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THE SYMMETRY OF THE EL2 DEFECT IN THE METASTABLE STATE

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We measured recovery of the optical absorption of EL2 under [100] and [111] uniaxial stress during heating of the crystal. The recovery step, occurring at about 45 K in *n*-type GaAs, splits into two components under [111] stress, and no splitting is observed under [100] stress. The same behavior under uniaxial stress shows the recovery occurring at 125 K in semi-insulating GaAs. A fraction of centers recovering at lower temperature can be altered by excitation of metastability with polarized light or by excitation under stress. These results indicate that EL2 in the metastable state is trigonally distorted from the tetrahedral symmetry of the ground state.

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The native deep donor EL2 in GaAs is technologically important and has the rare property of undergoing, at low temperatures, an optically induced transition from a normal to a metastable state. Piezospectroscopic investigations [1, 2] of the 1.039 eV no-phonon line of the EL2 defect indicated that EL2 has tetrahedral T_d symmetry in its normal configuration. Recent measurements [3] of a narrow luminescence line at 703 meV due to EL2 performed under uniaxial stress confirm this symmetry, supporting the isolated arsenic antisite As_{Ga} model of the normal state of EL2. Until now there was no experimental data on the symmetry of the metastable configuration of EL2. To determine that, we have measured thermal recovery of the optical absorption of EL2 under [100] and [111] uniaxial stress during heating of the crystal.

The near-infrared absorption due to the normal state of EL2 can be bleached by illumination of the crystal at helium temperature with light of energy 1.0 to 1.3 eV [4], i.e. from the band of intracenter transitions of EL2 [5]. The absorption recovers when the crystal is heated above 125 K in the case of semi-insulating (SI) GaAs, and above 45 K in the case of *n*-type GaAs [6]. The metastability is attributed to a large lattice relaxation following optical excitation of the defect.

In the experiments *n*-type ($n \approx 10^{16} \text{ cm}^{-3}$) and SI GaAs single crystals were used. Typical sample dimensions were $2 \times 2 \times 7 \text{ mm}^3$ with the long axis oriented along [111] or [100] crystallographic direction to within 1° by the X-ray back-reflection Laue technique. The sample was placed in an uniaxial stress apparatus in an optical cryostat. The transmission of the sample was measured with

a low intensity light with a wavelength of $1 \mu\text{m}$. The experimental procedure was as follows. The sample was first cooled to 10 K in the dark, after which the EL2 was excited to the metastable state by illumination with white unpolarized light. Uniaxial compressive stress was then applied. Finally, the recovery of the EL2 absorption was investigated during heating of the sample at a rate of approximately 5 and 2.6 K/min for *n*-type and SI GaAs samples, respectively. After the EL2 had completely recovered, the stress was removed.

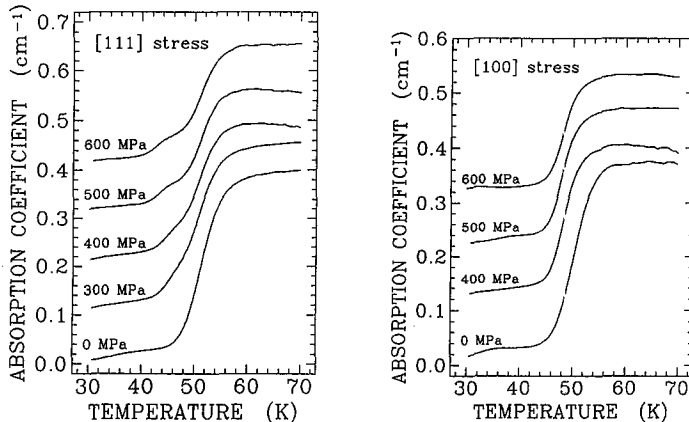


Fig. 1. Thermal recovery of the EL2 absorption in *n*-type GaAs under [111] and [100] uniaxial stress. Curves for different values of the stress are shifted vertically for clarity.

Figure 1 shows thermal recovery of the EL2 absorption for *n*-type GaAs under [111] and [100] uniaxial stress of selected values from 0 to 600 MPa. The recovery step starting at 45 K clearly splits into two components for large values of [111] stress and no splitting is observed under [100] stress. Qualitatively the same behavior is observed for the recovery step starting at about 125 K in SI GaAs. The observed splitting of the recovery is obvious evidence for an orientational degeneracy of EL2 in the metastable state. This follows from the fact that if the EL2 defect in the metastable state had T_d symmetry, then all the defects would be equivalent with respect to the stress and no splitting would be possible. The splitting into two components under [111] stress and lack of splitting under [100] stress indicates that EL2 in the metastable state has trigonal C_{3v} symmetry [7]. The numbers of EL2 defects recovering at lower and higher temperature under [111] stress amount to about 1/4 and 3/4 of the total number of defects, respectively. This implies that the defects recovering at lower temperature are oriented along the direction of the stress and those recovering at higher temperature are oriented aslant the direction of the stress.

We have also studied the effect of different methods of excitation of the metastability on the splitting of the recovery (see Fig. 2). The number of centers recovering at lower temperature (i.e. oriented along the stress) is increased when metastability is excited with light polarized parallel to the direction of stress, and

it is decreased when excitation is performed with light polarized perpendicularly. When excitation is performed under stress all the defects recover at higher temperature, i.e. are oriented aslant the direction of the stress. The ability of the defect to assume different orientations in the metastable state results from the T_d symmetry of the normal state. The defect prefers distortions in certain directions when it is excited with polarized light or when the excitation is performed under [111] stress which differentiates the distortion along the stress from the others.

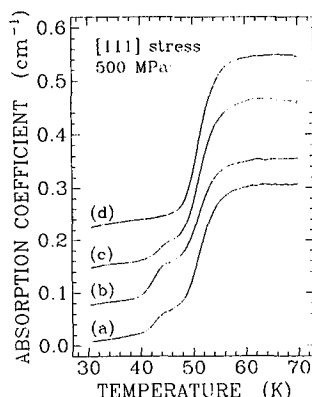


Fig. 2. Thermal recovery of the EL2 absorption in *n*-type GaAs under [111] uniaxial stress of 500 MPa. Curve (a) shows, for reference, the recovery after excitation of metastability with unpolarized light; curves (b) and (c) were obtained after excitation with light polarized parallel (b) and perpendicularly (c) to the direction of stress which was applied after the excitation; curve (d) was recorded after excitation performed under a stress of 500 MPa with unpolarized light. During excitation in cases (a), (b), and (c) no stress was applied.

Recent theoretical investigations [8–10] of the As_{Ga} support the original proposition [11] that a metastable state of C_{3v} symmetry is possible for this defect. According to these investigations, the metastable state is formed when the central As atom breaks one of its four As–As bonds and moves about 1.2 Å along [111] direction to an interstitial position. The metastable state is a tightly bound gallium-vacancy-arsenic-interstitial $V_{Ga}As_i$ defect pair of C_{3v} symmetry. Therefore, this model of the metastable state is in agreement with the presented experimental results.

In conclusion, on the basis of the studies of thermal recovery of EL2 under uniaxial stress, we have shown that the metastable state of EL2 is orientationally degenerate and has trigonal C_{3v} symmetry. The presented experimental results strongly support the attribution of the metastability of EL2 to the transformation of the isolated arsenic antisite As_{Ga} to a tightly bound gallium-vacancy-arsenic-interstitial $V_{Ga}As_i$ defect pair of trigonal symmetry.

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