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Mott barrier behavior by enhanced donorlike level neutralization in semi-insulating GaAs Schottky diodes

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The Mott barrier behavior of metal-semi-insulating GaAs diodes is explained by the compensation mechanism due to bulk donorlike centers. In such diodes the quasineutral region extends from metallization to a buried space charge region and widens with increasing bias. To assess the dependence of this behavior on the electronic levels associated with bulk deep donors, their density was increased by proton irradiation. We observed that the net space-charge density decreases and, correspondingly, the quasineutral region extent increases. The correlation between electric field distribution and deep levels confirms the strong influence of defects on the compensation process.

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Mechanisms responsible for the electric field behavior and charge compensation in semi-insulating (SI) GaAs are still the object of debate in the scientific community in spite of experimental and theoretical studies carried out in the last two decades. The spatial distribution of the electric field $\mathcal{E}$ across SI GaAs Schottky diodes has been extensively investigated. Theoretical and experimental studies[1–5] have allowed for a better understanding of the intervening mechanisms, although no definite conclusions have been drawn yet.

Attention has been mainly focused on the defect EL2, the dominant donor trap located at $E_C - 0.75$ eV, commonly found in concentrations of 10^{16} cm^{-3}. This defect is believed to control the electrical properties of GaAs given that it strongly determines the compensation degree together with the residual bulk impurities.[6] Its peculiar property is an electric field enhancement of the capture cross section,[7] increasing its ability to capture electrons, thus neutralizing it. EL2 neutralization occurs for $\mathcal{E}$ higher than a threshold value of some kV/cm and, as a result, a quasineutral region originates at the injecting contact.[1–3] Across such a quasineutral region the electric field $\mathcal{E}$ is constant, giving rise to a plateau at the edge of which an approximately square space-charge-region exists, characteristic of a Mott barrier.[8] This buried space-charge-region contains a charge density resulting from the net effective charge $N_{\mathrm{eff}} = N_D{}^+ + N_{\mathrm{EL2}}{}^+ - N_A{}^-$, where $N_D{}^+$ is the density of donors shallower than EL2, $N_{\mathrm{EL2}}{}^+$ is that of ionized EL2 and $N_A{}^-$ is that of ionized acceptors. However, the net charge carrier density measurement[9] results much lower (on the order of 10^{13} cm^{-3}) than what was predicted considering EL2 alone. This finding clearly implies the presence of levels other than EL2 that also act upon compensation. Consequently, studying diodes with different defect densities, as occurs before and after irradiation, would help to determine the actual role of EL2 and other defects. To achieve this goal, this work deals with a comparison of the electric field distribution and defect density in as-prepared and proton-irradiated metal-GaAs diodes.

We investigated SI GaAs grown by the liquid encapsulated Czochralski method, unintentionally doped, (100) oriented, with n-type resistivity $\rho = 1 - 3 \times 10^7\ \Omega\,\mathrm{cm}^{-2}$. The diodes were 100 μm thick and the Schottky contacts were obtained by Au metallization. Irradiation was carried out at room temperature with 24 GeV protons with fluence equal to 1.2×10^{14} cm^{-2}. All the diodes were analyzed before and after irradiation. The determination of the electric field distribution was carried out by surface potential (SP) and optical beam induced current (OBIC) measurements. Energy level positions in the gap and defect concentrations were obtained by different kinds of junction spectroscopy.[12] The experimental details together with the spectroscopy results are reported elsewhere.[3,9]

The diodes exhibit a Mott barrier behavior both before and after irradiation, but with markedly different features. The main differences are the following:

(1) Mott barrier behavior is evident for voltage $V_a > 30$ V in nonirradiated diodes and for $V_a > 10$ V in irradiated ones (Fig. 1);
(2) the quasineutral region width w, which corresponds to the extent of the electric field plateau, widens after irradiation and the electric field value $\mathcal{E}$ at the plateau decreases (Fig. 1);
(3) w increases with bias and approximately doubles after irradiation;[9]
(4) the buried space charge region of thickness d (Fig. 1 and inset therein) has a net effective carrier density N_{eff} that almost halves after irradiation, as does the surface charge $Q = \int_0^d N_{\mathrm{eff}}(x)dx$ (inset in Fig. 2).

