

Energy Parameters in the Three-Minima Model for the DX center

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Photoconductivity measurements were performed in Si-doped AlGaAs, aiming to determine the energy parameters related to the three-minima model for that impurity. The equilibrium conduction electrons density for the sample under illumination was measured as a function of the light intensity and temperature. In conditions of equilibrium the kinetic equations which describe the electrons emission from the DX-center and their return from the conduction band become simple algebraic equations. This is very convenient in order to obtain, through fitting the experimental data, the parameters involved in the model. The energy barrier between the conduction band and the DX^0 state, as well as between the states DX^- and DX^0 , could be obtained. The comparison of these values with the DLTS capture and emission energy barriers has provided an interpretation for the DLTS results on the light of the three-minima model.

Donor impurities in semiconductors usually have an effective mass hydrogenic or donor state (d^0) where they can be easily ionized (d^+) providing electrons to the conduction band. But in III-V semiconductors like GaAs or its aluminum alloy $Al_xGa_{1-x}As$, it is largely accepted that donor impurities can exist in a different state, called DX centers, in which the electrons are localized rather than extended as in the shallow donor impurities state. They have been intensively investigated not only because of their influence on electronic devices but also owing to their challenging physical properties. When the aluminum concentration x exceeds 22% in the alloy, or else when just GaAs ($x = 0$) is subjected to hydrostatic pressure over 20 kBar, the DX center has lower energy than the donor state which turns out to be metastable. The temperature dependent long lifetime of this donor state is responsible for the persistent photoconductivity (PPC) usually observed in these materials at low temperatures. Since the pioneering work by Lang et al.^[1], a great experimental and theoretic

cal effort has been done to understand the DX center and its formation mechanism. Most of this work has been reviewed by Mooney^[2] and by several articles published in a special issue of the Journal of Electronic Materials, some of which we would like to mention^[3-5]. From this effort it became accepted that the DX centers are formed solely by the doping ions through electrons' capture^[6-8] and that there are energy barriers between them and the donor states^[1] which are believed to be a consequence of a large lattice relaxation (LLR)^[3] of the defect. Pseudopotential calculations of the defect's energies by Chadi et al.^[8,9] show that the LLR model requires the DX center to be negative (Chadi-Chang DX^- model). Although some magnetic susceptibility results^[10] suggest the DX to be a paramagnetic center, in disagreement with this model, another^[11] points to a different conclusion. Also Electron Paramagnetic Resonance (EPR) experiments^[12,13] failed to find any unpaired spin, and practically all the experimental results on the center are consistent with the Chadi-Chang model, that has therefore become widely accepted.

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In addition to the above mentioned states for the

donor impurity another one is supposed to exist and to take part in the (d^0 or d^+) \rightarrow DX^- transformation. It should be a zero charge state and so is called DX^0 . Its existence was proposed in order to explain DX emission and capture rates^[14] and has also been seen by photoinduced EPR^[13]. Later evidences were also reported in transients studies of negative photoresistance^[15] and Photo-Hall^[16]. So, one can say that the model of a DX^- formed via the neutral DX^0 state is a three-minima model because it would ascribe to the crystal free energy an impurity contribution depending on some proper coordinates as represented in Fig. 1. The Q_{DX^-} represents the equilibrium ions' positions after the lattice relaxation which appears due to the DX^- center as proposed by the Chadi-Chang's mode^[18]. The Q_{DX^0} also is defined as the equilibrium configuration for the DX^0 state but the kind of coordinate it represents can be different from the one represented by DX^- . It is not even known whether the lattice is relaxed or not in the DX^0 state. Authors differ about this matter. In Theis and Mooney's paper^[14], for instance, DX^0 is considered to equilibrate very fast with the d^0 or d^+ states suggesting a negligible lattice relaxation. This assumption is also used by Mosser et al.^[17]. On the other hand, Dobaczewski and Kaczor^[15] argue that the barrier between DX^0 and d^+ can not be zero and that the one between DX^0 and DX^- has to be low. Similar conclusion was obtained by Sampaio et al.^[16] whose results also require the first barrier to exist but do not make any prediction about the second one.

