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# Splitting of the metastable *EL*2 acceptor state

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The results of electrical resistivity and Hall measurements of *n*-type GaAs under uniaxial stress in the [100] and [111] directions performed at low temperature are presented. After the transformation of the *EL*2 defect into its metastable configuration, a stress-induced decrease of both electron Hall concentration and mobility was observed. This effect was related to the capture of electrons by the acceptor state of the metastable *EL*2 ($[EL2^*]^{-/0}$). It was found that this level split under [111] stress into two orientationally degenerate components: the triplet and the singlet. The dependence of Hall concentration and mobility upon [111] stress obtained after the *EL*2 photoquenching performed under a high stress was different from that measured after *EL*2 photoquenching performed without an external stress. This difference was due to ordering of metastable *EL*2 centers after photoquenching performed under a high stress and it is consistent with the isolated $\mathrm{As_{Ga}}$ model of the *EL*2 defect. The stress coefficients for $[EL2^*]^{-/0}$ sublevels split under [111] stress are found to be $dE_T/d\chi[111]=-17$ meV/GPa and $dE_S/d\chi[111]=-41$ meV/GPa for triplet and singlet, respectively. The investigated level did not split under [100] stress.

## INTRODUCTION

The *EL*2 defect in GaAs has been very intensely investigated in recent years. Measurements of the no-phonon line of the *EL*2 intracenter absorption under uniaxial stress,[1,2] and measurements of a narrow luminescence line due to *EL*2 under uniaxial stress,[3] confirmed the tetrahedral $T_d$ symmetry of *EL*2 in its normal configuration. The recent measurements of the thermal recovery of the *EL*2-related absorption performed under uniaxial stress[4] showed that the *EL*2 in the metastable configuration has trigonal $C_{3v}$ symmetry. The dependence of the orientation of *EL*2 in the metastable configuration on the method of the *EL*2 photoquenching[5] confirmed the attribution of *EL*2 metastability to the transformation $\mathrm{As_{Ga}}\leftrightarrow\mathrm{V_{Ga}As_i}$.[6-8]

The *EL*2 defect in the metastable configuration cannot be observed by means of electrical or optical methods. However, under hydrostatic pressure in *n*-type samples the metastable *EL*2 defect can trap an extra electron, which leads to an increase of electrical resistivity directly observed in the experiment.[9] The acceptor level of the metastable *EL*2 ($[EL2^*]^{-/0}$), lying about 14 meV above the bottom of the conduction band, enters the gap under a hydrostatic pressure of 200–300 MPa. The stress-induced increase of the electrical resistivity due to occupation of the $[EL2^*]^{-/0}$ level was observed under uniaxial stress as well (for preliminary results, see Ref. 10). We have performed electron Hall concentration and mobility measurements under uniaxial stress in order to find the stress coefficients of the $[EL2^*]^{-/0}$ level. Measurements have been done at temperatures of 4.2 and 30 K.

## EXPERIMENT

The investigated material was *n*-type liquid-encapsulated Czochralski (LEC) GaAs. Two samples were prepared; they were x-ray oriented and a uniaxial stress could be applied along the [111] and [100] crystallographic directions. The electron concentration measured at room temperature was equal to $3.6\times10^{16}$ cm$^{-3}$ in the [111]-oriented sample, and $4.7\times10^{16}$ cm$^{-3}$ in the [100]-oriented one. The *EL*2 concentration measured by means of deep-level transient spectroscopy (DLTS) was equal to $4.5\times10^{15}$ and $6\times10^{15}$ cm$^{-3}$, respectively (the λ effect was taken into account). Uniaxial stress up to 700 MPa was obtained with a press spring apparatus attached to an optical cryostat. We have measured the electrical resistivity of samples using a four-probe method. The electron Hall concentration and mobility were measured in the van der Pauw configuration at $B=0.3$ T. Samples were illuminated with a white unpolarized light using a tungsten halogen lamp and Si-filter (Hall measurements) or monochromatic 1.05 μm light (resistivity measurements).

