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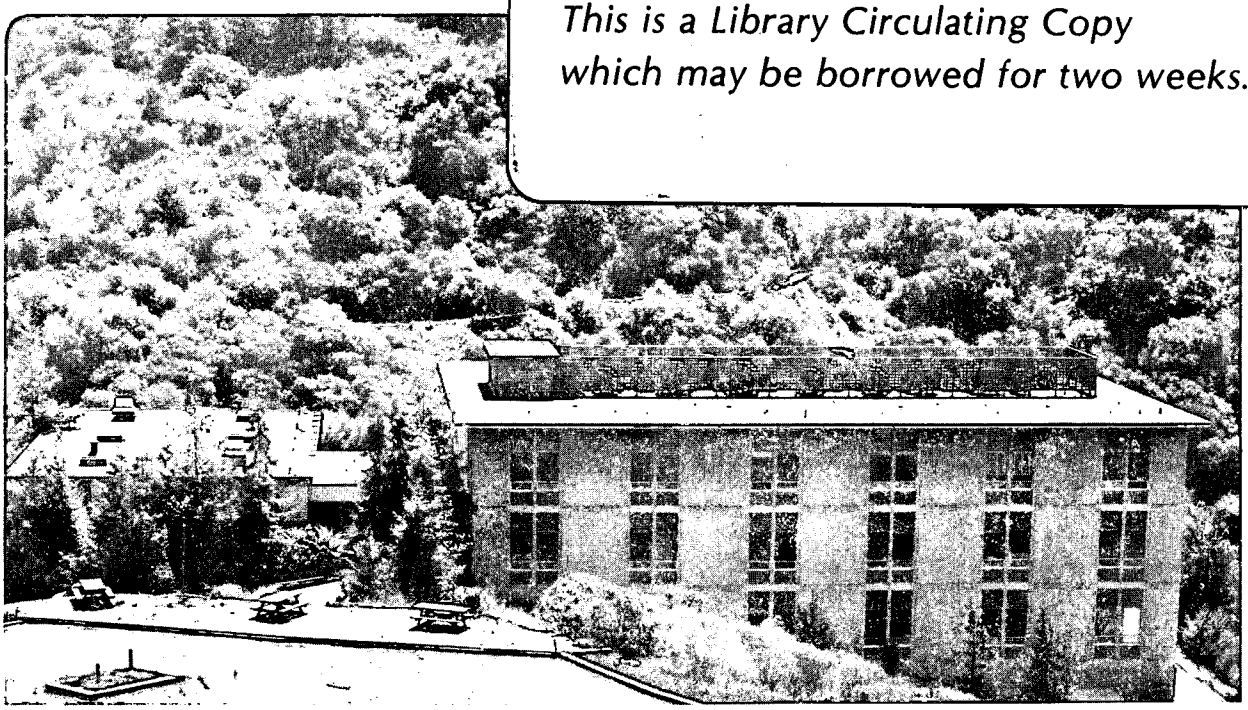

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# LATTICE RELAXATION OF THE DX CENTERS IN $Ga_{1-x}Al_xAs$ AND OF THE PRESSURE-INDUCED DEEP DONORS IN GaAs

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## ABSTRACT

Deep Level Transient Spectroscopies (DLTS) and capacitance transient techniques have been applied to GaAs:Si and to $Ga_{1-x}Al_xAs$:Te ($x$=0.35) under quasi-hydrostatic pressure using a diamond anvil cell. By substituting the experimental pressure coefficients of the defect energies into a model proposed by Li and Yu (Solid State Commun. 61, 13 (1987)) we concluded that both the DX center in the GaAlAs alloy and the pressure-induced deep donor (PIDD) in GaAs have large lattice relaxations associated with them.

