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LATTICE DEFECTS IN GaAs SUBJECTED TO MECHANICAL STRESSES

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Some of our recent results obtained with the DLTS method concerning lattice defects in GaAs depending on mechanical stresses are presented and discussed.

1. Introduction

Undoubtedly, dislocations are the most important stress-dependent defects in semiconductors. Usually, dislocations are generated during the crystal growth owing to thermally induced stresses. They can also be introduced into the crystal by artificial plastic deformation. Roughly above 2/3 of the melting point of a crystal, dislocations become essentially mobile and multiply themselves during the motion thus giving rise to an enhancement in their density.

Crystals can also be subjected to high mechanical stresses at low temperature under conditions of ultrasonic vibration. It is a feature of II–VI and III–V semiconductor compounds that ultrasound can induce some defect reactions in those materials. This offers an interesting possibility of studying some complex defects, that we have just started to deal with.

The problem of electronic states induced by dislocations in semiconductor materials is as old as semiconductor electronics itself. Unfortunately, up to now any reliable results concerning this problem are still very scarce. The reason for such a situation is rather simple. In order to reveal properties associated with dislocations, one commonly makes experiments with plastically deformed samples. But during the plastic deformation a huge number of point defects is also generated in a crystal. Electrical activity of those defects usually hides the effects originating from dislocation cores.

At this point one might doubt whether it is of any practical importance to study electrically active centres which represent a hidden minority in a crystal. But dislocations are exceptional defects in semiconductors. They are mobile and strongly interact with all other kinds of defects in a crystal eventually affecting its overall properties. It is essential that dislocation mobility depends on an electric charge carried on by a dislocation. The dislocation charge can also affect directly some properties of semiconductor devices. For instance, the charge accumulated at misfit dislocations at heterostructure interface can disturb the potential profile across the structure. The amount of dislocation charge depends on the positions of both the Fermi level and just the energy levels of dislocation core states in the band gap of a semiconductor.

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2. GaAs subjected to plastic deformation

GaAs is probably the only semiconductor for which we gathered the most reliable information on the electrical properties of dislocations. The first direct observation of dislocation-related level in the band gap of GaAs was done by Wosiński with the DLTS method [1]. He discovered in plastically deformed (at 400 °C) single crystals of n-type GaAs a hump on the low-temperature slope of the dominant peak associated with the EL2 trap (Fig. 1). He was able to deconvolute the as-observed DLTS peak into two separate peaks: one characteristic of EL2 and the other, called ED1, induced by plastic deformation. An apparent energy level of ED1 is $E_c - 0.68\ (\pm 0.01)$ eV.

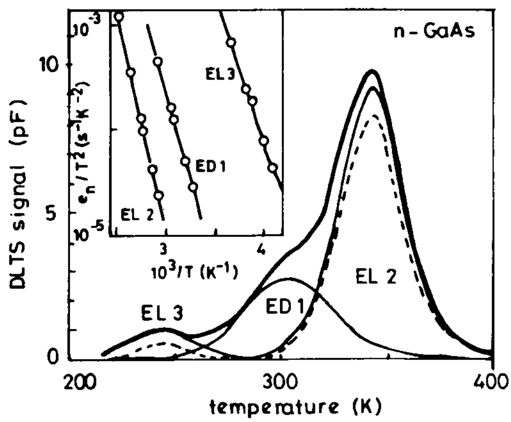

Fig. 1. DLTS spectra of undeformed (dashed line) and plastically deformed to the strain 3.4 % (thick solid line) n-type samples, recorded at a rate window 2.5 s^{-1}. Deconvoluted peaks of the latter spectrum are drawn with thin solid lines. Thermal activation plots of the electron emission rates are shown in the inset

This ED1 trap exhibits specific properties which allow to relate it with introduced dislocations. Firstly, the amplitude of the DLTS signal of ED1 shows a peculiar dependence on the filling time of the traps with electrons. Over six decades of the filling time the signal amplitude increases linearly with the logarithm of this time (Fig. 2). This non-standard behaviour points out that the ED1 traps are arranged in such a way that the Coulomb interaction between electrons captured at different traps limits their population. That is typical for dislocations where traps are arranged along a line. Furthermore, the concentration of ED1 traps is in accord with the concentration of possible core states of dislocations. Additionally, the DLTS peak of ED1 is essentially broadened suggesting probably the existence of one-dimensional energy bands at dislocations.