We have done experiments aiming to determine the barriers in this three-minima model. This was achieved by shining light on the sample, until a steady Hall voltage is reached, which means an equilibrium state between the rate of electrons rising from the DX centers to the conduction band, due to the light, and the thermal decay. Then the kinetic equations for the system will provide a relation between the light intensity and the conduction band electrons concentration (n). It involves the kinetic parameters of the system's move-

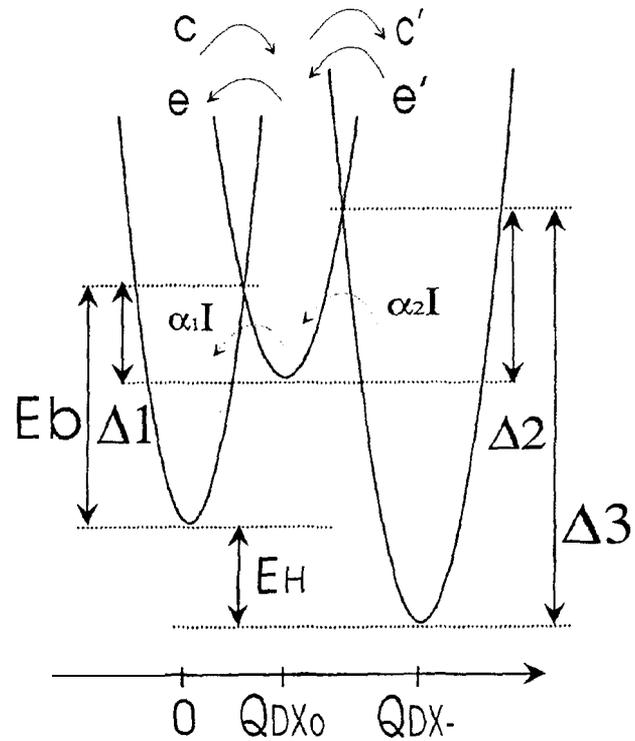


Figure 1: Coordinate Configuration representation of the impurities contribution to the crystal free energy in the three-minima model.

ment between the minima which depend on their energy barriers and temperature. So, if one takes the experimental dependence of n on the light intensity at several different temperatures, one can obtain the energy barriers from their fitting to the kinetic equations. For these ones we have used the following relations

$$\frac{dN^+}{dt} = -cN^+ + eN^0 + \alpha_1 N^0 I, \quad (1)$$

$$\frac{dN^0}{dt} = -(e + e')N^0 + cN^+ + e'N^- + (\alpha_2 N^- - \alpha_1 N^0) I, \quad (2)$$

$$\frac{dN^-}{dt} = e'N^0 - e'N^- - \alpha_2 N^- I, \quad (3)$$

where N^- , N^0 and N^+ denominate respectively the defects' concentrations in the DX^- , DX^0 and d^+ states and I is the light intensity. The coefficients c and c' are the probabilities per unit time that the impurity goes, respectively, from d^+ to DX^0 and from DX^0 to DX^- through the capture of one electron from the conduction band. On the other hand e and e' represent the