We observed that while *EL*2 is in its normal configuration (just after a sample was cooled down in the dark) the sample resistivity depends very weakly on applied stress (see Fig. 1). After the transformation of *EL*2 into the metastable configuration ($EL2^*$) with 1.05-μm light the stress-induced increase of the sample resistivity appeared. The effect was fully reversible at low temperatures ($T<40$ K). At $T=40$ K, relaxation of the resistivity during the application of stress was observed, and at $T=50$ K the effect was no longer observed. After a measurement done at $T=50$ K and a subsequent cooling down of the sample, the stress dependence of the sample resistivity was the same as before illumination. The observed stress-induced increase of the resistivity was due to the capture of electrons by the $[EL2^*]^{-/0}$ level, which moves downwards with respect to the conduction-band minimum when the stress is applied. At higher temperature ($T>40$ K) the thermal recovery of the $EL2^*$ defect into the normal configuration took place [$EL2^*$ in *n*-type

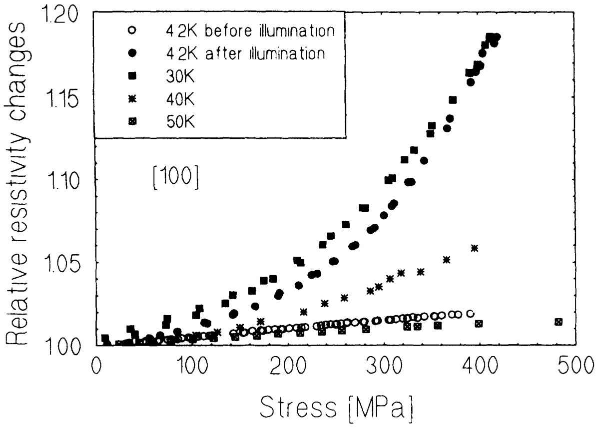

FIG. 1. The stress dependence of the sample resistivity measured at several temperatures under [100] uniaxial stress.

GaAs recovers at 40–50 K (Refs. 11 and 12)], and the $[EL2^*]^{-/0}$ level disappeared.

For a sample stressed along the [111] direction, we observed that the amplitude of the stress-induced resistivity increase depends on the method of *EL*2 photoquenching. If an unstressed sample was illuminated, the effect was larger than if a high stress (600 MPa) was applied during the illumination (see Fig. 2). We observed that after sufficiently long illumination performed at high stress the subsequent illumination without stress did not change the stress dependence of the resistivity. However, if *EL*2 photoquenching under high stress was not completed, then additional illumination without stress caused further changes in the stress dependence of the resistivity. This result means that after sufficiently long illumination performed at high stress, all *EL*2 centers are in the metastable configuration, and the ratio of centers created along and oblique to the axis of the stress cannot be changed during an experiment unless the temperature is too high (and thermal recovery becomes possible).

The observed effect was due to the dependence of the $EL2^*$ center orientation in a crystal on the method of *EL*2 photoquenching. If no stress is applied to a sample, the *EL*2 photoquenching with unpolarized light creates $EL2^*$ centers along all four [111] crystallographic directions. As a result the resistivity changes observed under the stress are due to the capture of electrons by both split $[EL2^*]^{-/0}$ sublevels; i.e., the singlet $[EL2^*]_S^{-/0}$ related to centers oriented along the axis of stress and the triplet $[EL2^*]_T^{-/0}$ related to centers oriented oblique to the axis of stress. If *EL*2 photoquenching is performed under high [111] stress, the pressure-induced optical recovery[13] becomes effective for the $[EL2^*]^{-/0}$ sublevel which is deeper in the forbidden gap. As a result, after a sufficiently long period of such illumination, mainly $EL2^*$ centers related to the higher-energy sublevel are present in a crystal. From the optical measurements of Trautman, Baranowski, and Babiński,[5] it is clear that such a situation can be produced either by illumination of a stressed sample with white unpolarized light (as in our experiment) or by illumination of an unstressed sample, but performed with light polarized perpendicularly to the direction of stress applied afterwards (i.e., after *EL*2 photoquenching). This means that centers present in our sample after *EL*2 photoquenching performed under high stress were oriented obliquely to the axis of stress, and the triplet sublevel of the split $[EL2^*]^{-/0}$ was of higher energy than the singlet level. Our results are consistent with the isolated $\mathrm{As_{Ga}}$ model of the *EL*2 center. In the

