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DLTS investigation of deep levels in bulk GaAs under uniaxial stress

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Abstract. This work reports uniaxial stress DLTS measurements on the EL2, EL3 and EL6 levels in n-type bulk GaAs. The stress was parallel to the $\langle 111 \rangle$ axis. The defect state EL6 seems unaffected by stresses up to 1.5 kbar. EL2 exhibits a pressure coefficient of 1.3 meV kbar^{-1}. EL3 shows a low-stress (2.8 meV kbar^{-1}) and a high-stress (4.6 meV kbar^{-1}) pressure coefficient. Our results are discussed in connection with previously reported data published in the literature. An anomalous electric field dependence of the emission rate of the EL3 level is also reported.

1. Introduction

The DLTS technique has become a powerful experimental tool, especially in studying quantitative aspects of defects in semiconductors. However, DLTS alone could not provide information concerning the origin of the deep levels and the structure of the corresponding defects. These inherent limitations of the technique could be, in general, overcome by studying the defects under uniaxial stress. In particular, pressure modifies deep-level potentials allowing access to structural information. Changes in the shape and the position of a peak in the DLTS spectra when a stress is applied could furnish valuable information about the symmetry properties of the associated wavefunction, the defect-lattice interaction and even the microscopic structure of the defect.

GaAs is a very important material both from the theoretical and the technological point of view. Nevertheless, the present understanding of the deep levels found in this material is rather limited and incomplete. Even the identity of the well investigated EL2 defect, which is always present in bulk and VPE (vapour phase epitaxy) GaAs, significantly affecting their properties, is not irrevocably known [1]. The main scope of this communication is to report uniaxial stress DLTS investigations on the EL2, EL3 and EL6 deep levels of GaAs.

2. Theory

General detailed-balance considerations yield the following expression for the electron emission rate e_n of deep levels

$$e_n = \sigma_n \langle v_n \rangle N_c g^{-1} \exp(-E/kT) \quad (1)$$

where σ_n is the electron capture cross section, v_n is the average electron thermal velocity, N_c is the effective density of states at the bottom of the conduction band ($\langle v_n \rangle N_c$ is proportional to $m_n T^2$ where m_n is the density of states effective mass), g is the degeneracy and $E = E_C - E_T$, the energy separation between the trap level and the lowest conduction-band minimum.

Assuming that the capture cross section and the density of states effective mass are essentially pressure independent the energy shift $\Delta E = E(P) - E$ of a trap level with pressure could be safely found [2] by using the well known expression

$$\Delta E = kT \ln \frac{e_n}{e_n(P)}. \quad (2)$$

In the case that the effect of stress on the density of states effective mass cannot be considered negligibly small one should use the more general expression (see appendix A)

$$\Delta E = kT \ln \frac{e_n}{e_n(P)} + kT \frac{dm_n}{m_n}. \quad (3)$$

Thermal emission measured by DLTS takes place to the lowest conduction band minimum which is Γ in the case of GaAs. This minimum does not split under uniaxial stress but it is lifted up by a rate of 12.6 meV kbar^{-1} relative to the valence band maximum [3]. If a deep level is coupled completely to one of the conduction band minima (i.e. its wavefunction is constructed entirely from

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functions belonging to that minimum) it should show the same splitting and movement as the corresponding band.

The following table shows the theoretically [4] expected energy changes in meV under 1 kbar stress for X-related and L-related levels under uniaxial stress in the ⟨111⟩ crystallographic direction:

X-like	L-like	
4.7	−1.6	high-energy stress-split component (triplet)
	2.4	centre of gravity
	14.4	low-energy component (singlet)

If a level is not purely X-like, L-like or Γ-like etc then its movement is a mixture of that of the bands.

We could in general distinguish between two kinds of splitting. A point defect in a crystal may populate a set of equivalent sites or orientations, each of them having its own symmetry. Hence, as a whole, such a defect is characterized by low symmetry and could be represented by an arrow. This arrow can point to different directions in the lattice. If a stress is applied in one crystallographic orientation, traps pointing to this direction react differently from others in perpendicular directions. Therefore the 'orientational degeneracy' is lifted by the stress (e.g. the A centre in Si [5]). In this case transitions between the different kinds of traps are not probable because of their distance in real space, so emissions from different traps to the conduction band are detected (with different activation energy). To demonstrate the second kind let us take the example of a trap with high symmetry (e.g. spherical potential). In this case all of the traps react to the stress in the same way. The ground state degeneracy can be lifted by the stress. The different split levels belong to the same trap, therefore the transition from one stress-split state to the other can have a high probability. Only the second case is considered in the following, since from the experimental results cited in the literature cases where the initial peak splits into two peaks under stress, as for example the A centre in Si [5], have not been reported so far for the EL2, EL3 and EL6 defects of GaAs.