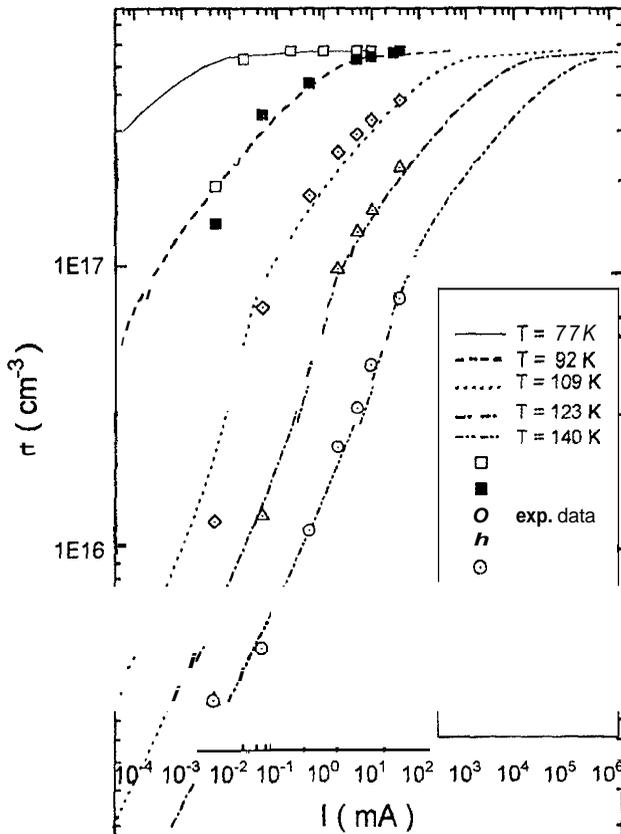


Figure 2: Hall carriers concentration versus LED current for different temperatures. Continuous line represent fitting results from the three-minima model.

respective probabilities of doing the opposite transformations with spontaneous emission of electrons to the conduction band; $\alpha_1 I$ and $\alpha_2 I$ represent the light induced probability time rates for these emissions. These definitions are summarized in Fig. 1.

In the absence of other impurities the defects' concentrations are related to the concentrations N_D and n of total donors and of free electrons in the conduction band:

$$N^+ + N^0 + N^- = N_D, \tag{4}$$

$$N^+ = N^- + n. \tag{5}$$

In all the above equations it was not considered the existence of non ionized donors in the shallow state d^0 . In steady state, the time derivatives of the concentrations are equal to zero and the equations above result in:

$$I = \frac{\sqrt{B^2 + 4D} + B}{2(1 - \eta)} \tag{6}$$

where

$$r \equiv \frac{n}{N_D}, \quad B \equiv \frac{c}{\alpha_1} r - (1 - r) \left(\frac{e}{\alpha_1} + \frac{e'}{\alpha_2} \right),$$

and

$$D \equiv \frac{(1 + r)cc' - (1 - r)ee' + rce'}{\alpha_1 \alpha_2}$$

The capture and emission probabilities depend on the activation energies E_b, Δ_1, Δ_2 and Δ_3 , defined in Fig. 1, as $c \propto n\bar{v}e^{-\beta(E_b - \xi)}$, $c' \propto n\bar{v}e^{-\beta(\Delta_2 - \xi)}f(E_b - \Delta_1, \xi)$, $e \propto e^{-\beta\Delta_1}$ and $e' \propto e^{-\beta\Delta_3}$, where $\beta \equiv 1/kT$ and $\xi, f(E, \xi)$ and \bar{v} are, respectively, the chemical potential, the Fermi-Dirac distribution as function of the energy E , and the mean velocity of the electrons in the conduction band. Then, the parameters B and D will take the following form:

$$= xrn\bar{v}e^{-\beta(E_b - \xi)} - (1 - r)(ye^{-\beta\Delta_1} + we^{-\beta\Delta_3}), \tag{7}$$

$$D = z(1 + r)n^2\bar{v}^2e^{-\beta(E_b + \Delta_2 - 2\xi)}f(E_b - \Delta_1, \xi) - yw(1 - r)e^{-\beta(\Delta_1 + \Delta_3)} + xwrn\bar{v}e^{-\beta(E_b + \Delta_3 - \xi)}, \tag{8}$$

where x, y, z and w are constants independent of the activation energies and of the electron concentration. Equations (6, 7 and 8) give a relation between n and the light intensity I , whose fitting to experimental data can provide the activation energies parameters.

The experiments were done on $3.8\mu\text{m}$ thick $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ layer with a nominal silicon doping of $6 \times 10^{17} \text{ cm}^{-3}$, separated from the semi-insulating (100) GaAs substrate by a non intentionally doped $0.7\mu\text{m}$ thick $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ and a GaAs buffer layers; the sample was covered by a cap layer of GaAs with 170\AA of thickness and doped with $8 \times 10^{17} \text{ cm}^{-3}$ of silicon. All the layers were grown by Molecular Beam Epitaxy at a temperature of 620°C . The alloy composition was determined by using conventional RHEED intensity oscillations to calibrate the effective incorporation rate of aluminum and gallium atoms. The piece of sample prepared for the experiment had the MBE layers shaped