## INTRODUCTION

Recently there is much interest in the DX centers in $Ga_{1-x}Al_xAs$ alloys due to their effect on the performance on devices such as modulation-doped field-effect transistors. DX centers were first identified and studied in great detail by Lang and coworkers [1,2]. To explain some of the unusual properties of the DX centers, such as their very small capture cross sections, the large difference between their thermal and optical ionization energies, Lang et al. [2,3] have suggested a model for the DX center involving a donor complex with large lattice relaxation (LLR). Recently, the discovery of similar deep donors in GaAs under pressure by Mizuta et al. [4] and the subsequent verification by Li et al. [5] using a different pressure technique, has prompted suggestions that DX centers may have relatively small lattice relaxation (SLR) [6,7]. To resolve this question of LLR vs SLR for the DX center and for the PIDD in GaAs, Li and Yu [8] have proposed a method based on the determination of the pressure coefficients of the defect's capture barrier height ($E_B$) and thermal ionization energy ($E_T$). Here we report the pressure coefficients of these defect energies for both the DX center in $Ga_{1-x}Al_xAs$:Te and the PIDD in GaAs:Si. Substituting these pressure coefficients into the model of Li and Yu we concluded that the results are consistent with the LLR model only and not with the SLR model.

## THEORY

The ideas behind the theory proposed by Li and Yu [8] are best illustrated by the configuration coordinate diagrams shown in Fig. 1(A) and (B). In these figures the parabola labelled $U_C$ represents the energy of the deep donor with its electron in the conduction band while the curve $U_T$ represents its energy after capturing an electron. In this model the equilibrium configuration coordinates of the deep donor before and after capturing the electron are different. As a result of this lattice relaxation the electron on curve $U_T$ has to overcome a barrier of height $E_B$ in order to be captured. The energy $E_S$ represents the lattice relaxation energy. As pointed out by Hjalmarson and Drummond [6] for a given pair of values of $E_B$ and $E_T$

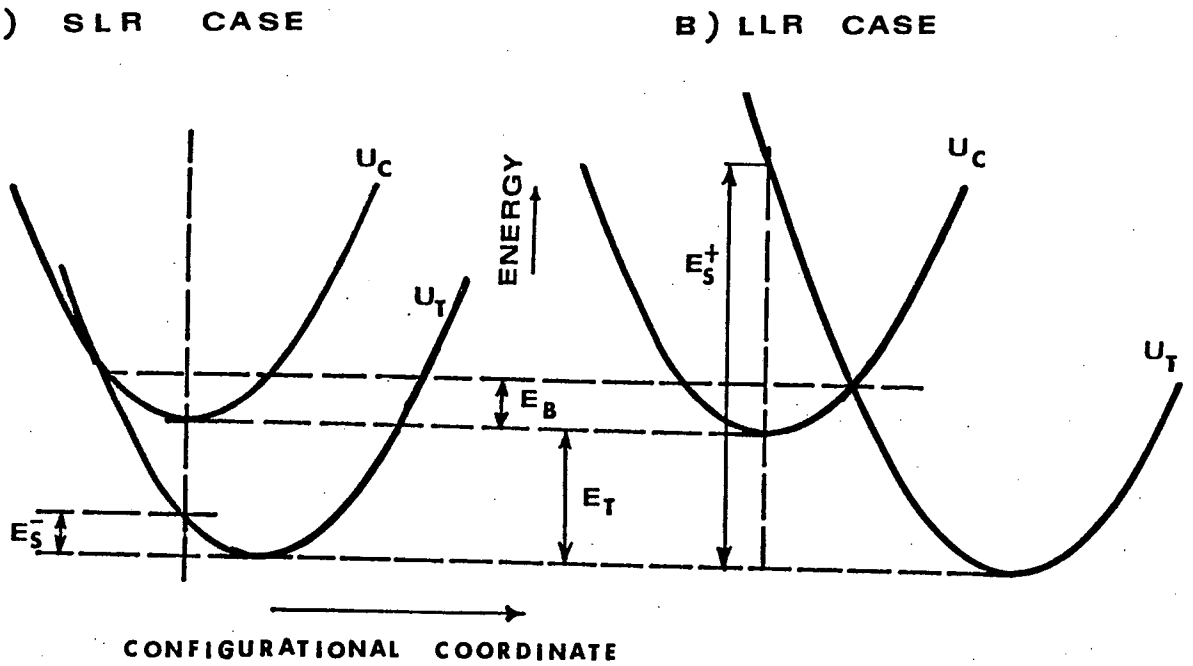


FIGURE 1 Configuration coordinate diagram for a defect center exhibiting (A) small lattice relaxation and (B) large lattice relaxation.

