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Lattice Relaxation of Pressure Induced Deep Center in GaAs:Si

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ABSTRACT

Deep centers induced by hydrostatic pressures in GaAs:Si have been studied by Deep Level Transient Spectroscopy and constant temperature capacitance transient techniques. The capture behavior of these centers has been studied in detail and found to be consistent with the multiphonon emission theory. The pressure coefficients of the ionization energy and the barrier height are consistent with the large lattice relaxation model proposed by Lang and Logan.

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Recently Mizuta et al.[1] found that when GaAs containing shallow donors are subjected to hydrostatic pressures in excess of 20 kbar deep centers similar in properties to the DX centers in AlGaAs alloys appeared. These results stimulated much discussions concerning the nature of these pressure induced deep centers (to be abbreviated as PIDC in this article) and of the related DX centers. In particular the question whether large lattice relaxations proposed by Lang and Logan[2] is necessary to explain the persistent photoconductivity (PPC) of the DX centers in AlGaAs alloys and of the PIDC in GaAs has not been resolved. Several authors, such as Hjalmarson and Drummond[3] and Henning and Ansems,[4] have proposed alternate electronic mechanisms of PPC. The difference between the large lattice relaxation model and the model proposed by Hjalmarson and Drummond[3] is shown schematically in Fig. 1. Recently Li and Yu[5] proposed that hydrostatic pressure measurements can distinguish between those two models. In this Letter we present measurements of the thermal ionization energy (E_T)and capture barrier height (E_B) of the PIDC in Si doped GaAs as a function of pressure. Our results for these PIDC are consistent with the large lattice relaxation model of Lang and Logan[2] but not with the model of Hjalmarson and Drummond.[3]

Our experiments were performed on Si doped bulk GaAs crystals with $N_D - N_A = 2\times10^{17}$ cm^{-3}. Schottky diodes were fabricated by first evaporating Au-Ge alloy on one side of the wafer and annealing at 450 °C for one minute to form an ohmic contact. This was followed by evaporating Al on the other side of the wafer which was then cut into small 200x200 $(micron)^2$ chips. The cut

sides of the samples were etched to reduce the reverse-biased leakage current before loading into a diamond anvil high-pressure cell. Details of this cell and the technique for introducing wires into the cell have been described elsewhere[6]. Powder of calcium sulfate was used as the pressure transmitting medium. The pressure inside the cell was determined by measuring the fluorescence of ruby chips placed adjacent to the sample. The accuracy in the pressure measurement is better than 1 kbar. Deep Level Transient Spectroscopy (DLTS) and constant temperature capacitance transient measurements were made using a Boonton Model 72B capacitance meter and a dual channel boxcar integrator. The temperature of the sample was measured with a calibrated Si diode in thermal contact with one of the diamond anvils. To minimize the temperature difference between the sample and the sensor, temperature scans in DLTS were made extremely slowly.

Figure 2 shows some typical DLTS spectra of two samples under pressure. Pulse widths long enough for saturated transient amplitudes were used to avoid any possible distortion of the DLTS spectra due to temperature dependence of the capture rates. Our results are qualitatively similar to those reported by Mizuta et al.[1] Quantitatively there are significant differences: (1) The shift in our DLTS peaks with pressure is much smaller than that reported by Mizuta et al. (2) The density of our PIDC also increases at a slower rate with pressure. Mizuta et al.[1] found that at 30 kbar the amplitude of the capacitance transient, ΔC, becomes comparable to the junction capacitance C. To avoid