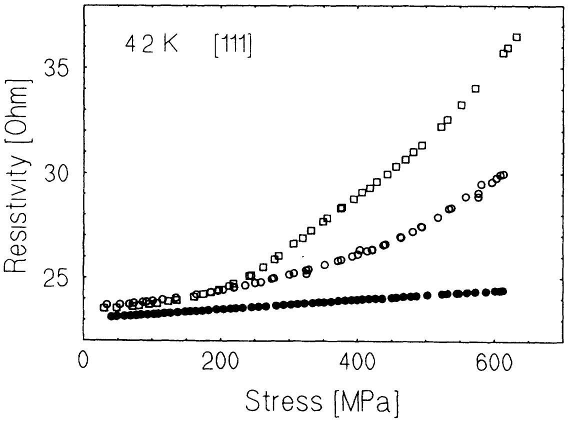

FIG. 2. The stress dependence of the sample resistivity under [111] uniaxial stress at $T=4.2$ K measured just after cooling down a sample in the dark (full circles), after full *EL*2 photoquenching without stress (squares), and after *EL*2 photoquenching performed under a high (600 MPa) stress (open circles).

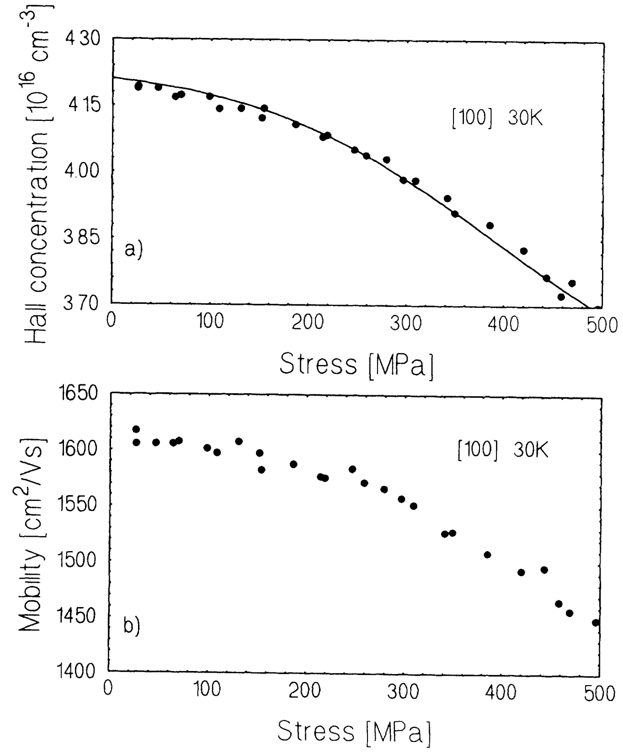

FIG. 3. The dependence of electron Hall concentration (a) and mobility (b) on [100] uniaxial stress at $T=30$ K. The measurements were performed after the transformation of *EL*2 into the metastable configuration. The full line is calculated with parameters taken from Ref. 9.

