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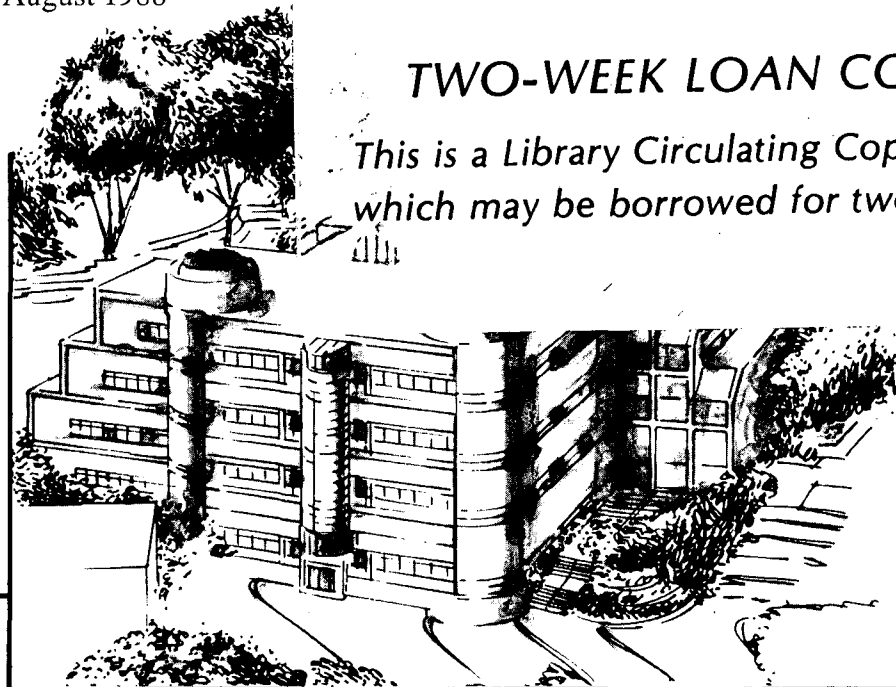**Center for Advanced Materials**

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Donors in GaAs:Si and the DX Centers
in GaAlAs:Si Alloys**

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DISCLAIMER

A COMPARISON OF THE PRESSURE-INDUCED DEEP DONORS IN GaAs:Si
AND THE DX CENTERS IN GaAlAs:Si ALLOYS

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A comparison is made between the emission and capture
activation energies of the pressure-induced deep donors
in GaAs (both with and without boron) and the DX center
in AlGaAs. It is suggested that the emission and
capture activation energies of the DX center are
influenced by its next nearest neighbors.

We have successfully implemented capacitance transient techniques
such as DLTS and photocapacitance under high pressure inside a diamond
anvil cell. These techniques have been used to study the pressure-
induced deep donors (PIDD) in GaAs which were first reported by Mizuta
et al.[1] using a Bridgman cell. Here we summarize our results on the
emission, capture and photoionization properties of these deep
centers. These results are compared with the corresponding properties
of the DX centers in GaAlAs alloys first reported by Lang et al.[2].

Two types of GaAs samples have been studied. Sample #1 is a bulk
GaAs grown by the horizontal Bridgman technique and doped with Si
(N_d-N_a=2x10^{17} cm^{-3}). Sample #2 is a liquid encapsulated Czochralski
grown bulk GaAs doped with Si(N_d-N_a=4x10^{16} cm^{-3}). Sample #2 was found
by SIMS to contain 2x10^{17} cm^{-3} of B. Schottky diodes were formed by
evaporating Al onto the wafers. Chips of about 200 microns square were
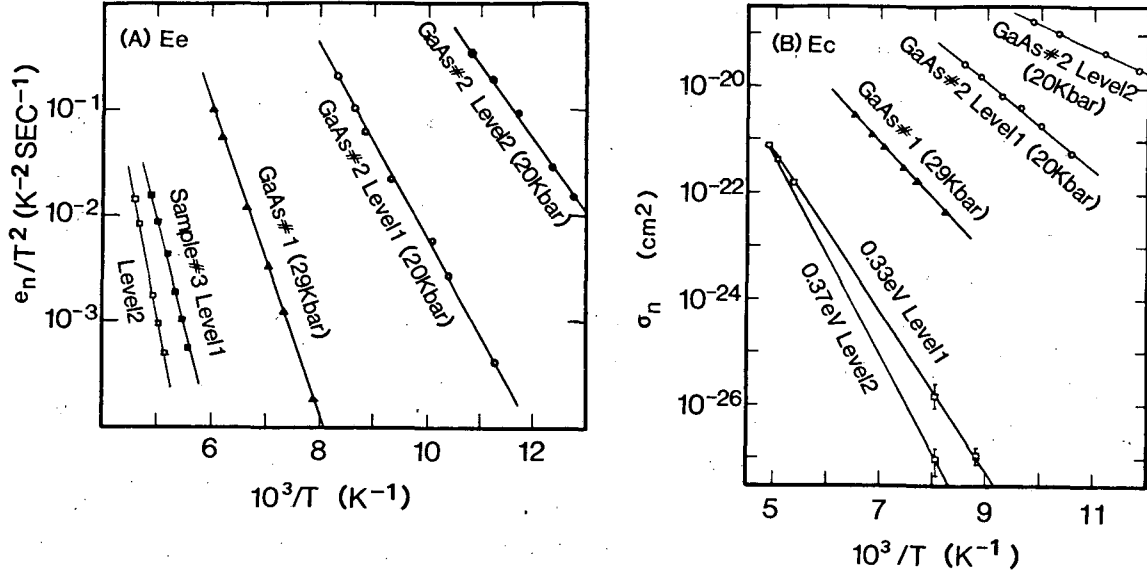cut and mounted into the cell using CaSO$_4$ as the pressure medium [3].