complications due to pressure dependence of the carrier concentration and nonlinear relationship between ΔC and the PIDC concentration, we have limited the pressure we applied to the sample to below 29 kbar where $\Delta C/C$ is still less than 2 %. We note that in Sample #3 the DLTS spectra indicate the existence of several peaks as have also been observed by Mizuta et al. From the DLTS spectra the emission rates (e_n) of the PIDC were obtained as a function of temperature and pressure. Plots of e_n versus temperature at 29 kbar for both samples #3 and #4 are shown in Fig.3. The capture rate (τ_e^{-1}) was measured by a standard majority-carrier pulse method[7] at constant temperatures corresponding to the DLTS peaks. In this case the transient signal amplitudes were recorded as a function of pulse widths. The capture time constant, τ_e, was determined by the half-signal point method of Lang.[8] The temperature dependence of the capture rates at 29 kbar in the two samples are also shown in Fig. 3. In sample #3 the DLTS cuvre was found to shift <u>en bloc</u> with pressure so we assumed all the levels contributing to the DLTS peak had the same pressure dependence. In spite of the multiplet nature of the DLTS peak in sample #3 the slopes of the curves in Fig. 3 for sample #3 and #4 are quite similar.

We have interpreted the temperature dependence of the emission and capture rates of the PIDC in GaAs:Si with the multiphonon emission theory (MET).[9,10] The capture and emission rates are related to the capture cross section σ_n, by

$$\tau_e^{-1} = \sigma_n \langle v \rangle n \qquad (1)$$

and

$$e_n = N_c \langle v \rangle \sigma_n \exp[-E_T/KT] \qquad (2)$$

respectively. In Eqs. (1) and (2) $\langle v \rangle$ is the electron thermal velocity, n is the carrier concentration, N_c is the effective conduction band density-of-states, E_T is the thermal ionization energy of the PIDC and K is the Boltzmann constant. In the high temperature limit of the MET the capture cross section depends on temperature as:[9,10,11]

$$\sigma_n = \sigma_{n\infty} \exp[-E_B/KT], \qquad (3)$$

where $\sigma_{n\infty}$ is the capture cross section at infinite temperature. The quantity $N_c\langle v \rangle$ depends quadratically on temperature.[7] By fitting the curves in Fig.3 with the above equations we obtained the values for E_T+E_B and E_B as 0.30 ± 0.01 eV and 0.22 ± 0.01 eV respectively for the PIDC in GaAs:Si at P=29 kbar. The values for samples #3 and #4 are identical within experimental uncertainties. We note that both the magnitude of the emission and capture cross sections and the activation energies for the PIDC in GaAs are very close to that of the DX center in AlGaAs reported in Ref. 2. This lends further support to the proposal by Mizuta et al. that the PIDC in GaAs are related to the DX centers found in AlGaAs under ambient pressure.

We have also determined the pressure coefficients of the energies E_T and E_B. Following previous work[11,12] we neglected the pressure dependence of the pre-exponential factors $\sigma_{n\infty}$, N_c, and $\langle v \rangle$ in Eqs.(1) to (3). From the pressure dependence of the DLTS peaks and of the capture rate, we obtained the pressure-induced shifts $\Delta(E_T+E_B)$ and ΔE_B as shown in Fig. 4. By a least-square fit of these data points to a straight line we obtained: $dE_B/dP = -2.1\pm0.4$ meV/kbar and $dE_T/dP = 0.8\pm0.4$ meV/kbar.

Recently Li and Yu[5] proposed a method for determining whether the large lattice relaxation (LLR) model of Lang and Logan[2] or the small lattice relaxation (SLR) model of Hjalmarson and Drummond[3] applies to a deep center. According to this method the pressure coefficient dE_B/dP given by:

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

(where $\varepsilon_S = E_S/E_T$ and E_S is the lattice relaxation energy as shown in Fig. 1) should be quite different for the two models. The reason is because in the LLR $E_S > E_T$ so that $\varepsilon_S > 1$ while in the SLR model $\varepsilon_S < 1$. In calculating dE_S/dP Li and Yu[5] used the equation:

$$dE_S/dP = -2E_S \, d\ln\omega/dP \qquad (5)$$

suggested by Barnes and Samara.[11] In Eq. (5) $\hbar\omega$ is the energy of the phonon in the MET and is usually assumed to be an optical phonon. However, for the DX centers in AlGaAs alloys Lang[8] has argued that the zone edge transverse acoustic (TA) phonon is involved in the mulitphonon emission. In GaAs the sign of $d\ln\omega/dP$ for the optical phonons is opposite to that for the TA phonon. In view of this uncertainty we do not use Eq. (5) to calculate dE_S/dP. Instead we note that in the same MET

$$\sigma_{n\infty} = \left(\frac{A}{E_T-E_S}\right)\left(\frac{4\pi E_B}{KT}\right)^{1/2} \qquad (6)$$

