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A NEW PROPOSED METHOD FOR DETERMINING INNER OR OUTER CROSSING LATTICE RELAXATION OF DX CENTERS IN $Al_xGa_{1-x}As$ BASED ON PRESSURE EFFECTS

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ABSTRACT

It is proposed that hydrostatic pressure measurements can be used to settle the recent controversies surrounding the model of the DX center in $Al_xGa_{1-x}As$ alloy. The method can in general distinguish the two possible cases of lattice relaxations in defect configuration coordinate diagrams: one with large lattice relaxation which we labelled as "outer crossing," and the other with small lattice relaxation labelled as "inner crossing".

The DX center in the $Al_xGa_{1-x}As$ alloys system has attracted much interest in recent years. Lang et al.[1] suggested in their original work that the DX center is a complex involving a donor atom and an anion vacancy. The main feature of this model is the large lattice relaxation (LLR) of the defect center in order to explain many of the unusual properties of the DX centers[1]. Recently, Mizuta et al.,[2] based on their pressure experiment and Hjalmarson and Drumond,[3] based on theoretical analysis, both suggested that the DX center is probably only a simple substitutional donor, and not a complex. Contrary to Lang et al., Hjalmarson and Drumond suggested that a deep donor with small lattice relaxation can explain most of the characteristics associated with the DX centers, such as persistent photoconductivity (PPC). In this communication, we propose a definitive way to resolve this controversy by determining whether a defect has a LLR or SLR. Our method is based on measuring the pressure coefficients of two energies which characterize the defect: the thermal barrier energy E_B and the thermal ionization Energy E_T. Since the pressure coefficients of these energies are not yet available for the DX center, we have illustrated our method by applying it to the B traps in GaAs[4]. In this case we concluded that the B hole traps in GaAs have SLR associated with them.

Our analysis of the problem of lattice relaxation of a defect starts with the multiphonon theory of Huang and Rhys.[5] The electron capture cross section of deep levels at high temperature is approximated by:[5,6]

$$\sigma(T) = \sigma_\infty e^{-E_B/kT} \qquad (1)$$

$$E_B = (E_T - E_S)^2/4E_S \qquad (2)$$

where σ_∞ is the pre-exponential factor, E_B is the thermal barrier energy, E_T is the thermal ionization energy from deep level to the conduction band, and $E_B = S\hbar\omega$ is the lattice relaxation energy, S is the Huang-Rhys factor and $\hbar\omega$ is the phonon energy. It was pointed out by Hjalmarson and Drumond that there are two possible solutions of E_S for a given pair of values of E_T and E_B:

$$E_S^{\pm} = E_T + 2E_B \pm 2 \; (E_B^2 + E_T E_B)^{1/2} \qquad (3)$$

Fig. 1 shows the configuration coordinate (CC)

diagrams for the two possible cases. Fig. 1(a) depicts the case of SLR for the DX center. It corresponds to the solution E_S^- in Eq. (3) or in terms of the dimensionless quantity $\epsilon_S = E_S/E_T$, it corresponds to $\epsilon_S < 1$. In this case, the minima of curves U_C and U_T are located at the same side of the crossing of the two curves. We labelled this case as "inner crossing".[1,7] Fig. 1(b) depicts the case of LLR suggested by Lang et al. It corresponds to the solution E_S^+ in Eq. (3) or $\epsilon_S > 1$. In this case, the minima of curves U_C and U_T are located at opposite sides of the crossing of the two curves. We labelled this case as "outer crossing".[1,7] From Eq. (2), we can derive the following equation for the hydrostatic pressure (p) coefficient of E_B:

$$\frac{dE_B}{dp} = \frac{(\epsilon_S^{-1} - 1)}{2}\frac{dE_T}{dp} - \frac{(\epsilon_S^{-2} - 1)}{4}\frac{dE_S}{dp} \qquad (4)$$

The first term on the RHS of Eq. (4) describes the contribution to dE_B/dp due to change of E_T under pressure. From Figure 1, this corresponds to a vertical shift between U_C and U_T. Evidently, the changes in E_B induced by the same shift in E_T have opposite signs for the two cases. This is essentially the method we propose to distinguish between the two cases described by Figs. 1(a) and (b). The second term on the RHS of Eq. (4) describes dE_B/dp due to variation of the lattice relaxation under pressure. This corresponds to a horizontal shift between the U_C and U_T curves in Fig. 1. Again, ΔE_B induced by the same shift ΔE_S have opposite signs for the outer crossing and inner crossing cases. The above conclusions about the relative signs of the contributions to dE_B/dp by the two terms dE_T/dp and dE_S/dp in Eq. (4) can also be obtained simply by noting that $(\epsilon_S^{-1} - 1)$ and $(\epsilon_S^{-2} - 1)$ both change sign depending on whether ϵ_S is larger or smaller than 1. As shown by Barnes and Samara[4], dE_S/dp can be expressed as:[4]

$$\frac{dE_S}{dp} = -2E_S \frac{d \ln \omega}{dp} \qquad (5)$$

where $d \ln \omega/dp$ is the Gruneissen parameter γ of the phonon. For GaAs, the values of γ for different phonon modes can be found in