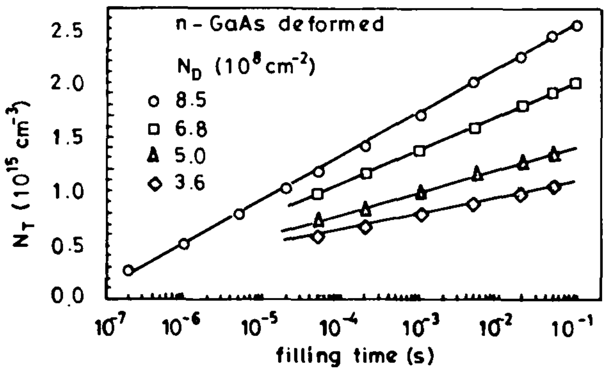

Fig. 2. Concentrations of electrons trapped at ED1 traps vs filling pulse duration time measured in plastically deformed n-type samples with different dislocation densities shown in the Figure

Later on, another deformation-induced DLTS peak, called HD1, was revealed by Wosiński in p-type GaAs [2] (Fig. 3). This hole trap exhibits similar properties as ED1 does, which enables one to relate it also to dislocation states. An apparent energy level of HD1 is $E_v + 0.37$ (± 0.01) eV.

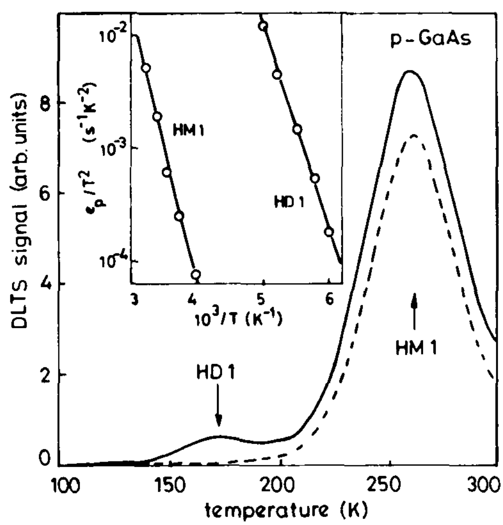

Fig. 3. DLTS spectra of undeformed (dashed line) and plastically deformed to the strain 2 % (solid line) p-type samples, recorded at a rate window 17 s^{-1}. Thermal activation plots of the hole emission rates are shown in the inset

Additionally, we looked for an electrical activity of dislocations introduced into GaAs by micro-indentation [3]. To avoid any disturbing effects of EL2, we used in the experiment an n-type GaAs thick layer grown by liquid phase electro-epitaxy (LPEE) which was completely free of EL2. Indentations were performed as in the microhardness test. An array of 10×10 indents separated from each other by a distance of 100 μm was made on the surface of the sample at a temperature of 250 °C in air. A gold disc was evaporated onto the indented area to form a Schottky diode. DLTS measurements performed with this diode revealed just the ED1 trap at a concentration of about 10^{13} cm^{-3} as a dominant deep trap introduced by the indentation (Fig. 4).

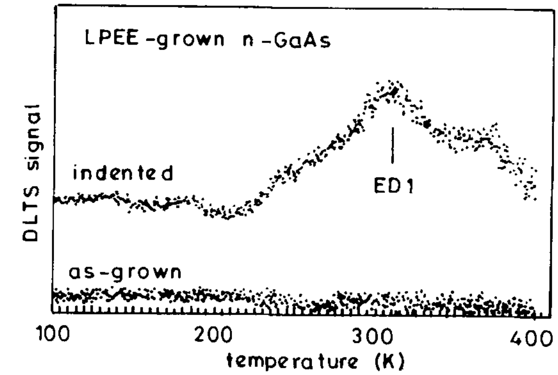

Fig. 4. DLTS spectra of LPEE-grown n-type GaAs recorded at a rate window 11 s^{-1}. Lower spectrum corresponds to as-grown sample and the upper one to the sample subjected to local plastic deformation by micro-indentation

Thus we believe that the ED1 and HD1 traps correspond to dislocation core states and a question arises as to which particular types of dislocations the traps belong. In the samples investigated by us always the 60° dislocations dominated and therefore we have a choice between α and β dislocations, if to ignore a complication resulting from dissociation of dislocations into partials. It is commonly accepted that real dislocations in III–V's correspond to the so-called glide set. Then α and β dislocation means that an extra atomic half-plane of the dislocation terminates with arsenic and gallium atoms, respectively.