Barnes and Samara have found that $\sigma_{n\infty}$ is independent of pressure for the B traps in GaAs and we have found this to be true also for the PIDC in GaAs. Using this result and Eq. (6) we obtain the following expression for the pressure coefficient of dE_S/dP:

$$\frac{dE_S}{dP} = \frac{dE_T}{dP} - \frac{(E_T-E_S)}{2E_B}\frac{dE_B}{dP} \qquad (7)$$

Substituting the experimental values of $E_B = 0.22$ eV,

E_T=0.08 eV, dE_T/dP=0.8 meV/kbar and dE_B/dP= -2.1 meV/kbar into the above equations, we obtin the following results for the PIDC in GaAs at 29 kbar:

a) In the LLR model

$$dE_S/dP = -3.7 \text{ meV/kbar and } dE_B/dP = -1.3 \text{ meV/kbar.}$$

b) In the SLR model

$$dE_S/dP \doteq 1.116 \text{ meV/kbar and } dE_B/dP = -83 \text{ meV/kbar.}$$

Clearly the experimental value of dE_B/dP=-2.1 meV/kbar is more consistent with the LLR model than with the SLR model. Thus we conclude that our results on the PIDC in GaAs are completely consistent with the MET in which the defect has a large lattice relaxation similar to that proposed by Lang and Logan[2] for the DX centers in the AlGaAs alloys. In addition substituting our values for E_T and E_B into the LLR model we obtained the value of 1 eV for the lattice relaxation energy E_S.

Finally the small value of the pressure coefficient dE_T/dP we measured is not consistent with the suggestion that this PIDC level in GaAs is formed from the L conduction minima only. If this were true, dE_T/dP would be given by $dE_\Gamma/dP-dE_L/dP$= 6 meV/kbar. On the other hand since the PIDC in GaAs originate from substitutional donors, it shows that it is not necessary to invoke complexes involving donors and vacancies to have many of the properties of the DX center in AlGaAs alloys. The results presented in this paper should be taken into consideration in any theory attempting to explain the origin of the DX centers.

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FIGURE CAPTIONS

Fig. 1 Configuration coordinate diagrams for a defect center exhibiting (a) small lattice relaxation and (b) large lattice relaxation.

Fig. 2 DLTS spectra in two Si doped GaAs under pressure. These spectra were obtained with window times of t_1=1 ms and t_2= 0.5 ms while the width of the filling pulses was 10 ms.

Fig.3 Plots of the electron emission and capture rates versus temperature for the PIDC in two samples of GaAs under 29 kbar of pressure.

Fig.4 The pressure-induced shifts of E_B and E_T+E_B for the PIDC in GaAs versus pressure. The vertical and horizontal bars around the experimental points represent the estimated experimental errors. The straight lines drawn through the experimental points represent least square fits to the data points.

