Symmetry of the $EL2$ center in GaAs

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(Submitted 9 April 1991; resubmitted 12 May 1991)
Pis'ma Zh. Eksp. Teor. Fiz. **53**, No. 8, 548–553 (10 June 1991)

Optical absorption under conditions of uniaxial compression of GaAs single crystals makes it possible to identify the model of an $EL2$ center. In this model the charge states of a double donor (D°, D^+, and D^{++}) reveal a C_{3v} symmetry and are formed from the wave functions L, Γ, and X, respectively, of the conduction band valleys.

A deep double donor $EL2$ and GaAs ($D^\circ/D^+ \rightarrow E_c - 0.75$ eV–$EL2$ level, $D^+/D^{++} \rightarrow E_V + 0.52$ eV) is a system which constantly is being studied in various ways, since its presence in single crystals and epitaxial layers simultaneously accounts for the high mobility of the carriers and for the semi-insulating properties of the material.[1] The basis of $EL2$ center is the antistructure donor AsGa, which manifests itself in the total correlation of the spectral dependences of the "family" quenching (1.0–1.3 eV) of the photocapacitance, of the photoconductivity, and of the corresponding ESR spectrum.[1-3] According to the data on ESR, DENR, and piezocapacitive spectroscopy, the $EL2$ center is associated with the $\mathrm{As_{Ga}} + \mathrm{As}_i$ complex. As a result, it has a C_{3V} symmetry.[4-6] The results of experimental studies of the optical absorption under conditions of uniaxial compression of GaAs single crystals, which contain $EL2$ centers, are interpreted, however, on the basis of the model of an isolated $\mathrm{As_{Ga}}$ defect of the T_d symmetry.[7,8] The behavior of the 1.039-eV zero-phonon suggests that the optical transitions responsible for the quenching processes indicated above, which are attributable to the transition of the $EL2$ center to the metastable state, occur inside the center.[7] The nature of the metastable state and the symmetry of the $EL2$ center thus remain unresolved problems. In our study we have identified the model of the $EL2$ center on the basis of the data obtained in a multifaceted study of the optical absorption under conditions of hydrostatic and uniaxial compression of GaAs single crystals. A correlation has been established between the metastable properties and the symmetry of the various charge states of the deep-seated defect with a conduction-band structure.

Piezospectroscopic studies of the optical transmission (0.8–1.3 eV) of the n-type GaAs samples [$n(77\ \mathrm{K}) = 1.5\times10^{16}\ \mathrm{cm}^{-3}$], which were synthesized by the Bridgman method, were carried out at $T = 4.2$ K under conditions of hydrostatic and uniaxial compression. In the case of uniaxial compression we used GaAs single crystals ($3\times3.5\times7$ mm in size), whose longest side was oriented in the direction of one of the crystallographic axes ([111], [100], or [110]) and corresponded to the direction of compression. The measurements were carried out in parallel and perpendicular polarizations of light with respect to the direction of uniaxial compression. It should be noted that the intensity of monochromatic light was maintained at a high level in order to avoid a transition of the $EL2$ center to the metastable state.

In the course of the experiments we obtained optical absorption spectra (Figs. 1a

