Chadi, Chang, and Walukiewicz Reply: We have recently proposed a structural model involving a large lattice relaxation for the *DX* center in GaAs which accounts for many of the physical properties of this defect.[1] The results of our calculations indicate that *DX* is stable in the proposed configuration only when *negatively* charged.

In their Comment, Maude *et al.*[2] raise the question of whether this charge state is consistent with the observed pressure dependence of the mobility in heavily degenerate *n*-type GaAs samples.[3] In these samples the Fermi level E_F at zero pressure lies 0.25–0.30 eV above the conduction-band minimum, close to the position of the *DX* resonance. As pressure is applied the energy of the Γ_1 conduction state rises more rapidly than *DX*, forcing some electrons to become trapped on *DX* centers. This results in a decrease of the free-electron concentration but an *increase* in the mobility. Maude *et al.*[2] suggest that the observed trends are better explained by a neutral defect center. However, they are able to account for only *half* the observed percentage increases in the mobility ratios $\mu(P=10\text{–}15\text{ kbar})/\mu(P=0)$ for various samples. In the following we show that the experimental observations are consistent with a negatively charged *DX* center.

The unique feature of the pressure and mobility measurements for the heavily doped GaAs samples[3] is the degeneracy of the energies of electrons in *DX* states with those at E_F. In addition, at the doping levels and the temperature of 300 K at which pressure is applied, the electrons at E_F and the *DX* centers are in full thermal equilibrium. The total density of electronic states at E_F, therefore, which needs to be used in the calculation of the screening parameter is given by

$$n(E_F)=\frac{3n}{2E_F}+\frac{n(P=0)-n(P)}{W}\,. \tag{1}$$

In Eq. (1) $n(P)$ is the pressure-dependent free-carrier concentration, W is the width of the *DX* level energy distribution, and the concentration of *DX* centers is assumed to be negligible at zero pressure. Only the first term on the right side of Eq. (1) is used by Maude *et al.*[2] in calculating the screening parameter λ from

$$\lambda^2 \simeq 4\pi e^2 n(E_F)/\epsilon\,. \tag{2}$$

For the case of a negatively charged *DX* center, we find that, for either Si- or Sn-doped samples, a value of W in the range of 0.03–0.04 eV completely corrects the underestimation in the mobility increases with pressure and leads to results in good agreement with experimental data.[3] If *DX* were a neutral defect, a substantially larger value of 0.2 eV for W would be needed to bring theory in agreement with experiment. Such a large value for W is *inconsistent* with experimental data, which exhibit a much more sharply defined Fermi-level pinning position.[3,4] The estimate $W \simeq 0.03\text{–}0.04$ eV for DX^- centers is consistent with that resulting from fluctuations in the screened Coulombic potential at these centers arising from the presence of other DX^- and ionized donor centers. In the regime where the concentration of DX^- is smaller than that of the free electrons, the repulsive interaction between DX^- centers introduces correlations in their positions which may also play a critical role in reducing the scattering rate of the conduction electrons.[5]

Finally, the inverse correlation of mobility with carrier concentration in heavily degenerate GaAs is opposite to that observed in *n*-type $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ alloys, in the composition range where *DX* is a bound state (i.e., for $x \geq 0.22$). Strong enhancements (by a factor as large as 5) in the mobility with an *increase* in the carrier density are observed in AlGaAs alloys.[6,7] In addition, unlike the case reported by Maude *et al.*[3] an increase in mobility with photoexcitation is seen.[6,7] The observed trends in the moderate doping regime, where the maximum free-carrier density is $10^{17}\text{–}10^{18}\text{ cm}^{-3}$, are also inconsistent with a neutral-state model for the *DX* center. For neutral *DX*, photoexcitation would lead to a sharp increase in the density of charged impurity scatterers leading to a decrease in the mobility. For a negatively charged *DX* center releasing its two electrons to the conduction band, the density of charged impurity centers would remain unchanged and the extra screening provided by the free carriers would lead to an increase in mobility according to Eq. (1) of Ref. 2.

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