Hu and co-workers[4] modeled the above findings on the electric field and the buried space charge distribution. They modified a previous model of McGregor *et al.*[1] with the assumption that the triggering of a field enhancement of the EL2 capture cross section takes place even for low electric fields (on the order of 1 kV cm^{-1}). Moreover, with low energy positron annihilation techniques, they observed that the electric field dependence on the applied bias is well reproduced with N_{eff} on the order of some 10^{13} cm^{-3}, in agreement with our SP results.[3]. Figure 2 shows our experimental data and those obtained by Hu and co-workers.

The low value of N_{eff} brings into play a stronger compensation, which can be explained only by including other de-

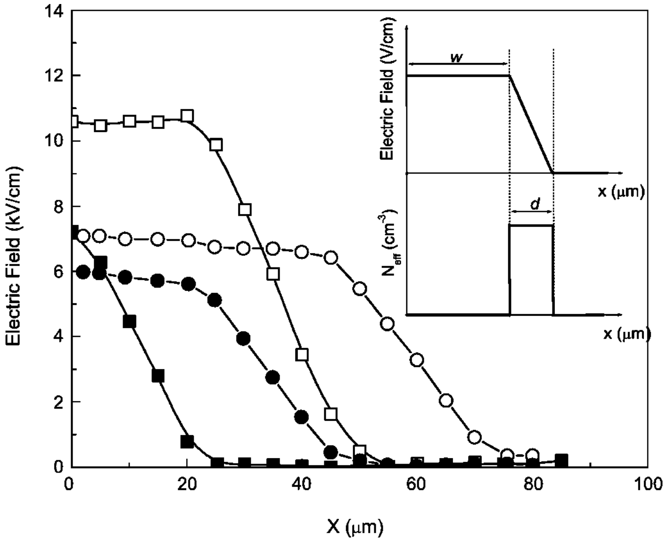

FIG. 1. Electric field as measured before (squares) and after (circles) irradiation for biases 20 V (full symbols) and 40 V (open symbols). In the inset a schematic view of the Mott barrier spatial distribution of electric field (top) and of space charge (bottom). The origin of the *x* axis corresponds to the metallization side. *w* is the quasineutral region extent, *d* is the space charge distribution extent into the bulk.

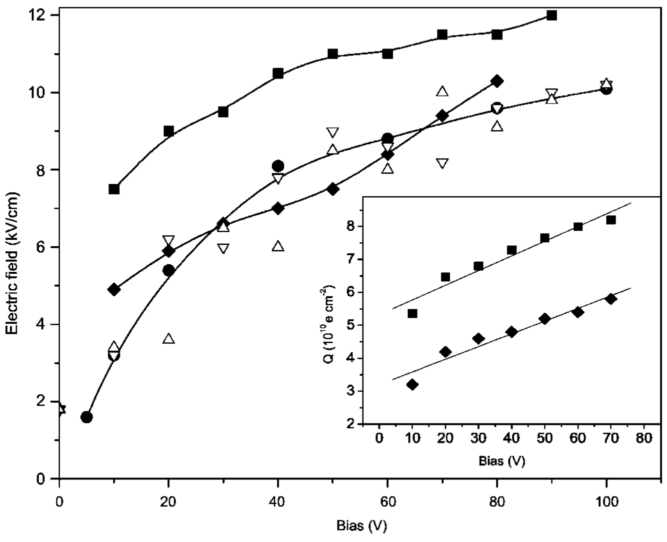

FIG. 2. Experimental data as obtained by Hu *et al.* (Ref. 4) by the positron annihilation technique (open triangles) and by SP results (full symbols) (Refs. 3 and 9). ● refers to unirradiated SI GaAs cited in Ref. 3, ■ refers to unirradiated SI GaAs cited in this work and in Ref. 9, ◆ refers to irradiated SI GaAs cited in this work and in Ref. 9. In the inset the surface charge density as obtained by spatial integration of the buried space charge region for samples cited in this work. Lines are drawn to guide the eye.

TABLE I. Deep level spectroscopy results concerning the traps most influenced by irradiation: energy levels and densities in as-processed diodes ($N_T{}^{\mathrm{ap}}$) and in irradiated diodes ($N_T{}^{\mathrm{ir}}$) are reported. Details of such findings have been already published by the authors in Refs. 9, 12, and 13.