there are two solutions for $E_S$. The case where $E_S$ is smaller than $E_T$ is shown in Fig. 1(A) and corresponds to SLR while the case where $E_S$ is larger than $E_T$ is known as LLR. In the model of Henry and Lang [9] $E_B$,$E_T$ and $E_S$ are related via the expression:

$$E_B=(E_T-E_S)^2/4E_S \tag{1}$$

In principle whether a deep center has LLR or SLR can be uniquely determined if $E_T$ and $E_S$ are known. Unfortunately it is usually impossible to determined $E_S$ directly. On the other hand the pressure coefficient $d(\ln E_S)/dP$ can be calculated if the phonon which couples to the deep center is known. For example Barnes and Samara [10] have shown that if $\hbar\omega$ is the phonon energy then the pressure coefficient of $E_S$ is given by:

$$d(\ln E_S)dP = -2d(\ln\hbar\omega)/dP \tag{2}$$

where $d(\ln\hbar\omega)/dP$ is the Gruneisen parameter of the phonon mode. In case the mode Gruneisen parameter is not known, Li et al. [5] have suggested an alternate method. In the multiphonon emission theory [9] at temperature $kT>>\hbar\omega$ the capture cross section $\sigma_{n\infty}$ is given by:

$$\sigma_{n\infty} =(A/|E_T-E_S|)(4\pi E_B/kT)^{1/2} \tag{3}$$

If experimentally it is found that $\sigma_{n\infty}$ is independent of pressure, then Eq. (3) implied that:

$$\frac{dE_S}{dP} = \frac{dE_T}{dP} - \frac{(E_T-E_S)}{2E_B}\frac{dE_B}{dP} \tag{4}$$

It should be noted that the Eq. (4) is only true when $\sigma_{n\infty}$ is independent of pressure. This has been found to be true for the B traps in GaAs by Barnes and Samara [10]. We have also found this to be true for the PIDD in GaAs and for the DX center in GaAlAs:Te.

Li and Yu [8] pointed out that if $dE_S/dP$ was known then whether LLR or SLR was valid could be determined conclusively by testing if the three pressure coefficients of $E_T$, $E_B$ and $E_S$ satisfied this equation:

$$\frac{dE_B}{dP} = \left(\frac{\epsilon_S^{-1}-1}{2}\right)\frac{dE_T}{dP} - \left(\frac{\epsilon_S^{-2}-1}{4}\right)\frac{dE_S}{dP} \qquad (5)$$

In Eq. (5) $\epsilon_S$ is the ratio $E_S/E_T$ and is smaller than 1 for SLR and larger than 1 for LLR. Thus using Eq. (1) and (5) one can decide not only whether a given deep center has LLR or SLR but also whether the theory of multiphonon emission proposed by Henry and Lang [9] applies to this center.

## EXPERIMENTAL DETAILS AND RESULTS

Experiments have been performed on both GaAs:Si and on $Ga_{1-x}Al_xAs$:Te as a function of pressure using a diamond anvil cell. Details of the construction of the cell and the technique for making electrical measurements with this cell are similar to those described by Erskine et al. [11]. The samples were fabricated into Schottky barrier diodes as described in Ref. 5. The relevant defect energies were determined by Deep Level Transient Spectroscopies (DLTS) and constant temperature capacitance transient techniques. From the DLTS spectra the emission rates ($e_n$) of the deep center were determined while the capture rates ($\tau_c^{-1}$) were measured by a standard majority-carrier pulse method at constant temperatures [12]. In both samples we found that the peaks in the DLTS spectra showed activated temperature dependence according to the equations:[3]

$$e_n/T^2 = A_e \exp-(E_e/kT) \qquad (6)$$

$$(\tau_c)^{-1} = A_c \exp-(E_c/kT) \qquad (7)$$

where $E_e$ and $E_c$ denote respectively the activation energies for emission and capture of the electron.