Ref. 8. There are, however, no available data for the value of γ in $Al_xGa_{1-x}As$ or AlAs. For simplicity, we neglect the effect of a small fraction of Al, and use the value of γ = 1.2 in GaAs for the value γ in $Al_xGa_{1-x}As$ and obtain:

$$\frac{d \ln \omega}{dp} = 1.60 \times 10^{-3} \text{ kbar}.$$

Substituting this value into Eq. (5), we find:

$$\frac{dE_S}{dp} = -3.2 \times 10^{-3} E_S \text{ eV/kbar}.$$

Thus, dE_S/dp is uniquely determined by the value of E_S and is always negative. This can be understood from Fig. 1 since pressure always decreases the distance between the minima of U_C and U_T in the CC diagram.

For the DX center in $Al_xGa_{1-x}As$, with x ~ 0.35, we use the following values: E_B = 0.20 eV and E_T = 0.15 eV from Hjalmarson and Drumond. Substituting these values into Eqs. (3) and (4) we obtain these results for the two cases:

i) "Inner crossing" case:
$E_S^- = 0.021$ eV, $\epsilon_S = 0.14$,
$dE_S/dp = -0.067$ meV/kbar,

and

$$\frac{dE_B}{dp} = +3.1 \left(\frac{dE_T}{dp} + 0.27 \text{ meV/kbar}\right) \qquad (6)$$

ii) "Outer crossing case":
$E_S^+ = 1.08$ eV, $\epsilon_S = 7.19$,

$$\frac{dE_S}{dp} = -3.5 \text{ meV/kbar}$$

and

$$\frac{dE_B}{dp} = -0.43 \left(\frac{dE_T}{dp} + 1.97 \text{ meV/kbar}\right) \qquad (7)$$

Eqs. (6) and (7) are plotted in Fig. 2(a). Now, dE_B/dp and dE_T/dp are experimentally measurable quantities. By measuring dE_B/dp and dE_T/dp and plotting the experimental point in Fig. 2, it should be possible to determine uniquely whether the deep level has a large or small lattice relaxation, except for the very coincident case that the experimental point lies at the intersection of the two lines. Lifschitz et al.,[9] from their Hall measurements, asserted that the energy difference between the DX level and the L minimum of the conduction band E_L is constant at specific range of X and pressure. If their assertion is correct, we can roughly

estimate dE_T/dp by:

$$\frac{dE_T}{dp} \doteq \frac{dE_\Gamma}{dp} - \frac{dE_L}{dp} \doteq (11.5-5.5) \text{ meV/kbar}$$

$$= 6 \text{ meV/kbar.}$$[9]

Substituting into Eq. (6) and (7), we obtain dE_B/dp = +19 meV/kbar for the SLR case or -3meV/kbar for the LLR case. Thus, PPC should be strongly enhanced in the SLR case and suppressed in the LLR case. In the absence of direct experimental data for the DX center in $Al_xGa_{1-x}As$, we will apply our method to the B traps in GaAs as an illustration of its validity. In this case, the relevant pressure coefficients have been determined by Barnes and Samara.[4] According to Barnes and Samara, E_B = 0.248 eV, E_T = 0.715 eV for the B traps. Substituting into Eqs. (3) and (4) we obtain for the "inner crossing" case, E_S^- = 0.234 eV, and

$$\frac{dE_B}{dp} = 1.03 \left(\frac{dE_T}{dp} + 1.52 \text{ meV/kbar}\right) \qquad (8)$$

and for the "outer crossing" case, E_S^+ = 2.188 eV, and

$$\frac{dE_B}{dp} = -0.34\left(\frac{dE_T}{dp} + 4.46 \text{ meV/kbar}\right) \qquad (9)$$

Equations (8) and (9) are plotted in Fig. 2(b). In this case, Barnes and Samara determined that $d(U_{T,min} - E_V)/dp$ = 4.9 meV/kbar, where $U_{T,min}$ is the energy minimum of the U_T curve and E_V is the valence band edge. From Ref. 10 we obtain the pressure coefficient of the band gap in GaAs: $d(U_{C,min}-E_V)/dp$ = 11.4 meV/kbar. Combining these two results we obtain dE_T/dp = 6.5 meV/kbar. Substitute it into Eq. (8) and (10), we find dE_B/dp = +8.3 meV/kbar for the "inner crossing" case and dE_B/dp = -3.8 meV/kbar for the "outer crossing" case. The experimental values of dE_B/dp determined by Barnes and Samara is +8.6 meV/kbar. We thus conclude that the "inner crossing" case is valid for the B traps in GaAs.