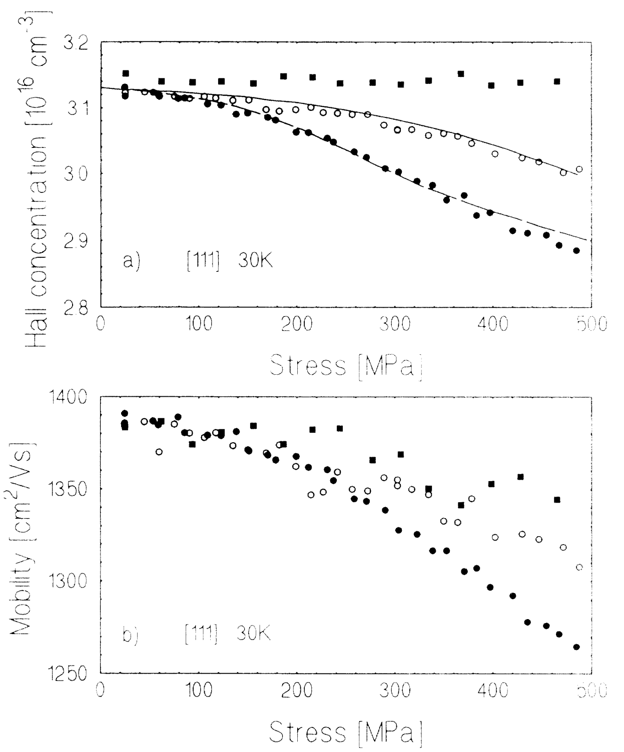

FIG. 4. The stress dependence of the electron Hall concentration (a) and mobility (b) on [111] uniaxial stress at $T=30$ K. The measurements were performed just after cooling down the sample (squares), after *EL*2 photoquenching with a white unpolarized light without an external stress (full circles), and after *EL*2 photoquenching under a high stress (500 MPa) (open circles). The theoretical stress dependences were obtained with the following parameters: $E_0=14$ meV, $dE_T/d\chi[111] = -17$ meV/GPa, and $dE_S/d\chi[111]=-41$ meV/GPa.

model, which is the only one based on total-energy calculations, the transition to the metastable configuration is connected with the transition of the antisite $\mathrm{As_{Ga}}$ atom into the interstitial position along the [111] direction.[7,8]

Figures 3–6 present results of Hall concentration and mobility measurements performed at $T=30$ and 4.2 K. It was found that while *EL*2 was in its normal configuration, the electron Hall concentration did not depend on applied stress, and only a weak stress-induced decrease of electron mobility was observed. After *EL*2 photoquenching a stress-induced decrease of electron Hall concentration as well as mobility appeared. The observed stress-induced decrease of the electron concentration was due to the capture of electrons by the $[EL2^*]^{-/0}$ level. The stress-induced decrease of the mobility was due mainly to the appearance of charged $[EL2^*]^-$ centers which act as scattering centers. It is interesting to note that the relative changes of mobility and concentration are very similar.

## NUMERICAL ANALYSIS

We have performed a numerical analysis of the obtained stress dependences of the electron concentration at $T=30$ K. Let us consider the most general situation

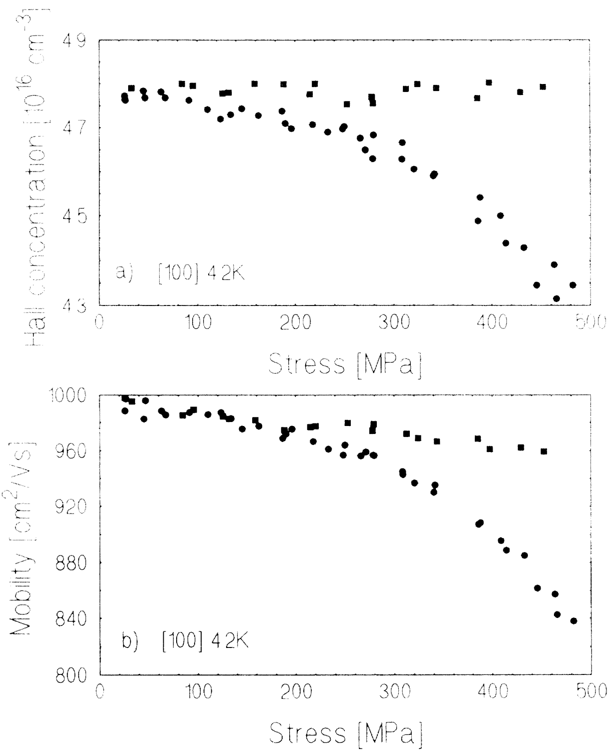

FIG. 5. The stress dependence of the electron Hall concentration (a) and mobility (b) on [100] uniaxial stress a $T=4.2$ K. The measurements were performed just after cooling down the sample (squares), and after *EL*2 photoquenching with a white unpolarized light (circles).