TABLE I

Defect energies and pressure coefficients for the PIDD in GaAs and for the DX center peak in $Ga_{0.65}Al_{0.35}As$. For P>6 kbar $Ga_{0.65}Al_{0.35}As$ has an indirect gap and the values shown in parentheses corresponds to capture via the X valley.

| | | GaAs:Si (29 kbar) | $Ga_{0.65}Al_{0.35}As$:Te (1 bar) | (7.4 kbar) |
|---|---|---|---|---|
| $E_c$ | (meV) | 220 | 237 | 224 |
| $E_e$ | (meV) | 300 | 273 | 281 |
| $dE_c/dP$ | (meV/kbar) | -2.1 | -3.6 | 1.4 |
| $dE_e/dP$ | (meV/kbar) | -1.3 | 2.4 | -1.4 |
| $E_{LD}$ (D=Γ or X) | (meV) | 110 | 62 | 32 (0) |
| $dE_{LD}/dP$ | (meV/kbar) | -6 | -6 | 7 (0) |
| $E_B=E_c-E_{LD}$ | (meV) | 110 | 175 | 192(224) |
| $dE_B/dP$ | (meV/kbar) | 3.9 | 2.4 | -5.6 (1.4) |
| $E_T=E_e-E_B$ | (meV) | 190 | 108 | 89 (57) |
| $dE_T/dP$ | (meV/kbar) | -5.2 | 0 | 4.2 (-2.8) |

Details of our experimental results on the PIDD in GaAs:Si has already be presented in Ref. 5 while the results in $Ga_{1-x}Al_xAs$ will be presented elsewhere [13]. In this paper we summarize in Table I the values of $E_e$ and $E_c$ for the PIDD in GaAs and for the DX center in $Ga_{1-x}Al_xAs$ together with their pressure coefficients.

Based on the pressure dependence of the DX center several authors [7,14,15] have suggested that the DX center energy level was formed predominantly from the L valleys of the conduction band. As a result it has been proposed [16] that if the electrons are initially in the lowest conduction band minimum (either $\Gamma$ or X) they have to be thermally excited into the L valleys before they encounter the capture barrier height $E_B$. Based on this model the experimentally determined capture barrier height $E_c$ is equal to $E_B+E_{LD}$ where $E_{LD}$ is the energy separation between the L valleys and the lowest conduction minimum D. For the PIDD in GaAs at P<40 kbar and for the DX center in $Ga_{1-x}Al_xAs$ with a direct band gap D is the valley at $\Gamma$. Taking into consideration the energy $E_{LD}$ and its pressure coefficient we obtain the true capture barrier heights $E_B$ and their pressure coefficients in Table I. Within this model a similar correction has to be applied to the experimental emission activation energies to obtain the thermal ionization energy $E_T$. The corrected values are listed in Table I also. In case of the DX center we found that the pressure coefficient of $E_e$ changes discontinuously around 5 kbar where the conduction band minimum changes from $\Gamma$ to X. To explain this result we propose that when the X valley is lower than the L valley the electron can be captured into the DX center via the X valley. The values of $E_B$ and $E_T$ corresponding to capture via the X valleys are shown in Table I in parenthesis.

## DISSCUSSIONS

In order to apply the model of Li and Yu [8] to test whether the PIDD in GaAs or the DX center have LLR or SLR it is necessary to know $dE_S/dP$. We have calculated $dE_S/dP$ by using two different methods. In method 1 we use Eq. (2) and the fact that Lang [3] has shown the DX center coupled most strongly to the zone-edge transverse acoustic (TA) phonons. We have made similar conclusions about the PIDD in GaAs based on both the temperature dependence of the capture cross section [5] and on the photon energy dependence of the photoionization cross section [17]. The values of $dE_S/dP$ calculated with Eq. (2) assuming a TA phonon Gruneisen parameter of $-2.5\times10^{-3}$ $(kbar)^{-1}$ [18] are shown in Table II. In the second method we noted that within our typical experimental uncertainty of a few percents the capture cross sections $\sigma_{n\infty}$ for both the PIDD in GaAs and for the DX centers in $Ga_{1-x}Al_xAs$ are independent of