E_T	$E_C-0.15$ eV	$E_C-0.37$ eV	$E_C-0.75$ eV
$N_T{}^{\mathrm{ap}}$ (cm^{-3})		4×10^{13}	1.2×10^{16}
$N_T{}^{\mathrm{ir}}$ (cm^{-3})	2×10^{15}	1.2×10^{15}	9×10^{16}

fects further than EL2. Actually, other traps have been observed as playing an important role in the determination of the diode electrical characteristics.[10–14] Deep level spectroscopy reveals that in our diodes the electronic levels mostly affected by irradiation are at $E_C-0.15$ eV, $E_C-0.37$ eV, and $E_C-0.75$ eV,[9,12,13] as reported in Table I. These levels are common in *n*-type GaAs and are well-known to be donorlike traps. Namely, the level at $E_C-0.75$ eV is identified with EL2, $E_C-0.37$ eV corresponds to EL6 in Martin's notation,[15], and also the trap at $E_C-0.15$ eV has been widely studied.[16] In our diodes the level at $E_C-0.15$ eV is absent in as-processed diodes while its density is 2×10^{15} cm^{-3} after irradiation. The density of the level at $E_C-0.37$ eV increases by two orders of magnitude and that of EL2 by about one.

It is well known that "compensation in GaAs means the mechanism by which the bound electrons and holes of shallow donors and acceptors are transferred to the deep level EL2 where thermal excitation to the conduction or the valence band is improbable."[11] This definition emphasizes the importance of including defect-related deep levels, present in concentrations on the order of 10^{15} cm^{-3}, in the compensation model. Bearing in mind this definition, an explanation will be given below for the following findings:

(a) the neutral region extent increases after irradiation;
(b) the net effective charge density N_{eff} is orders of magnitude lower than the density of ionized EL2 and further decreases after irradiation.

(a) Neutral region extent: It has already been observed that the introduction of donors, even in concentrations sensibly lower than EL2, can cause a dramatic shift of the Fermi level E_F.[11] For the purpose of clarifying the role of defects shallower than EL2, we determined the Fermi level position before and after irradiation employing Shockley diagrams [Figs. 3(a) and 3(b)]. For this analysis, the charge balance equation is graphically solved by plotting positive and negative charge as a function of E_F. The interception between these two diagrams provides the actual Fermi level position. We considered the densities of grown-in shallow donors [Si] and acceptors [C] in addition to the densities of the deep traps EL2, EL6, and $E_C-0.15$ eV as reported in Table I. The difference between E_F values explains the diversity in the extent of the quasineutral regions before and after irradiation. In nonirradiated diodes E_F is located at about midgap [Fig. 3(a)] and pinned to EL2, thus the Mott barrier behavior is mainly controlled by EL2. Accordingly, the extent of the quasineutral region is associated with the field enhanced neutralization of this level and the buried space charge region initiates at the interception of E_F with EL2 [Fig. 4(a)].

The introduction by irradiation of donor levels shallower than EL2, namely EL6 and $E_C-0.15$ eV, causes E_F to be pinned at EL6 [Fig. 3(b)], as reported in the literature[17] when