Recently, we have proposed the following correspondence between the traps and dislocation types: ED1 $\Leftrightarrow$ α dislocation, HD1 $\Leftrightarrow$ β dislocation [3]. Such a conclusion is consistent with recent results obtained by Watson et al [4]. They observed deep level states induced by misfit dislocations created between InGaAs and GaAs layers grown by MOCVD method. They could change the density of α and β dislocations separately by altering the size of rectangular mesas fabricated from the structure. Using the DLTS method they found an electron trap with an energy level at 0.58 eV below the conduction band edge, which had features characteristic of dislocations and whose concentration correlated with the density of α dislocations. Although this level is 0.1 eV shallower than the ED1 level in GaAs, we believe that both belong to a trap of the same nature.

The correspondence proposed by us is consistent with the results of photoplastic experiments performed by Maeda et al [5]. During the plastic deformation GaAs crystals were irradiated with an electron beam or illuminated with laser light generating electron–hole pairs. The authors observed radiation-induced changes in the dislocation velocities under applied stress at variable temperature. The principal results of those investigations are the following. In a low temperature range the activation energy for dislocation motion is essentially reduced by irradiation. This reduction depends on the type of dislocation involved: α, β or screw but it is independent of the irradiation intensity.

Let us recall that the dominating mechanism of dislocation motion in III–V crystals is glide actuated by kink-pair formation and subsequent kink migration along the dislocation lines. Both of these elementary steps of dislocation motion are thermally activated processes. Consequently, the photoplastic effect described above can be considered as a recombination-enhanced process of kink formation and migration [6]. It means that an energy released in the electron–hole recombination event at a dislocation assists to overcome the potential barrier for kink formation and migration. Then the observed activation energy for dislocation motion should be reduced by the amount of released energy.

Maeda et al [5] obtained the following irradiation-induced reduction of the activation energy for dislocation motion: 0.7 eV for α dislocations, and 1.1 eV for β dislocations. These values coincide very well the energies which are expected to be released in nonradiative recombination events occurring via the ED1 and HD1 trap levels, respectively.

It is worth paying attention at the end of this part of the paper to recent results by Jones et al [7] concerning the theoretical examination of electronic structure of dislocations in GaAs, using an *ab initio* density functional cluster method. This work predicts the positions of dislocation energy levels that are in general accord with those obtained in our experiments.

3. GaAs subjected to ultrasonic vibration

Now we pass to the effect of high-intensity ultrasonic vibration on the spectrum of deep traps in GaAs [8]. Since GaAs is a brittle material at low temperature, our samples were subjected to ultrasonic vibration under a high hydrostatic pressure of 1 GPa to avoid their possible fracture. The investigated samples were put in an ultrasonic resonator, operating at 17.5 kHz, combined with a high-pressure vessel. The samples prepared from n-type HB-grown single crystal were subjected to ultrasonic vibration of different amplitudes for 600 s at a temperature of 0 °C.

In as-grown samples there were three deep electron traps detectable with DLTS, labeled EL2, EL3 and EL6 according to the conventional notation. In the samples subjected to the vibration the concentration of the EL6 traps was strongly reduced and two new traps, EL5 and EL18, appeared, while the concentration of the EL3 traps increased.