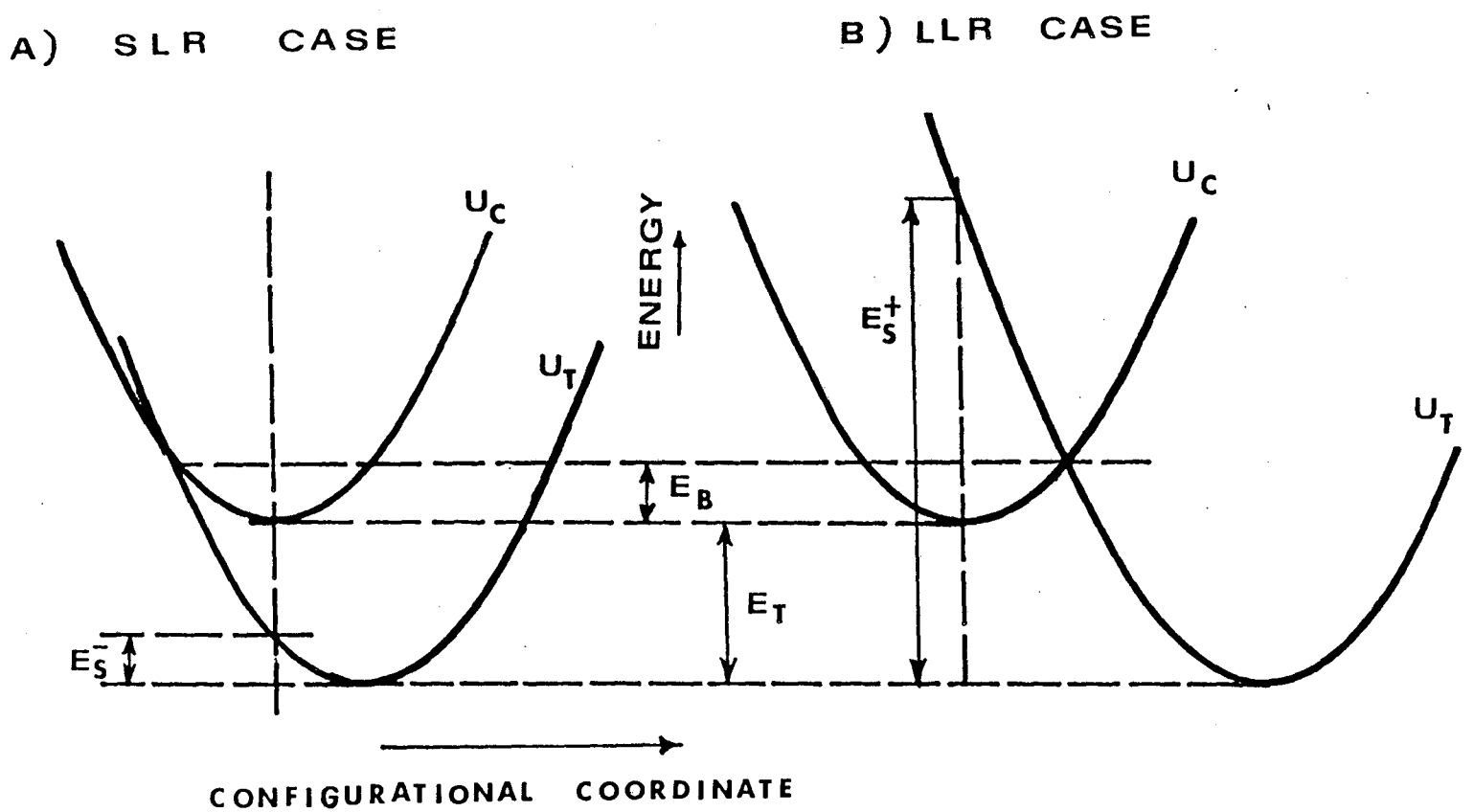
A) SLR CASE
B) LLR CASE
U_C
U_T
ENERGY
E_B
E_T
E_S^-
E_S^+
CONFIGURATIONAL COORDINATE