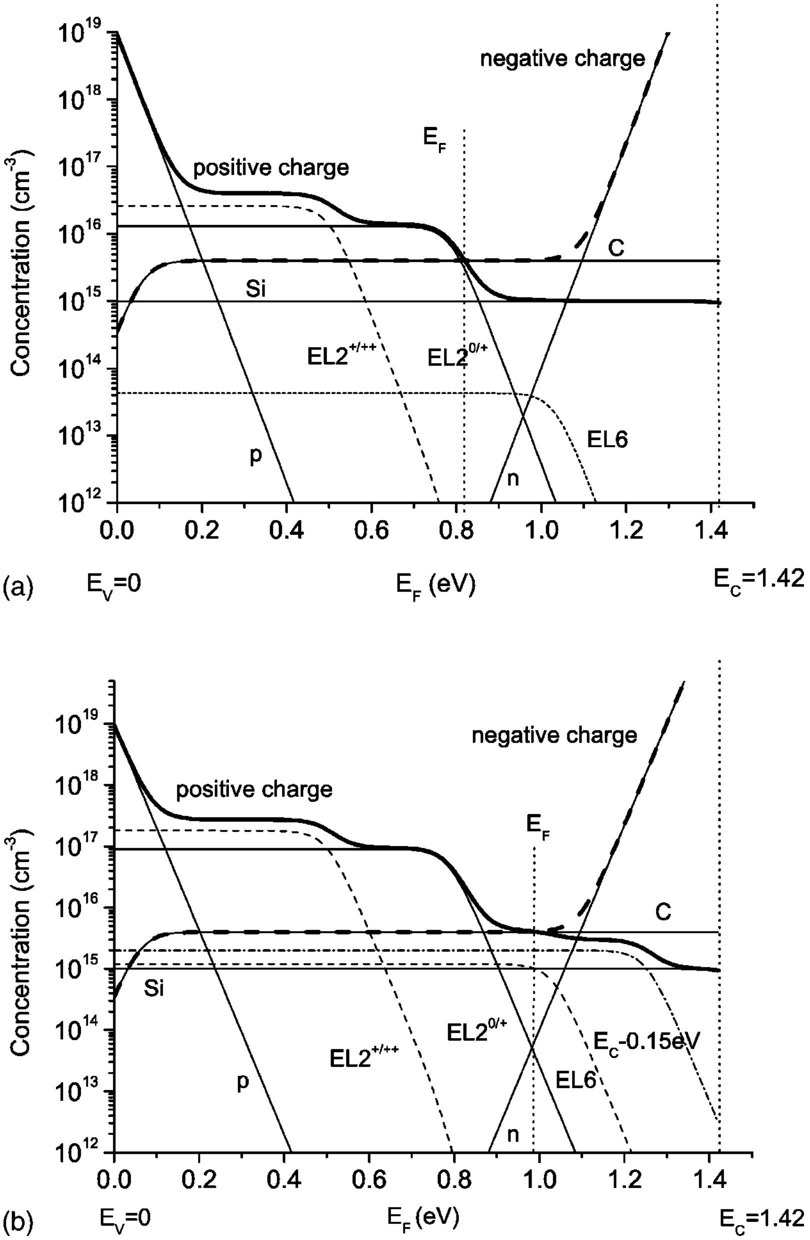

FIG. 3. (a) A Shockley diagram for the nonirradiated material: the positive charge includes [Si] unintentional doping, the two charged states of EL2, i.e., $[EL2^{0/+}]$ and $[EL2^{+/++}]$, the free density of holes p and [EL6]. Negative charge includes [C] unintentional doping and free density of electrons n. The intercept of positive and negative charge gives the Fermi-level energy value. In this view the Fermi level is pinned to EL2. (b) A Shockley diagram for the irradiated material: the positive charge includes [Si] unintentional doping, the two charged states of EL2, i.e., $[EL2^{0/+}]$ and $[EL2^{+/++}]$, the free density of holes p, [EL6] and the level at $E_C - 0.15$ eV. Negative charge includes [C] unintentional doping and free density of electrons n. The introduction of donor levels at 0.15 eV and 0.37 eV from the conduction band in concentrations in the order of 10^{15} cm^{-3} shifts the Fermi level toward the conduction band.

this level is present in high concentration. When the EL2 energy level lies well below E_F, the defect is mainly in the neutral state and the space-charge region begins at the interception of E_F with EL6, as shown in Fig. 4(b).

(b) Net effective charge density: The other crucial point of our investigation is that the net charge density N_{eff} in the buried space charge region is of the order of 10^{13} cm^{-3}, further decreasing after irradiation from 3.0×10^{13} cm^{-3} to 1.6×10^{13} cm^{-3}. When EL2 field enhanced neutralization no longer exists, the compensation by other deep donors must intervene to justify the value $N_{\text{eff}} \approx 10^{13}$ cm^{-3}.

Recently, Ling *et al.*[14] analyzed the electric field decay as a function of temperature by positron lifetime spectroscopy and suggested that "apart from the processes of ionization of EL2 and the field enhancement of the EL2 capture cross section which determine the electric field strength close to the contact, there exists another thermally activated process neutralizing the net charge density in the space charge region." The activation energy of this process is $E_T = (1.03 \pm 0.15)$ eV, which could correspond to the levels EL6 or EL5,[14,15] located at $E_C - 0.35$ eV and $E_C - 0.42$ eV, respectively, known as strong recombination centers.[18] These levels could then play a significant role in determining the electrical characteristics of SI GaAs Schottky diodes. Thus, a further mechanism of neutralization occurring in the space charge region can be invoked beside the compensation among the different defects. This hypothesis is strengthened when considering the similarity in the structures of the above cited defects. Many models have been proposed concerning the nature of the levels at $E_C - 0.15$ eV and $E_C - 0.37$ eV,[10,16–22] but with no definite confirmations.