Figure 1 Arrhenius plot of (a) capture cross section and (b) electron emission rate for the PIDD or DX center in the three kinds of samples.

In Fig. 1 the Arrhenius plots of the electron emission rate e_n: $e_n = T^2 A_e \exp(-E_e/kT)$; and capture cross-section σ_n: $\sigma_n = A_c \exp(-E_c/kT)$ of PIDD for both types of samples are shown. The results are compared with those of a MBE grown $Al_{0.3}Ga_{0.7}As$:Si with 1×10^{17} cm^{-3} of free carrier (to be referred to as sample #3 in this paper) reported by Zhou et al.[4].

The activation energies obtained for the three kinds of samples from Fig. 1, the photoionization threshold (E_{op}) and pressure coefficients deduced from data not shown here [3,5,6] are quite different and are summarized in Table 1. These differences in energies cannot be accounted for even after correcting for the difference in sample pressures using the pressure coefficients listed in Table 1. On the other hand these results are consistent with recent experiments by Mooney et al. [7] who found that the DX center in heavily-doped GaAs and in AlGaAs with low Al concentrations can show as many as three level with values of E_e (in eV) and log A_e (with A_e in units of $K^{-2}sec^{-1}$) equal to (0.33,7.69), (0.40,7.63) and (0.43,7.45) respectively. The values of E_e and A_e obtained by Mooney et al. in highly doped GaAs:Si are in excellent agreement with our PIDD results in sample #1 if we extrapolate our data from 29 kbar to atmospheric

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Table 1. Summary of data for the PIDD in GaAs:Si with and without B and the DX center in AlGaAs:Si determined from their DLTS and photoionization spectra.

	Sample #2		Sample #1	Sample #3	
	level 2	level 1		level 1	level 2
Pressure (kbar)	20		29	0.001	
E_e (eV)	0.14	0.18	0.30	0.40	0.51[a]
log A_e	7.2	6.9	7.4-7.9		
dE_e/dP (meV/kbar)	2.9	1.4	-1.3		
E_c (eV)	0.09	0.16	0.22	0.33	0.37
log A_c	-13.1	-11.5	-13.2		
dE_c/dP (meV/kbar)	-1.3	-1.4	-2.1		
E_{op} (eV)			1.44[b]	1.25[c]	
Phonon energy (meV)			8[b]	10[c]	

[a] after T^{-2} correction.

[b] Ref.5.

[c] Ref.8.

pressure using the pressure coefficients given in Table 1. The values of E_e for the other peaks measured by Mooney et al.[7] are very close to those obtained by Zhou et al.[4] after a correction for the T^{-2} term. Lang [8] has reported observing only one level with $E_e=0.43$ eV for the DX center in $Al_{0.4}Ga_{0.6}As$:Si.

Thus these differences in properties between the PIDD in the GaAs samples and the DX centers in sample #3 must be due to their different environments. In particular the crucial difference between these three kinds of samples is that the next nearest Ga sites of their Si_{Ga} impurity are occupied all by Ga (sample #1), or may contain B (sample #2) or Al (sample #3). Although in sample #2 the concentration of B is relatively low there is evidence that Si and B are attracted to each other to form Si-B pairs[9]. B, Al and Ga are isovalent but they differ in their electronegativity and in their atomic s-level energies. These are listed in Table 2 for comparison. We note that the s-electron energy decreases from B to Al and this may be related to increase in E_c and E_e in Table 1 from left to right. Hjalmarson et al.[10] have used the relation between impurity atomic energies and short range potentials to predict the chemical trends of deep centers.

Table 2. Energy of s-electrons and electronegativity for B, Al and Ga.

	B	Ga	Al
Energy of s-electrons[a] (eV)	-13.46	-11.55	-10.70
Electronegativity[b]	2.00	1.13(1.6)	1.18(1.5)

[a] C.E. Fisher, Atomic Data, 4, 301 (1972).

[b] J.C. Phillips, **Bands and Bonds in Semiconductors**, (Academic Press, New York, 1973). The values in brackets are Pauling's values.

It is possible that the atomic energies of the next nearest atom may affect the DX center short range potential and hence change the lattice relaxation and the capture barrier height.

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