobility is complete before more than 20% of the impurity centers are full, it does not appear that it can be due to a change in their charge state or to a type of trap-controlled mobility.[11] These effects would be expected to continue to higher pressure and not saturate until most of the centers contained electrons.

Usually it is necessary to perform a numerical iterative solution of the Boltzmann equation when a number of scattering mechanisms are active to include accurately the energy dependence of the scattering rates. However, over the limited energy range sampled in the experiment, we can use Matthiessen's rule to separate out the mobility limited by resonance scattering, $\mu_{\text{c.c.}}$. Hence we can determine the average scattering rate $\langle 1/\tau_{\text{c.c.}}\rangle$, over the electron distribution, from $\mu_{\text{c.c.}} = e\tau_{\text{c.c.}}/m^*$. This is shown in Fig. 3. The scattering rate has a peaked structure centered around $\simeq$4–5 kbar with a width of about 2.5 kbar which corresponds to a movement of the deep level of $\sim kT$ at room temperature relative to the electron distribution.

Sankey, Dow, and Hess[5] discuss the scattering rate for resonant central-cell impurity scattering and give, as a function of electron energy E,

$$[\tau_{\text{c.c.}}(E)]^{-1} = [2N_I/\hbar\pi D(E)]\sin^2\phi(E),$$

$$\sin^2\phi(E) = [\pi d(E)]^2/\{[V_s^{-1} - g(E)]^2 + [\pi d(E)]^2\},$$

where N_I is the impurity density, $D(E)$ is the total conduction-band density of states, and the real functions $g(E)$ and $d(E)$ are given by

$$g(E) - i\pi d(E) = \langle S \mid G_0(E) \mid S\rangle,$$

where $G_0(E)$ is the host-crystal Green's function with outgoing wave boundary conditions and $|S\rangle$ is an atomiclike orbital centered on the impurity atom. V_s is the impurity central-cell potential. Resonance occurs at $V_s^{-1} = g(E)$, where $\sin^2\phi = 1$. To obtain the shape of the resonance it is not necessary to know the exact values of V_s and $g(E)$. All that is required is the derivative $g'(E)$ at $g(E) = V_s^{-1}$, for we then have

$$\sin^2\phi(E) = \{[(E - E_r)g'(E)]^2/\pi^2 d^2(E) + 1\}^{-1},$$

where E_r is the energy of the resonant level.

Calculation of $g'(E)^4$ gives a value of about 1 eV^{-2} and, using this, we have calculated the average scattering rate over the electron distribution as

$$\langle 1/\tau_{\text{c.c.}}\rangle = \frac{\int_0^\infty ED(E)f(E)[\tau(E)]^{-1}dE}{\int_0^\infty ED(E)f(E)dE},$$

where $f(E)$ is the Fermi-Dirac distribution. Results of this calculation are given by the solid line in Fig. 3, with the resonance taken as centered at the experimental maximum and with the measured pressure coefficient of the trap, $d(E_D - E_F)/dp = 10.7$ meV/kbar. When we consider the approximate nature of the analysis, the agreement is very good.

Resonant scattering is characterized by a small width in energy and so only electrons with energies close to the resonance will experience strong scattering. For this scattering to be observed through its effect on the mobility, a substantial fraction of the electron population and also empty states into which they can scatter must be present at the resonance energy. Scattering will therefore not be strong in a heavily doped, highly degenerate sample. It can thus be seen that quite stringent conditions must be satisfied if central-cell scattering is to be observed: The resonance maximum, the band edge, and the Fermi level must all be close in energy for the maximum effect. In the case studied here these conditions are satisfied and the resulting mobility depression is still small, corresponding to a mobility limited by central-cell scattering of about 30000 cm^2/V·s at the resonance peak. Therefore, at room temperature, central-cell scattering will only have a large influence on the mobility in a heavily compensated sample with the level just coincident with the conduction-band minimum. Hydrostatic pressure will normally remove this degeneracy and pro-

vides an excellent test of the presence of central-cell scattering.

In conclusion, we have reported, for the first time, experimental results showing the influence on the mobility of electrons in a semiconductor of resonant scattering from the central-cell potential of an impurity. The resonance was observed as the level was brought through the conduction band under hydrostatic pressure. The scattering rate could be well described by the model of Sankey, Dow, and Hess.[5]

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