We are now in the process of determining the corresponding pressure coefficients for the DX center.

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Figure captions

Fig. 1 Configuration coordinate diagram for defect center in GaAs or $Al_xGa_{1-x}As$. (a) "Inner crossing" case, (b) "Outer crossing" case.

Fig. 2 Calculated dE_B/dp vs dE_T/dp curves for both "inner crossing" and "outer crossing" cases: (a) for the DX centers in $Al_xGa_{1-x}As$ with X = 0.35 and (b) for the B traps in GaAs. The solid circle in (b) is the experimental result of Ref. 4.

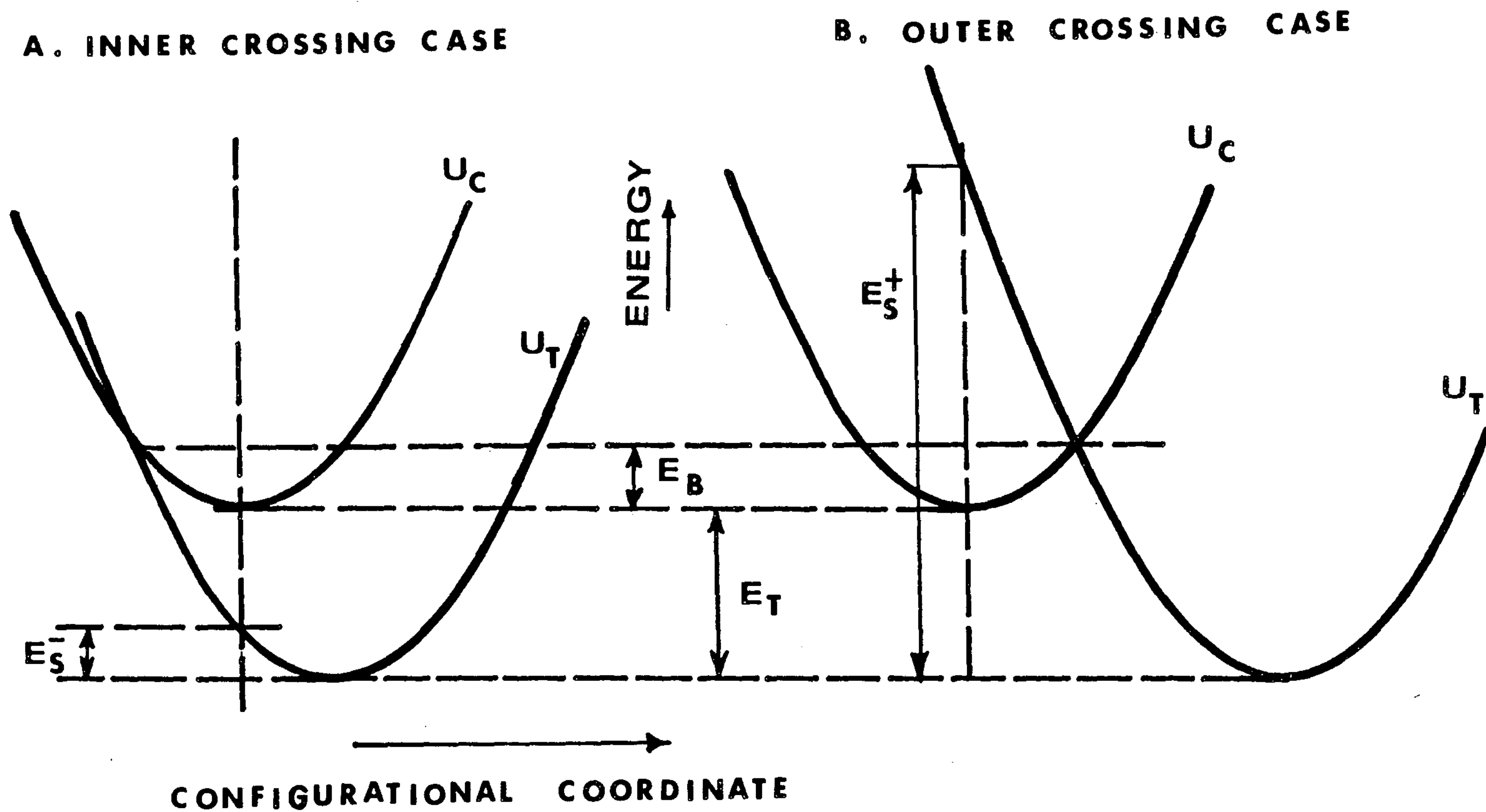
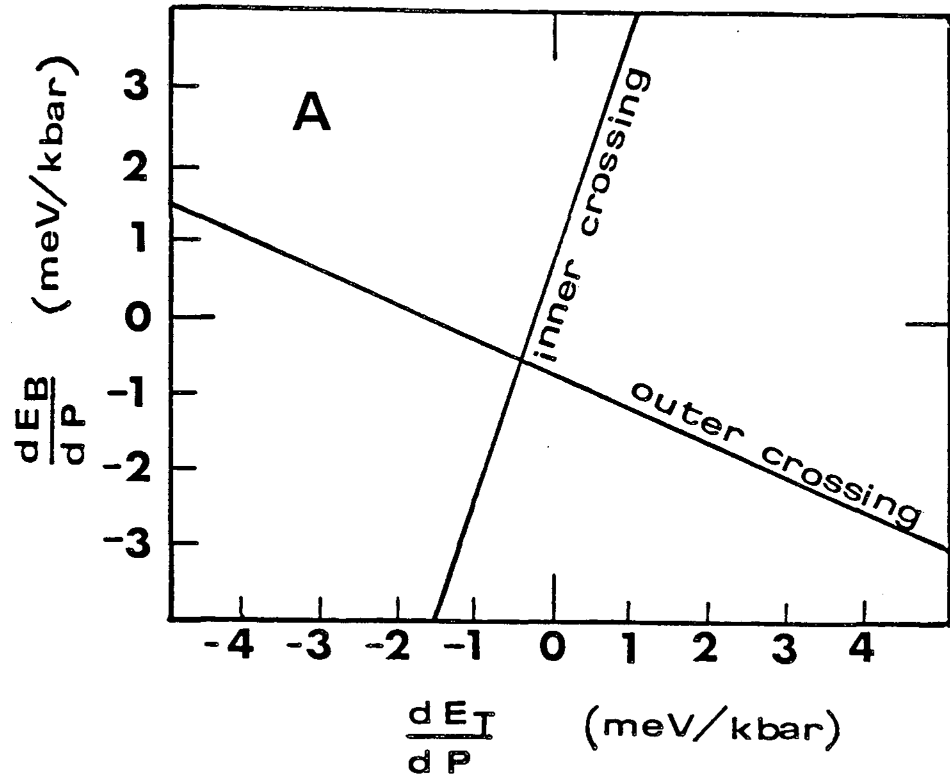