with two sublevels $T$ and $S$ for centers oblique to and along the axis of stress involved. The concentration of these centers are $N_T$ and $N_S$ and their energies are equal to $E_T$ and $E_S$, respectively. For the measurements performed under [100] stress both kinds of centers are equivalent ($N_T+N_S=N_{[EL2^*]}$, where $N_{[EL2^*]}$ is the total concentration of metastable *EL*2 and $E_T=E_S=E$). If the *EL*2 photoquenching was performed under a high [111] stress, only one sublevel is involved ($N_T=N_{[EL2^*]_T}=N_{[EL2^*]}$ and $N_S=0$). If the *EL*2 photoquenching was performed without an external stress both split sublevels are present ($N_T=N_{[EL2^*]T}$ and $N_S=N_{[EL2^*]S}$). We used the following formulas.

(a) The equations for the equilibrium population of the $[EL2^*]^{-/0}$ levels are

$$N_T^-/N_T^0=\exp[(E_F-E_T)/kT] ,$$

$$N_S^-/N_S^0=\exp[(E_F-E_S)/kT] ,$$

where $N_T^-$ and $N_T^0$ are the concentrations of triply orientationally degenerate $EL2^*$ in negative and neutral charge states, respectively; $N_S^-$ and $N_S^0$ are the concentrations of singly orientationally degenerate $EL2^*$ in negative and neutral charge states, respectively, $E_F$ is the Fermi level, and $E_T$ and $E_S$ are the energies of triplet and singlet levels, respectively, including the entropy change. For both $E_T$ and $E_S$, we assume a linear dependence of

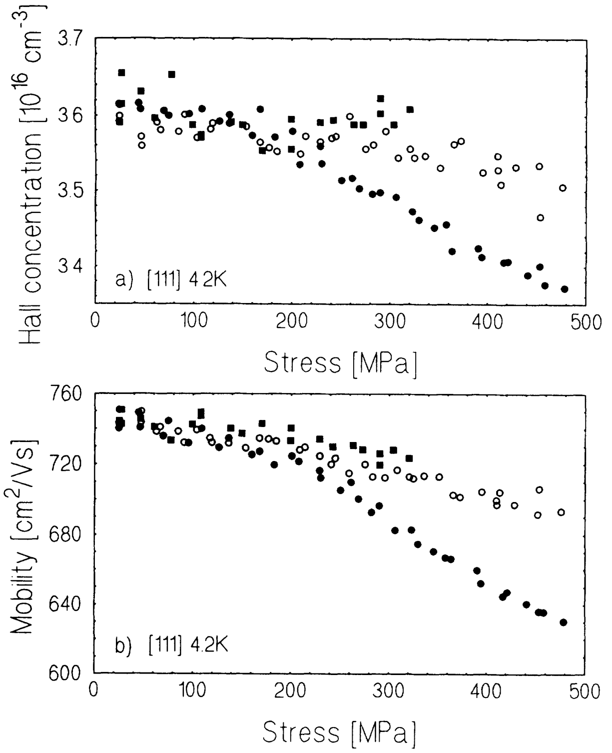

FIG. 6. The stress dependence of the electron Hall concentration (a) and mobility (b) on [111] uniaxial stress at $T=4.2$ K. The measurements were performed just after cooling down the sample (squares), after *EL*2 photoquenching with a white unpolarized light without an external stress (full circles), and after *EL*2 photoquenching under a high stress (500 MPa) (open circles).

the level energy on stress, i.e., $E_{T,S}(\chi)=E_0+(dE_{T,S}/d\chi)\times\chi$, where $\chi$ is the uniaxial stress.