**TABLE II**

The lattice relaxation energies and their pressure coefficients calculated for both LLR and SLR using Eq. (2) (method 1) or Eq. (4) (method 2). Figures in parentheses correspond to capture via the X valley.

| | GaAs:Si (29 kbar) | $Ga_{0.65}Al_{0.35}As$:Te (1 bar) | $Ga_{0.65}Al_{0.35}As$:Te (7.4 kbar) |
|---|---|---|---|
| $E_S^+$(LLR) (meV) | 773 | 903 | 938(1006) |
| $E_S^-$(SLR) (meV) | 47 | 13 | 8 (4) |
| $dE_S^+/dP$(1)(meV/kbar) | 3.9 | 4.4 | 4.4(4.4) |
| $dE_S^+/dP$(2)(meV/kbar) | 5.1 | 5.4 | -8.2(0.16) |
| $dE_S^-/dP$(1)(meV/kbar) | 0.24 | 0.06 | 0.04(0.02) |
| $dE_S^-/dP$(2)(meV/kbar) | -7.7 | -0.62 | 5.4 (-2.9) |

pressure. These results allow us to use Eq. (4) to calculate $dE_S/dP$ and the results are also shown in Table II. We note that the values of $dE_S/dP$ obtained by both methods agree rather well for the LLR model but not for the SLR model. The only exception is the the case of the DX center in the indirect gap region. In this case the sign of $dE_S/dP$ obtained by the two methods are opposite. By assuming that the capture occurs via the X valleys at least the two methods gave the same sign for $dE_S/dP$.

Substituting the values of $E_T$, $dE_T/dP$ in Table I and the values of $E_S$ and $dE_S/dP$ in Table II into Eq. (5) we obtained four sets of values for $dE_B/dP$, two sets for LLR and two for SLR. These values are compared with the experimental values listed again in Table III. Overall we find that the values of $dE_B/dP$ calculated from the LLR model are in much better agreement with experiment. In case of the DX center in the indirect gap region we found that agreement with experiment is much better if we assume that electrons are captured via the X valley rather than the L valley.

**TABLE III**

The experimental pressure coefficient $dE_B/dP$ compared with calculated values based on either LLR or SLR using the pressure coefficients of the lattice relaxation energy calculated by two different methods (Method 1 uses Eq. (2) and Method 2 uses Eq. (4)). Figures in parentheses correspond to capture via the X valley.

| | GaAs:Si (29 kbar) | $Ga_{0.65}Al_{0.35}As$:Te (1 bar) | $Ga_{0.65}Al_{0.35}As$:Te (7.4 kbar) |
|---|---|---|---|
| $dE_B/dP$ (Exp) (meV/kbar) | 3.9 | 2.4 | -5.6 (1.4) |
| $dE_B/dP$(LLR,1)(meV/kbar) | 2.9 | 1.1 | -0.81(2.6) |
| $dE_B/dP$(LLR,2)(meV/kbar) | 3.2 | 1.3 | -3.93(1.4) |
| $dE_B/dP$(SLR,1)(meV/kbar) | -8.9 | -2.1 | 16.2(-29.3) |
| $dE_B/dP$(SLR,2)(meV/kbar) | 21.7 | 21.2 | -97.8(300) |

## CONCLUSIONS

$E_B$, $E_T$ and their pressure coefficients for the PIDD in GaAs:Si and for the DX center in $Ga_{1-x}Al_xAs$:Te have been determined experimentally. The pressure coefficients of $E_S$ have been calculated by two different methods. From the theoretical values of $dE_S/dP$, values of $dE_B/dP$ have been calculated using both the LLR and SLR models. It was found that overall the experimental values of $dE_B/dP$ are consistent with the LLR model only and not with the SLR model. In case of the DX center in $Ga_{1-x}Al_xAs$ in the indirect band gap region good agreement between theory and experiment is obtained if we assume that carriers are captured into the DX centers via the X valleys. In the direct gap region our results are consistent with carrier capture via the L valleys of the conduction band.

## ACKNOWLEDGEMENTS

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