3. Experimental details

n-type bulk GaAs Schottky diodes were used. The samples had a typical geometry of 2 × 2 × 6 mm. Their longest dimension was in the ⟨111⟩ crystallographic direction. From C–V profiling the shallow doping level of the material was found to be $N_D = 6 \times 10^{16}\,\mathrm{cm}^{-3}$. N_T/N_D (N_T is the trap concentration) was calculated to be about 10^{-1} for EL2 and EL6 and about 10^{-2} for EL3.

A bath-type compound-lever uniaxial stress cryostat was built for the investigations, with a force magnification of 35. To avoid breaking the samples the maximum applied stress was limited to 1.5 kbar. Its direction was parallel to the long axis ⟨111⟩ of the samples. Isothermal DLTS technique [6] was used to investigate the influence of stress on the emission process. In the above technique the sample is held at a constant temperature and the rate window (v) is scanned. The temperature was adjusted in such a way that the emission rate was adequately high, allowing a short measuring time for a DLTS spectrum. Immediately before and after every scan a measurement at zero stress was carried out to allow the accurate observation of stress effects. In this way the influence of the long-term temperature change could be eliminated. (In the case of a 0.6 eV trap such as the EL3 level, at room temperature, a 0.1 meV change in energy corresponds to a 0.05 K change in temperature. The short-time (60 s) temperature stability of our cryostat was better than 0.05 K.)

The isothermal DLTS technique was also used to measure the influence of the electric field on the emission of the carriers. A double-pulse sequence of a filling pulse V_1 followed by a clear pulse V_2 was applied. The difference in the two pulse amplitudes was chosen to be sufficiently small to allow us to consider unchanged electric field strength in the investigated section of the space-charge region.

4. Results and discussion

Figure 1 shows a typical DLTS spectrum due to majority carrier traps for the samples used in the present study. Three peaks with corresponding activation energies $E_c = 0.80$, 0.60 and 0.34 eV have been identified as EL2, EL3 and EL6 respectively by comparisons of their Arrhenius plot (e_n/T^2 against $1/T$) signatures with those reported in the literature [7].

Figure 2 shows the variation of the activation energy of EL2 as a result of the applied stress. The estimated coefficient is 1.3 meV kbar^{-1}. This value is larger than the previously reported values of 0.8 meV kbar^{-1} [8] and 0.9 meV kbar^{-1} [9] but consistent with hydrostatic pressure data of 3.8 meV kbar^{-1} [10]. Energy shifts by hydrostatic pressure are expected to be larger by a factor of three than the uniaxial stress shifts.

Deviations in the reported values of the pressure coefficient found in the literature might be due to the different experimental techniques used and the special difficulties of these delicate experiments. We consider our isothermal DLTS measurements to be very accurate and

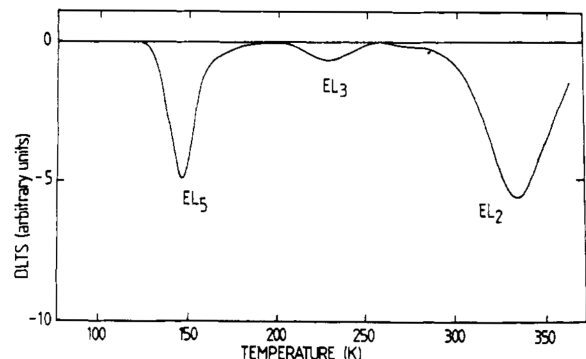

Figure 1. Typical DLTS spectrum of our samples from n-type bulk GaAs ($e_n = 2.5\,\mathrm{s}^{-1}$).

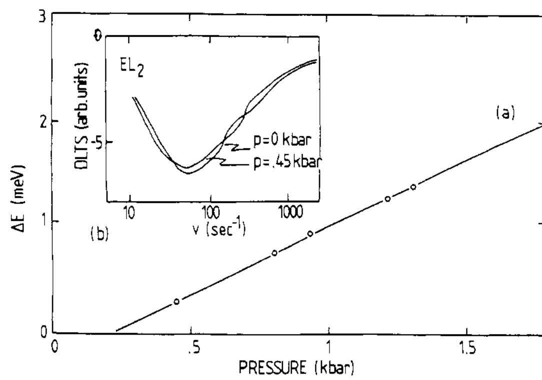

Figure 2. The variation of the activation energy of EL2 as a function of ⟨111⟩ uniaxial stress. In the inset are shown isothermal (T = 384 K) DLTS spectra of EL2 with (P = 0.45 kbar) and without the application of stress.

trustworthy. For EL2 in particular it is common knowledge that it is not a unique defect but a family of defects, and thus various authors may not refer to exactly the same defect structure. The inset of figure 2 shows two DLTS spectra for EL2 without stress and under uniaxial stress. Simultaneously with the shift in peak position a monotonic decrease in amplitude was also observed, which might indicate changes in the electron occupancy of the level under stress.