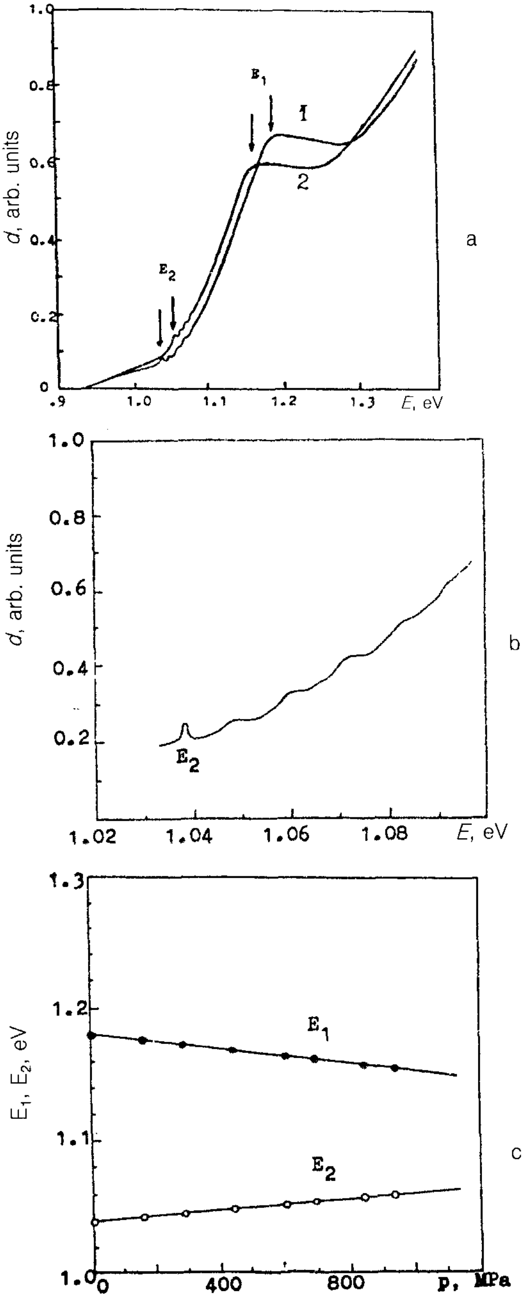

FIG. 1. GaAs: *EL* 2. (a) Optical absorption spectrum. 1—$p = 0$; 2—$p = 950$ Mpa; the arrows indicate the position of the optical transition to the metastable state (E_1) and the position of the zero-phonon line (E_1); (b) fragment of the optical absorption spectrum with a zero-phonon line (E_2); (c) the energies E_1 and E_2 versus the hydrostatic pressure. The solid lines were calculated on the basis of the data of Ref. 9.

and 1b), whose emission has made it possible to determine the changes in the energy positions of the zero-phonon line (at 1.039 eV) and of the optical transition of the *EL* 2 center to the metastable state (at 1.18 eV) as a function of the hydrostatic compression (Fig. 1c). We see that the energy of the optimal transition to the metastable state,

E_1 (in the 1.0–1.3-eV band) decreases with increasing pressure, while the zero-phonon line (E_2) shifts up the energy scale. The phonon repetition frequency (at 11 eV) in this case remains constant. The results we obtained are in good agreement with the data of Ref. 8 and show that the optical transitions (E_1 and E_2) are induced by different charge states of the $EL\,2$ center in GaAs. The magnitudes of the shifts ΔE_1 and ΔE_2 correlate completely with the corresponding changes in the energy gaps between the valleys of the conduction band[9] of GaAs (Fig. 1c): $\Delta E_1 = \Delta_{X\Gamma}(p)$ and $\Delta E_2 = -\Delta_{L\Gamma}(p)$.

Such a relationship between optical transition with a structure of the conduction

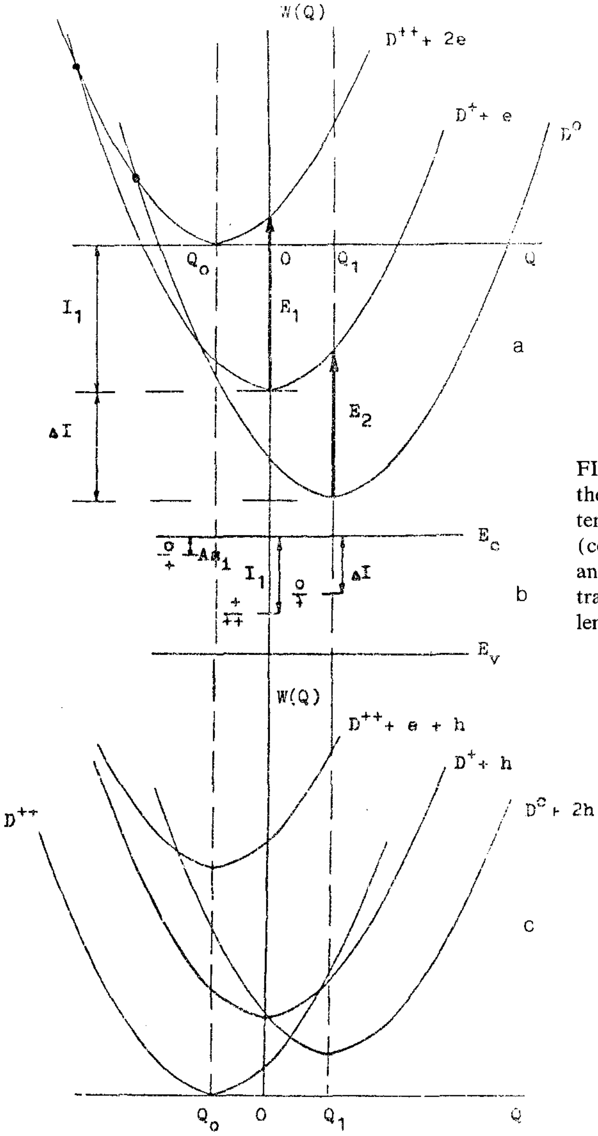

FIG. 2. Adiabatic potentials (*a* and *c*) of the different charge states of the $EL\,2$ center in a GaAs measured in the (defect)–(conduction band) optical transition (a) and a (valence band)–(defect) optical transition (c); $I_2 = I_1 + \Delta I$; (b) equivalent band diagrams; $Q \parallel [111]$.