(b) The balance between both types of $EL2^*$ is

$$N_{[EL2^*]}=N_S+N_T\ .$$

Centers created along the axis of stress or oblique to that axis were not able to change their orientation during an experiment, and all *EL*2 centers were in the metastable configuration.

(c) The balances between various charge states of the metastable centers are

$$N_S=N_S^-+N_S^0\ ,$$

$$N_T=N_T^-+N_T^0\ .$$

(d) The condition of crystal neutrality is

$$n=N_D-N_A-N_T^--N_S^-\ ,$$

where $n$ is the electron concentration and $N_D-N_A$ is the net ionized shallow donor concentration.

The above formulas were used to calculate the free-electron concentration. The Fermi integral was calculated with an assumption of a spherical and parabolic conduction band with the effective mass dependent only on the hydrostatic component of the stress.[14]

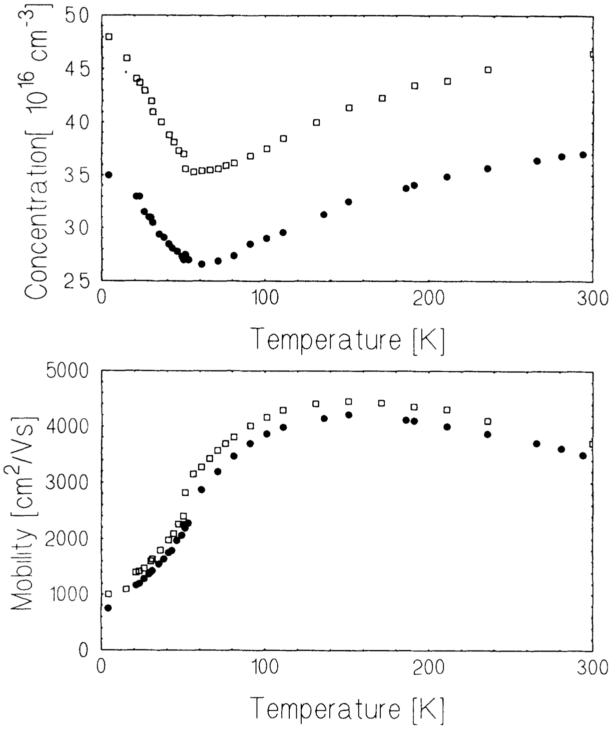

FIG. 7. The temperature dependence of the electron Hall concentration and mobility for a sample measured in a piezo-Hall experiment (squares—[100]-oriented sample, circles—[111]-oriented sample).

The approximate character of the above assumptions has to be noted. The results obtained at $T=30$ and 4.2 K (compare Fig. 3 with Fig. 5 and Fig. 4 with Fig. 6) are very similar. They cannot be explained by assuming that the electrons are only in the conduction band. The temperature dependence of the Hall concentration and mobility (see Fig. 7) with a characteristic minimum[15] suggests that at $T=30$ K band tailing[16] has to be taken into account. It means that the measured Hall concentration is a function of the actual electron concentrations and mobilities in the conduction band and in the impurity band. It is not known, however, what is really the electron concentration in the conduction band and the impurity band, and what density of states at the bottom of the conduction band is the best approximation for our experimental situation.

## RESULTS OF THE ANALYSIS

In our analysis we assume that the measured electron Hall concentration is equal to the electron concentration $n$ and that $N_D-N_A$ is equal to the electron concentration before *EL*2 photoquenching. For $N_{EL2}$ we take the value obtained from DLTS measurements. For $E_0$ we consider in our calculations the value 14 meV, reported in Ref. 9.