Figure 3 presents the variation of the activation energy of EL3 with stress. The inset demonstrates two DLTS spectra of EL3 taken with and without stress. A significant outcome of the present study is the shape of $E = E(P)$ in figure 3, indicating that the pressure coefficient is not the same at 'high' and 'low' stresses. On physical grounds, one intuitively expects that the variation of E with pressure is not precisely linear. Deep levels are characterized by strong potentials which act to localize the electronic wavefunctions near the sites of defects. Such potentials are dominated by short-range forces which are strong functions of the interatomic separation. A change of pressure results in the change of the interatomic separation which in general may enhance

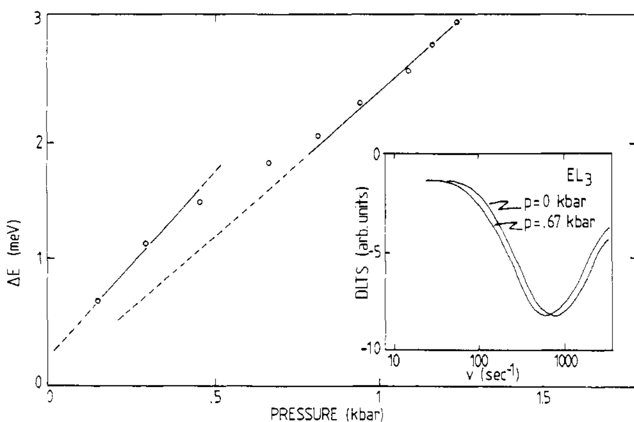

Figure 3. The variation of the activation energy of EL3 as a function of ⟨111⟩ uniaxial stress. In the inset are shown isothermal (T = 296 K) DLTS spectra of EL3 with (P = 0.67 kbar) and without the application of stress.

the electron–lattice coupling thus increasing the localization of the electronic wavefunctions. Hence, $\partial E/\partial P$ the pressure coefficient may not be the same at various pressures.

In an attempt to explain the above results we have distinguished two cases: the high-stress case, where the energy separation between the stress-split components is much higher than the thermal energy kT, and the low-stress case, when this separation is of the order of kT or less. In the high-stress case the emission from a low-energy stress-split component can take place in two ways: in one step to the conduction band or in two steps, first to the high-energy component and then to the conduction band. The two- (or more) step process is more probable, so practically all observed emission takes place through the highest split level. Therefore only the high-energy stress-split component is seen in high-stress measurements. (Most of the published uniaxial stress DLTS data were taken in high-field conditions.) Let us now consider the low-stress case. If the stress-split components are close to each other, a direct transition of carriers takes place from any of the levels to the conduction band. In this case the observed change in the energy is the average of the movement of the different stress-split components. The low-stress condition is realized only as an asymptotic case.

In the measured results the transition from the low-stress case to high-stress case appears as follows: the starting slope of the curve is determined by the movement of the centre of gravity of the multiplet, and then with increasing stress the ratio $\partial E/\partial P$ decreases, the new slope is determined by the movement of the high stress-split component relative to the Γ minimum.

The high-stress slope is 2.8 meV kbar^{-1} in complete agreement with the result of reference [8]. The starting slope (low stress) is 4.35 meV kbar^{-1}. If the influence of the stress dependence of the effective mass is taken into account, then (see appendix B)

$$\partial E/\partial P = 4.35 + 0.22 \text{ meV kbar}^{-1} \approx 4.6 \text{ meV kbar}^{-1}.$$

On the basis of this result we can conclude that the EL3 level splits under uniaxial stress in the ⟨111⟩ crystallographic orientation. The stress dependence of the centre of gravity of the stress-split levels corresponds to the theoretical prediction for X-like centres (4.7 meV kbar^{-1}). This is supported by the conclusion of reference [8] based on results measured in the ⟨100⟩ direction. It is important to note that the saturation straight line goes close to the origin, as is expected.

Figure 4 shows the electric field dependence of the emission rate of EL3, indicating an anomalous behaviour at low fields. It must be pointed out that besides the well known Poole–Frenkel effect, other mechanisms have also been suggested to explain the enhancement of the emission rate as a function of the electric field. Among them, phonon-assisted tunnelling [11,12] has been used to interpret the anomalous variation of the carrier emission rate at low fields. However, the results of figure 4 could also be successfully explained by simply considering the Poole–Frenkel effect, taking into account that

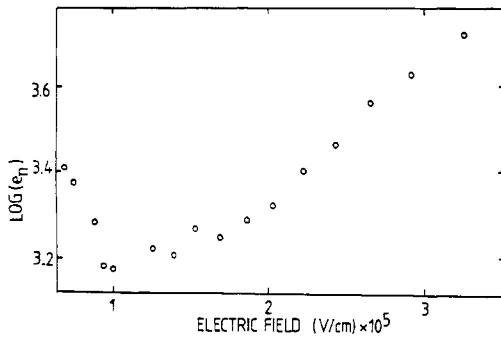

Figure 4. Changes in the electron emission rate of EL3 as a function of the applied electric field.

parallel to the emission process recapture from the Debye tail also takes place [13]. The latter mechanism becomes significant for low fields where the investigated interval of the depletion layer is near to the edge region.