Figure 1.



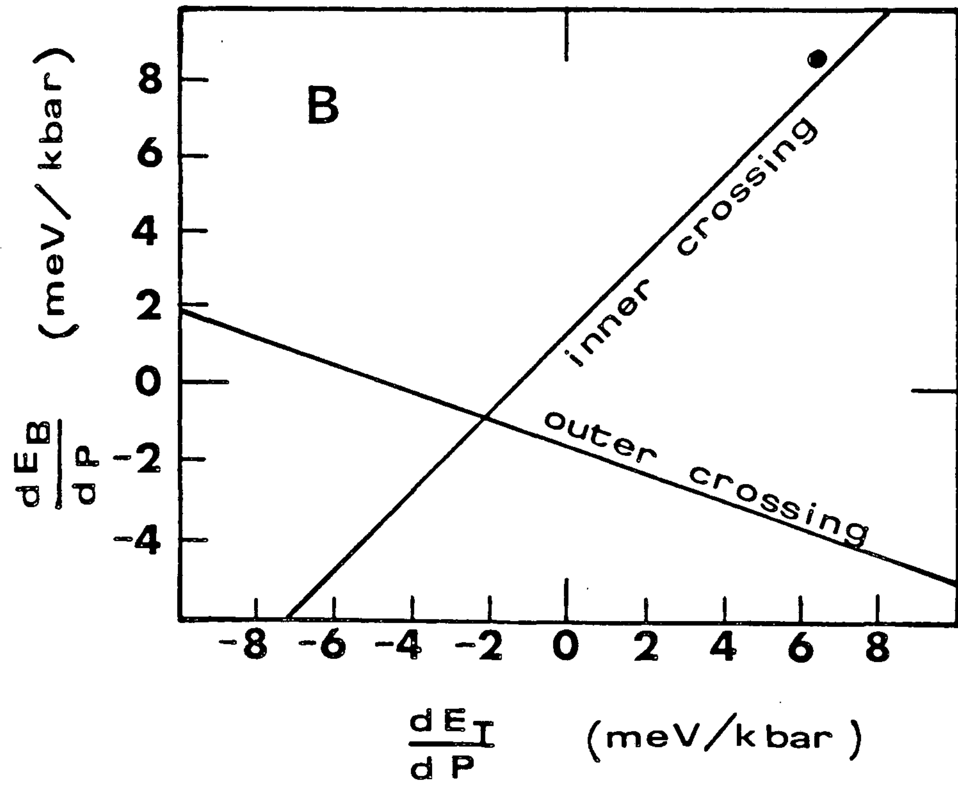


Figure 2.

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