Fig. 1

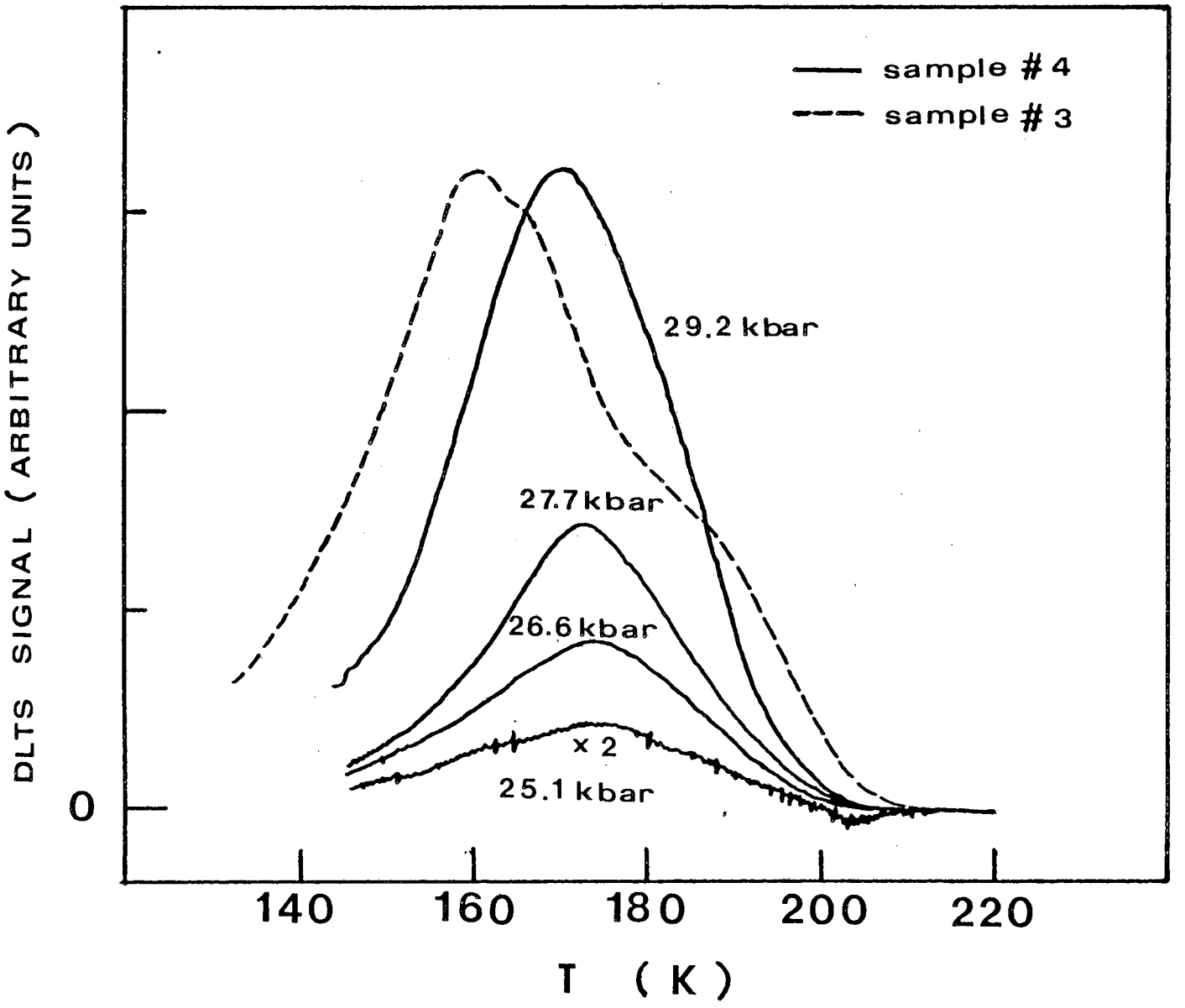
sample # 4
sample # 3
29.2 kbar
27.7 kbar
26.6 kbar
x 2
25.1 kbar
DLTS SIGNAL (ARBITRARY UNITS)
0
140
160
180
200
220
T (K)