Previously, the role of EL2 as being uniquely responsible for the properties of SI GaAs was questioned and a strong

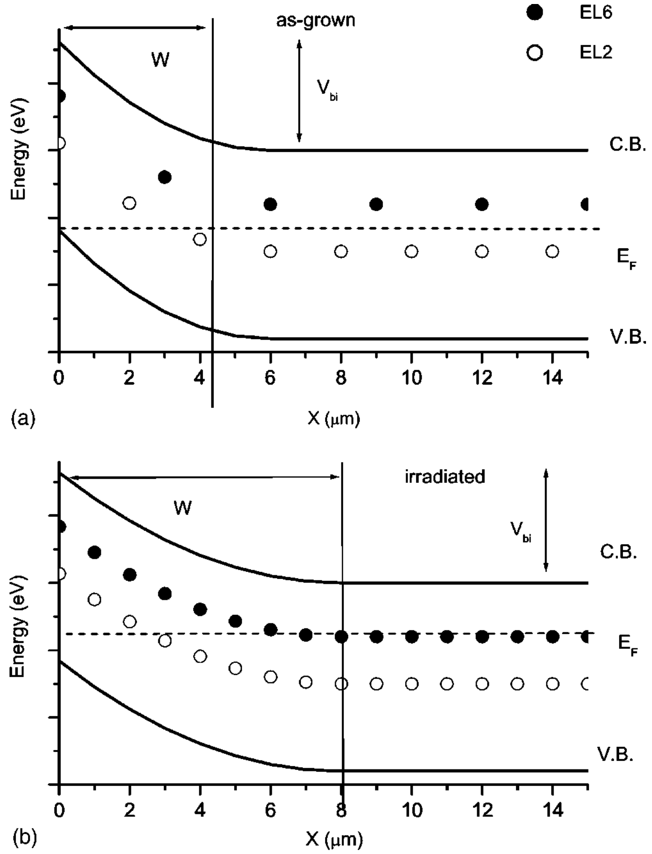

FIG. 4. Band diagram simulation for the unirradiated (a) and irradiated (b) materials. The intercept of the Fermi level deep in the bulk with EL2 (before irradiation) or EL6 (after irradiation) determines the quasineutral region extent. Calculations have been made for $V_{bi}=0.8$ eV.

interaction was suggested between EL2 and other defects, principally EL6,[19–21] whose microscopical origin could involve the EL2 defect among its constituents.[22] Furthermore, a similarity of the $E_C-0.15$ eV behavior with that theoretically predicted for the complex defect As_{Ga}-V_{As} has been observed.[16] Such observations can provide the key to explaining why the Mott barrierlike behavior persists when donors other than EL2 control the diode electrical properties, as observed in Fig. 1. If EL2 were the only trap undergoing a field-enhanced neutralization, we would expect that, when the electric field is controlled by EL6, a standard Schottky diode behavior would take place. Then a space charge would originate from the metallization and widen with applied bias, differently from what was observed.

Recent studies, however, suggest that the field-enhanced neutralization may be related to the fully nonradiative relaxation multiple phonon emission (MPE) capture process by the As_{Ga} defects assisted by the applied electric field.[23] Consequently, each defect containing this antisite should undergo this process in high field conditions, giving rise to the observed Mott barrierlike behavior. Since both EL6 and $E_C-0.15$ eV structures could contain As_{Ga},[16,22] their possible field enhanced neutralization can be invoked to account for the Mott barrier behavior observed after irradiation.

In summary, the Mott barrierlike behavior of SI GaAs diodes is controlled by defect-associated electronic levels. The study of the electric field distribution after irradiation has been correlated to the changes in the defect population induced by proton irradiation, generating levels at $E_C-0.37$ eV and $E_C-0.15$ eV. The introduction of such donors in addition to EL2 shifts the Fermi level towards the conduction band, significantly altering the ionization degree of EL2, which loses its dominance in the control of electrical characteristics. Moreover a field-enhanced neutralization effect, such as for EL2, is supposed to act for these donorlike traps, consistently with their proposed structure.

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