band can be explained in the terms of the model of the deep center in which the electron-vibrational coupling constant depends nonmonotonically on the charge state and the spin state (Fig. 2). The deep-lying defect in this case is a tunnel system, in which the lattice sites of different charge states are characterized by different symmetries and belong to the corresponding valley of the conduction band. As applied to the $EL\,2$ center in GaAs, the D^{+} state occupies a lattice site and is formed from the wave functions of the Γ valley of the conduction band, while the D° and D^{++} states are situated in the tetrahedral and hexagonal interstitial lattice sites and belong to the L and X valleys, respectively (Fig. 2). In other words, the state $D^{\circ} = (\mathrm{As}_i V_{\mathrm{Ga}})^{\circ}$ has a C_{3V} symmetry, while the $EL\,2$ level is formed from the wave functions of the L valley. At first glance, D^{+} and D^{++} states should have T_d and D_{2d} symmetry, respectively. The symmetry of the D^{+} state is lowered, however, to C_{3V} symmetry because of restructuring of the nearest arsenic site $(\mathrm{As}_i V_{\mathrm{As}})$. This is reflected in the DENR data which identify the $EL\,2$ center as the $\mathrm{As}_{\mathrm{Ga}} + \mathrm{As}_i$ complex.[5] The symmetry of the D^{++} state also tends to C_{3V}, but now because of the Stark effect which is induced because of the presence of the compensating acceptors.[10] The optical transition $D^{\circ} \to D^{+}$, whose optimum corresponds to the zero-phonon line (Fig. 2a), is thus accompanied by a tunneling of the $EL\,2$ center from the tetrahedral interstitial site to the lattice site, which gives rise to intervalley scattering of electrons $[\Delta E_2 = -\Delta_{L\Gamma}(p)]$, which are photoexcited from the $EL\,2$ level to the L valley of the conduction band. This process manifests itself most clearly under conditions of hydrostatic compression of GaAs single crystals (Fig. 1c). An electron which is photoexcited to the Γ valley of the conduction band as a result of a D^{+}/D^{++} transition $[\Delta E_1 = \Delta_{X\Gamma}(p)]$ undergoes an intervalley scattering in a similar manner.

During continuous light pumping $h\nu = E_1$, two-electron capture processes,[10] which stimulate a transition of the residual concentration of singly charged $EL\,2$ centers to the metastable state, begin to dominate (Fig. 2a):

$$\begin{array}{l} D^{+} + h\nu(E_1) \to D^{++} + e \\ D^{++} + 2e \to D^{\circ} \end{array} \;\Big\|\; 2D^{+} + h\nu(E_1) \to D^{\circ} + D^{++}. \tag{1}$$

A transition to the metastable state is accompanied by an abrupt decrease in the lifetime of nonequilibrium carriers as a result of the formation of auxiliary Auger-recombination channels because of the presence of interstitial arsenic near the antistructure donor

$$\begin{aligned} &\mathrm{As_{Ga}}^{\circ} + \mathrm{As}_i^{\circ} + 2(e+h) \to \mathrm{As}_{\mathrm{Ga}}^{+} + \mathrm{As}_i^{+} + 3e + h \to \mathrm{As}_{\mathrm{Ga}}^{+} + \mathrm{As}_i^{\circ} + 2e + h \\ &\to \mathrm{As_{Ga}}^{\circ} + \mathrm{As}_i^{+} + 2e + h \to \mathrm{As_{Ga}}^{\circ} + \mathrm{As}_i^{\circ} + e + h. \end{aligned} \tag{2}$$

Such a superfast recombination of nonequilibrium carriers may account for the quenching of the photocapacitance, of the photoconductivity, and of the ESR spectra in GaAs with $EL\,2$ centers.[4–6] An adequate verification of the model of metastability of the $EL\,2$ center of GaAs turned out to be, on the one hand, the detection of the optical generation of the D^{+} state when $h\nu = E_g - E_1$ (Fig. 2c):[11]

$$\begin{array}{l} D^{++} + h\nu(E_g - E_1) \to D^{+} + h \\ D^{\circ} + h \to D^{+} \end{array} \;\Big\|\; D^{\circ} + D^{++} + h\nu(E_g - E_1) \to 2D^{+}, \tag{3}$$

and, on the other hand, a good agreement between the experimentally determined energy of thermal annealing of the metastable state[4] and the height of the energy barrier of the reaction $D^{\circ}+2h\rightarrow D^{+}+h$ (Fig. 2c) which is responsible for thermal generation of the D^{+} state.