(a) [100] direction of stress. As was reported previously,[4] the $[EL2^*]^{-/0}$ level does not split under [100] uniaxial stress, and its energy shift is due to the hydrostatic component of the stress. We have performed a theoretical calculation of the electron concentration under [100] uniaxial stress using parameters taken from hydrostatic pressure data[9] $[(dE/d\chi)[100] = \frac{1}{3}X - 68$ meV/GPa $= -23$ meV/GPa]. The result of this calculation is presented in Fig. 3(a) (see continuous line). The agreement with experimental points is very good. It has to be noted that the values reported in Ref. 9 were obtained without taking into account mobility changes after $EL2$ photoquenching.

(b) [111] direction of stress. The best fit to the experimental points measured after $EL2$ photoquenching performed under a high stress, when only the $[EL2^*]_T^{-/0}$ sublevel is present (all $EL2^*$ centers are oriented oblique to the axis of stress), was obtained with $dE_T/d\chi[111] = -17$ meV/GPa [see continuous line in Fig. 4(a)]. Taking into account the hydrostatic pressure coefficient of the $[EL2^*]^{-/0}$ level, we can find the stress coefficient of the single orientationally degenerate sublevel $[EL2^*]_S^{-/0}$ to be equal to $dE_S/d\chi[111] = -41$ meV/GPa.[17]

If $EL2$ photoquenching is performed without external stress and with unpolarized light, both types of $[EL2^*]^-$ centers are created (along the axis of stress and oblique to that axis). However, it is not known how many singlet and triplet centers are created. The best fit to our experimental results was obtained with the assumption that $\frac{1}{3}$ of all $EL2^*$ centers were created along the axis of stress, and $\frac{2}{3}$ of the $EL2^*$ centers were oblique to the direction of stress [see the dashed line in Fig. 4(a)].

## CONCLUSIONS

It has been shown that after $EL2$ photoquenching a stress-induced decrease of electron Hall concentration and mobility are observed. These changes are related to the occupation of the $[EL2^*]^{-/0}$ level. A numerical analysis using a parabolic density of states in the conduction band has been performed. The stress coefficient of the $[EL2^*]^{-/0}$ level for uniaxial stress along the [100] direction ($dE/d\chi[100]$) results from the hydrostatic component of stress and it is equal to $-23$ meV/GPa. The $[EL2^*]^{-/0}$ level splits under [111] stress into two orientationally degenerate components: triplet and singlet. Stress coefficients of these sublevels are found to be equal to $dE_T/d\chi[111] = -17$ meV/GPa and $dE_S/d\chi[111] = -41$ meV/GPa, respectively. The schematic diagram of the $[EL2^*]^{-/0}$ energy levels under uniaxial stress is presented in Fig. 8. Our results are fully consistent with the trigonal $C_{3V}$ symmetry of the metastable $EL2$. The dependence of stress-induced resistivity under [111] stress on the method of $EL2$ photoquenching strongly supports the isolated $\mathrm{As}_{Ga}$ model of the $EL2$ center.

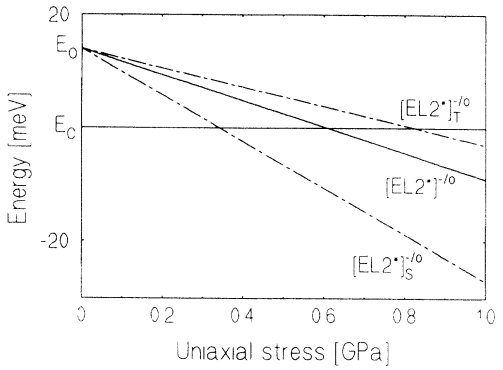

FIG. 8. The schematic energy diagram of the $[EL2^*]^{-/0}$ level under uniaxial stress. The $[EL2^*]^{-/0}$ level does not split under [100] stress (see continuous line). Under [111] stress the $[EL2^*]^{-/0}$ level splits into two orientationally degenerate sublevels: the triplet $[EL2^*]_T^{-/0}$ and the singlet $[EL2^*]_S^{-/0}$ (dashed line).

## ACKNOWLEDGMENTS

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