As far as EL6 is concerned virtually no stress dependence (figure 5) was observed in the range up to 1.5 kbar. The shape (i.e. height and half-width) of the corresponding peak was unchanged. Its position in the spectrum was virtually unaffected within experimental error, which is a proof that this level is coupled to the Γ minimum. Notably, there are some inconsistencies and conflicting results in the previously published data concerning the behaviour of EL6 under pressure. Values of the pressure coefficient as 1.8 meV kbar^{-1} [9] and 7.1 meV kbar^{-1} [14] have been given. No stress-induced effects [15] have also been reported, and this has been considered as an indication that the point defect may have the full site symmetry of the lattice. We ascribe the above discrepancies to similar reasons as mentioned previously for EL2.

Some additional remarks should be made. As is known, small values of the pressure coefficient are typical for shallow levels. However, in view of the diversity of the experimental results for EL6 as cited in the literature it seems premature to draw any definite conclusion. In contrast with this level, EL2 and EL3 are characterized by large pressure coefficients indicating deep centres with highly localized wavefunctions and short-range potentials. The positive values of the pressure coefficients indicate that the emission of the electrons from the latter two levels is accompanied by lattice expansion [16].

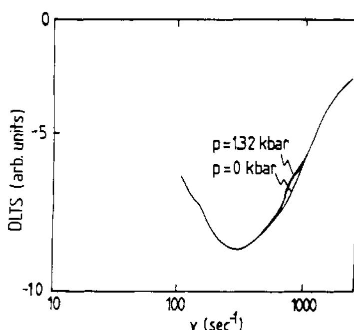

Figure 5. Isothermal (T = 186 K) DLTS spectra of EL6 with (P = 1.32 kbar) and without the application of stress.

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Appendix A

In the case of pressure dependence of the density of states effective mass m_n we can write for the electron emission rate

$$e_n = \sigma_n \langle v_n \rangle N_c g^{-1} \exp(-E/kT) \propto m_n T^2 \exp(-E/kT)$$

if $e_n(P)$ is the emission rate under the stress P then

$$e_n(P) = \sigma_n \langle v_n \rangle N_c g^{-1} \exp(-E(P)/kT) \propto m_n(P) T^2 \exp(-E(P)/kT).$$

From these two we obtain

$$\frac{e_n}{e_n(P)} = \frac{m_n}{m_n(P)} \exp(\Delta E/kT)$$

where $\Delta E = E(P) - E$ or

$$\frac{e_n}{e_n(P)} = \left(1 + \frac{dm_n}{m_n}\right)^{-1} \exp(\Delta E/kT)$$
$$= \exp\left[-\ln\left(1 + \frac{dm_n}{m_n}\right)\exp(\Delta E/kT)\right]$$
$$\simeq \exp\left(-\frac{dm_n}{m_n}\right)\exp(\Delta E/kT)$$
$$\simeq \exp\left[\left(\Delta E - kT\frac{dm_n}{m_n}\right)\Big/ kT\right].$$

Hence

$$kT \ln(e_n/e_n(P)) \simeq \Delta E - kT\frac{dm_n}{m_n}.$$

Appendix B

The variation of m_n under uniaxial stress is given by the expression

$$\frac{dm_n}{m_n} = \frac{1}{3}\left(\frac{dm_l}{m_l} + 2\frac{dm_t}{m_t}\right)$$

where m_t and m_l are the transverse and the longitudinal masses respectively. Under 3.33 kbar maximal stress the change in the effective mass in GaAs in different crystallographic orientations is as follows (reference [4]):

$$\langle 100 \rangle (dm_n/m_n)_l = -0.0076$$
$$(dm_n/m_n)_t = 0.0469$$
$$\langle 111 \rangle (dm_n/m_n)_l = 0.03$$
$$(dm_n/m_n)_t = 0.024.$$

From these values we get the change in the density of states effective mass $dm_n/m_n = 0.00864\ \text{kbar}^{-1}$ in both crystallographic directions. In DLTS measurements it appears as an 0.22 meV kbar^{-1} decrease in the measured activation energy at room temperature. Therefore this change should be taken into account in the interpretation of the results.

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