Fig. 2

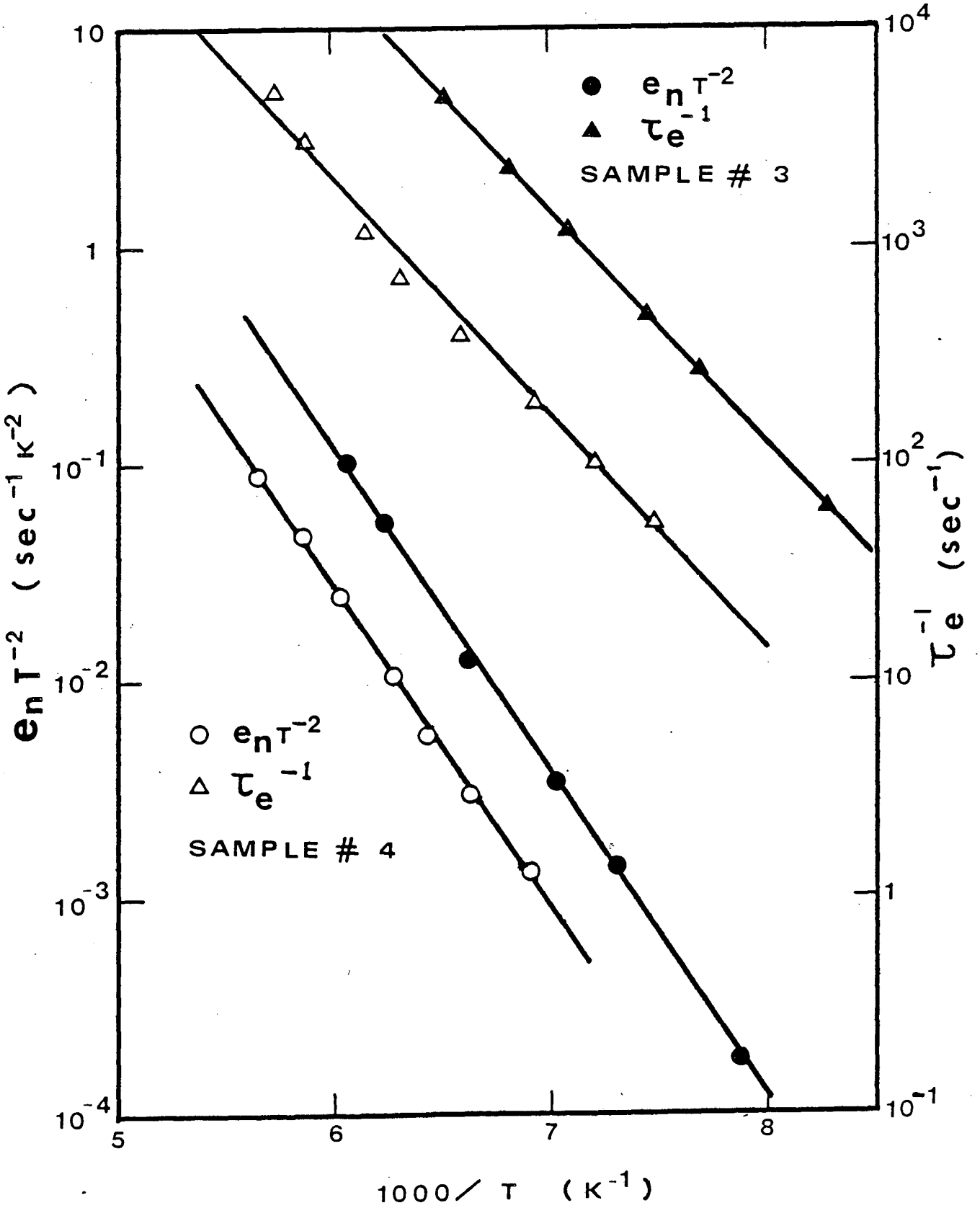
10
1
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{4}
10^{3}
10^{2}
10
1
10^{-1}
5
6
7
8
$e_n T^{-2}$ ($sec^{-1} K^{-2}$)
τ_e^{-1} (sec^{-1})
1000/ T (K^{-1})
● $e_n T^{-2}$
▲ τ_e^{-1}
SAMPLE # 3
○ $e_n T^{-2}$
△ τ_e^{-1}
SAMPLE # 4