by photolithographic process in a Hall bridge pattern with a current channel width of $300\mu\text{m}$ and a distance of $800\mu\text{m}$ between the voltage measuring arms. The electrical contacts were obtained by indium diffusion at a temperature of 400°C , for 10 minutes, in a hydrogen rich N_2 atmosphere. The sample was slowly (approximately 0.6 degree per min.) cooled down to a working temperature and a HP HEMT1001 infrared LED was used to irradiate on the sample. Its photon energy depends on the temperature, but it was always lower than the AlGaAs forbidden band gap. A variable electrical current through the LED was used to change its radiation intensity and for each current value the system was allowed, to reach steady conditions by monitoring the Hall voltage. Then, the steady carriers concentration, as measured by Hall effect, was obtained for several LED current values. This was repeated for five different temperatures and the results are shown by the discrete plot data in the Fig. 2.

The experimental results were fitted with the relations 6, 7 and 8, where the radiation intensity I was taken as the LED current because they resulted to be proportional to each other. The chemical potential ξ was numerically estimated for each temperature and each light intensity from the experimental values n of the Hall carriers concentration through the formula $n = \int_0^\infty g(E) f(E, \xi) dE$, where $g(E)$ is the conduction band density of states for the AlGaAs and $f(E, \xi)$ is the Fermi-Dirac distribution function. Then \bar{v} was also numerically calculated as the average of the absolute value of the carriers velocities.

The energy parameters relation $\Delta_3 - \Delta_2 + \Delta_1 - E_b$ is equal to the energy difference between the DX^- and the d^+ minima which is the activation energy E_H . It can be obtained by the temperature dependence of the Hall effect in the region of temperatures above 120 K as described by Theis et al.^[5]. Temperature dependence of the Hall electron concentration gives $E_H = 60$ meV for our sample and this value was used as a constraint to the energy parameters in the fitting. One could also

see that only the difference $\Delta_2 - \Delta_1$ is relevant to the fitting process rather than each parameter taken separately. So, the six parameters x, y, z, w, E_b and $\Delta_2 - \Delta_1$ were determined to give the best simultaneous fit of the experimental $n \times I$ curves corresponding to all the five temperatures. The best fitting curves obtained are shown in Fig. 2. They agree fairly well with the experimental data, except for the low temperature and low n results. This is quite understandable because at these ranges of temperatures and carriers' concentrations the conduction by impurities' band cannot be disregarded and the above model is expected to fail. The values obtained from the fitting for the energy parameters are $E_b = 270$ meV, $\Delta_2 - \Delta_1 = 50$ meV and from the known E_H value one obtains $\Delta_3 = 380$ meV. It is interesting to compare these results with the ones already in the literature. By Deep Level Transient Spectroscopy (DLTS) the DX-center emission energy is found to be 430 meV^[18]. However our result is in fairly good agreement with the value of 370 meV obtained more recently by Seguy and Yu^[19]. The literature describes a capture barrier in AlGaAs alloys dependent on the aluminum content, x . For $x = 30\%$ the capacitance method data by Mooney et al.^[20] predicts, by linear interpolation, a capture barrier about 310 meV. This value is significantly higher than our result for E_b but coincides very well with $E_b + (\Delta_2 - \Delta_1)$. Therefore, it appears that the capture barrier obtained by capacitance techniques represents the total energy barrier between the conduction band and the DX^- state, even if the crossing point of the d^+ and DX^0 energy wells is lower than the crossing of DX^0 and DX^- .

In conclusion we have shown that the curves of Hall carriers concentration versus light intensity are very useful for the determination of the energy parameters of the three-minima model for the DX-center. The results suggest that the emission and capture barriers measured by DLTS actually represent total effective energy barriers between the leftmost and rightmost energy minima. With the kind of experiments we have done,

the real barriers between these minima and the intermediate state DX^0 , i. e., E_b , Δ_3 , and $(\Delta_2 - \Delta_1)$, could be determined. This can be useful to determine these barriers for different aluminum concentrations in non degenerate AlGaAs alloy, or different hydrostatic pressures on GaAs, to get more insight on the DX^0 state.

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