The structure of the conduction band also has an effect on the optical absorption

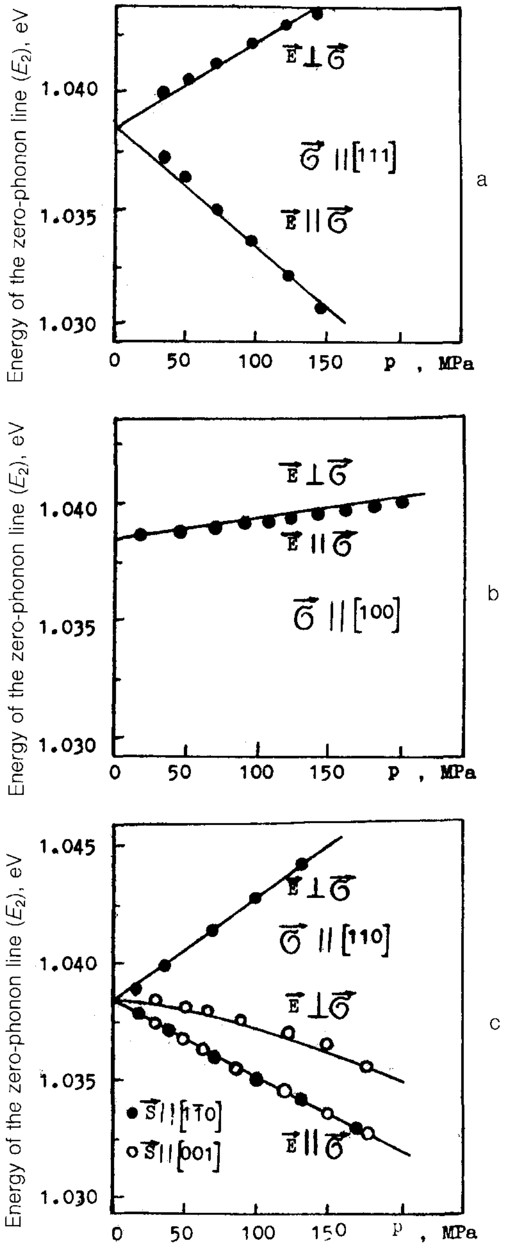

FIG. 3. Energy of the zero-phonon line versus the uniaxial compression. The solid line in Fig. 3b is the plot of the $|1/3\Delta_{L\Gamma}(p)|$ based on the data of Ref. 13.

due to uniaxial compression of GaAs single crystals with $EL\,2$ centers (Fig. 3). The strongest splitting of the zero-phonon line was observed upon a compression in the direction of the [111] axis. Compression of a single crystal in the [100] direction did not lead to a splitting of the zero-phonon E_2 line, whereas three of its components, whose behavior is evidence of the presence of the dynamic Jahn-Teller effect, were observed when $\vec{\sigma}\|\{110\}$. The characteristic features of induced splitting of the spectral lines, which correspond to the resolved transitions in a system with centers of different symmetries in the cubic crystals, were calculated by Kaplyanskiĭ.[12] The principal conditions for the splitting are the intensity, the degree of polarization, the number of split components, and the magnitude of their displacement from the position of the spectral line which was not split. Taking into account the data of Ref. 12, we conclude on the basis of our results (Fig. 3) that the $EL\,2$ center in GaAs has a C_{3V} symmetry. The whole pattern of splitting of the zero-phonon line is in good agreement with the results of hot-photoluminescence studies of the effect of uniaxial compression on the splitting of the L valley of the conduction band.[13] In particular, the displacement of the zero-phonon line with $\vec{\sigma}\|[100]$ (Fig. 3b) corresponds to the intervalley splitting: $\Delta = -1/3\Delta_{L\Gamma}$. This circumstance is an independent confirmation that the $EL\,2$ level belongs to the L valley of the conduction band. It also accounts for the presence of the zero-phonon line in the spectral dependence of the photocurrent.[14] The study of the optical absorption under conditions of hydrostatic and uniaxial compression of GaAs single crystals thus has shown that D°, D^+, and D^{++} states of the $EL\,2$ center have C_{3V} symmetry and are formed from the L, Γ, and X valleys of the conduction band. The transition of the $EL\,2$ center to the metastable state is a consequence of the optical charge exchange of the type $2D^+ \to D^\circ + D^{++}$ and is accompanied by a tunneling of an antistructure donor from the lattice site (the D^+ state) to a tetrahedral interstitial site (the D° state).

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Translated by S. J. Amoretty