Fig. 3

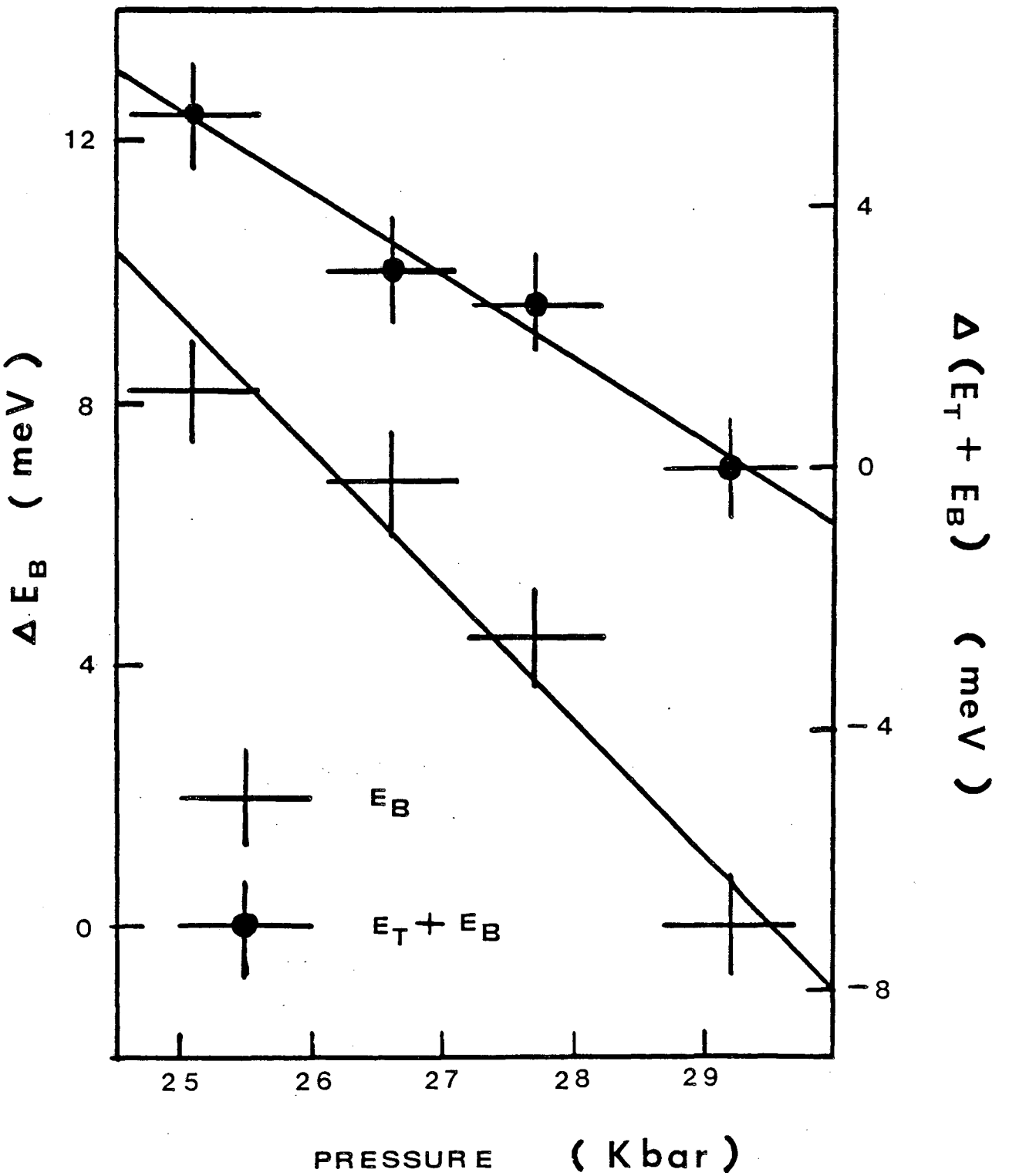
Δ (E_T + E_B) (meV)
4
0
−4
−8
Δ E_B (meV)
12
8
4
0
E_B
E_T + E_B
25
26
27
28
29
PRESSURE (Kbar)

Fig. 4

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