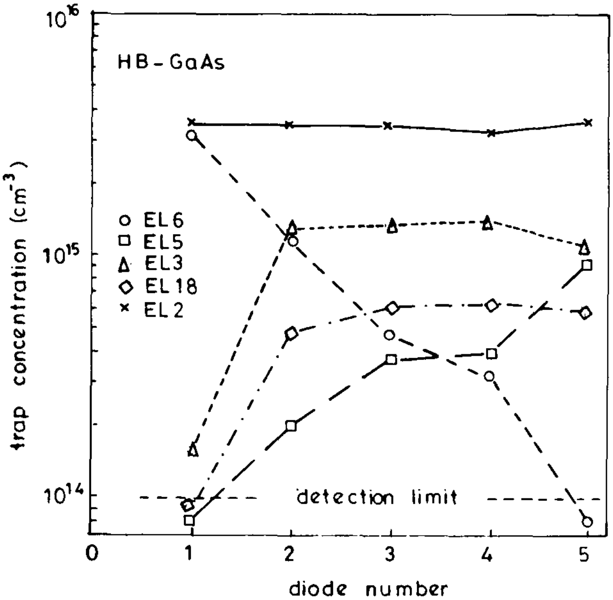

Fig. 5. Concentration of deep electron traps measured with DLTS in the reference diode (number 1) and the diodes subjected to increasing amplitude of the ultrasonic vibration (numbers 2 to 5)

In Fig. 5 the concentrations of deep traps are presented as a function of the diode number. The diode #1 represents the reference sample and the numbers from 2 to 5 correspond to the diodes subjected to increasing amplitude of the ultrasonic vibration. Only the EL2 concentration was not affected by the ultrasonic treatment. The EL6 concentration decreased monotonically with increasing ultrasonic stress applied and the concentration of three other traps, EL3, EL5 and EL18 increased at its expense. It means that the sum of the concentrations of all these traps remains almost unchanged during the ultrasonic treatment. These results point out a transformation of the EL6 traps into the EL5, EL18 and EL3 traps driven by the ultrasonic vibration. This finding, together with the data known from the literature, allows us to speculate on the microscopic nature of the defects associated with the observed traps.

It is well established that EL6, like EL2, is related to excess arsenic. To explain consistently our present results we postulate that EL6 is a complex defect composed of As anti-site and As vacancy: As_{Ga}–V_{As}. The EL3 trap has been recently identified as a defect associated with an off-centre oxygen atom in place of arsenic: O_{As}.

Further, we postulate that the defect responsible for EL5 is a divacancy complex V_{Ga}–V_{As}, and EL18 corresponds to a Ga vacancy, V_{Ga}. The energy levels of these defects, calculated theoretically using the self-consistent Green's function method by Baraff and Schlüter [9], are in accordance with the thermal activation energies obtained from DLTS measurements.

With these assumptions, the transformation of the EL6 trap into three other traps occurring under the ultrasonic treatment can be explained by the following defect reactions:

$$\begin{aligned} &As_{Ga}\text{–}V_{As} \rightarrow V_{Ga}\text{–}V_{As} + As_i, \\ &As_{Ga}\text{–}V_{As} + O_i \rightarrow O_{As} + V_{Ga} + As_i. \end{aligned}$$

The EL5 traps are produced in the first reaction, and both the EL3 and EL18 traps are produced in the second one. Arsenic interstitials, As_i, which are produced in both reactions are highly mobile, and probably quickly diffuse out from the bulk to some sinks, such as the sample surface and dislocations. The rate of the second reaction is limited by interstitial oxygen, O_i, which is not electrically active in GaAs.

To complete this part of the paper, it is proper to add that although we have not found any influence of ultrasonic treatment on the concentration of EL2, there is in fact an effect of ultrasound on the properties of this defect. Recently, Buyanova et al [10] investigated regeneration of EL2 from metastable to normal state under conditions of ultrasonic vibration. They found that in that case the regeneration occurs at a much lower temperature than without ultrasouund. This result is interpreted in terms of ultrasound-induced oscillations. These oscillations generate an alternating strain field, in particular nearby the EL2 centres. As a consequence, the local compressions reduce the energy barrier for the metastable-to-normal transition in the same way as under hydrostatic pressure. In a similar way the present authors have explained an unquenchability of some EL2 centres by the static strain field of dislocations [11].

In conclusion, we have identified with a high reliability two important core-state levels of dislocations in GaAs. Further, we have demonstrated that by subjecting GaAs to ultrasonic vibration one can learn much about the structure of complex defects in this compound.

Acknowledgement

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