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Defect models in electron-irradiated n-type GaAs

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1 MeV electron irradiation has been performed in degenerate, n-type \( (n\approx 2\times 10^{17} \text{ cm}^{-3}) \), molecular beam epitaxial GaAs layers, and Hall effect measurements have been carried out during the irradiation in order to get accurate defect production data. The results have been fitted with statistical models, and are most consistent with the usual \( E_1 (E_F=0.045 \text{ eV}) \) and \( E_2 (E_C=0.15 \text{ eV}) \) levels being the \((-\downarrow)\) and \((\uparrow/\downarrow)\) transitions of the As vacancy, respectively. Also, an acceptor well below \( E_C=0.15 \text{ eV} \) is produced at a much higher rate than that of \( E_1 \) and \( E_2 \).

I. INTRODUCTION

Over the last few years, an understanding of the defects in GaAs has become more important. These defects, which can greatly affect the electrical and optical properties of the material, may be present as a result of growth conditions, or also as a result of irradiation with high energy particles. For example, irradiation with 1 MeV electrons will produce intrinsic defects such as vacancies, interstitials, and possibly antisites.\(^1\)\(^-\)\(^3\) In as-grown material, such intrinsic defects may interact among themselves, or with impurities to form complex defects. However, it is first necessary to understand the simple defects before the complex ones can be identified. Another motivation for studying the effects of electron irradiation is the wealth of space applications for GaAs devices, because the damage caused by protons, neutrons, and gamma rays in space can often be usefully simulated by 1 MeV electron irradiation.\(^4\)

Much work has been done in an effort to identify the defects produced in GaAs by electron irradiation, and the situation is summarized in recent review articles.\(^1\)\(^-\)\(^3\) The most widely studied defects are electron traps, usually designated as \( E_1 \) (at \( E_C=0.045 \text{ eV} \)), \( E_2 \) (at \( E_C=0.15 \text{ eV} \)), and \( E_3 \) (at \( E_C=0.29 \text{ eV} \)). However, even these traps have not been firmly identified, although they are generally thought to be related to the As vacancy \( V_{As} \). One problem here is that \( V_{As} \) would naively be expected to be a donor, but yet the Fermi level continuously drops during irradiation of \( n\)-type GaAs. Thus, there should be acceptors, below midgap, which are being produced at a higher rate than \( E_1 \) and \( E_2 \) combined, or else \( E_1 \) and/or \( E_2 \) must themselves be acceptors. Recently this problem has been studied by Hall effect measurements\(^5\)\(^,\)\(^6\) in pure GaAs, but not in heavily doped material.

To further investigate these effects, we have designed and constructed an \textit{in situ} Hall effect apparatus which allows continuous measurements while the electron beam is on; thus, very detailed defect production rate data may be obtained.\(^7\) The donor and acceptor production rates are obtained through a solution of the charge-balance equation, corrected for degeneracy using the Ehrenberg approximation. We have chosen samples of high enough concentration that the Fermi level \( \epsilon_F \) is near the conduction band edge, so that \( \epsilon_F \) may be swept through \( E_1 \) and \( E_2 \) during the irradiation.

II. EXPERIMENT

For this experiment, the 1 MeV electrons were produced by a van de Graaff generator and traveled through a short span of air to hit the sample. Typical current densities were 0.4 \( \mu \text{A/cm}^2 \). The entire configuration has been described elsewhere,\(^7\) and therefore a detailed description will not be given here. The material studied was an \( n\)-type molecular beam epitaxial (MBE) layer, doped with Si at about \( 2\times 10^{17} \text{ cm}^{-3} \) to put \( \epsilon_F \) close to the conduction band edge. This concentration is also important for metal-semiconductor field-effect transistor applications. Thick samples (10 \( \mu \text{m} \)) were used in order to minimize the severity of surface and interface free carrier depletion effects, which typically totaled 0.1–0.5 \( \mu \text{m} \) (Ref. 8) for the conditions of this study. Although small, these corrections were included for completeness. All irradiations were performed at room temperature.

III. THEORY

It is well known that shallow impurities in semiconductors, such as Si in GaAs (at \( E_C=0.006 \text{ eV} \)), can form an energy band at high concentrations and produce a second conduction mechanism.\(^9\) As the concentration is further increased, this band can overlap the conduction band and the electrons in the two bands are indistinguishable. Lowney\(^10\) has shown that for a hydrogenic donor concentration greater than \( 1\times 10^{17} \text{ cm}^{-3} \) in GaAs, neither a bound state nor an impurity band exists at 300 K. This idea is supported by the lack of free carrier freeze-out, even at 4 K. Thus, we assume that each Si atom provides an electron which takes part in the conduction.

The measured carrier concentrations are related to physical parameters by means of statistical theory. The energy distribution function for electrons in an energy band is

\[
\begin{equation}
    f(\epsilon) = \frac{1}{1 + e^{(\epsilon - \epsilon_F)kT}},
\end{equation}
\]
where \( \varepsilon_F \) is the Fermi energy. In this work, we will measure all energies from the valence band. The distribution function for defects or impurities is often assumed to be of the form:

\[
f(\varepsilon) = \frac{1}{1 + Ke^{(\varepsilon - \varepsilon_F)/kT}},
\]

where \( K \) is a degeneracy factor. To apply these expressions we must find \( \varepsilon_F \), which is done by solving the charge balance equation:

\[
n + \sum_k N_{Ak} = p + \sum_k N_{Dk}.
\]

where \( N_{Ak} \) and \( N_{Dk} \) denote particular acceptor and donor concentrations, respectively. For single donors, i.e., centers that are either neutral or have a single, positive charge, the unoccupied state density (that of the charged state) can be written as

\[
N_{A+}^+ = N_A^+ e^{(\varepsilon_A^+ - \varepsilon_F)/kT},
\]

where \( N_A \) is the number of acceptors, \( \varepsilon_A \) is the energy of the donor level measured from the valence band, and the \( g_k \)'s are the degeneracies of the occupied (\( g_1 \)) and unoccupied (\( g_0 \)) states, respectively. Similarly, the number of charged (or occupied in this case) acceptors can be written

\[
N_{A-}^- = N_A^- e^{(\varepsilon_A^- - \varepsilon_F)/kT},
\]

where \( N_A \) is the number of acceptors, and \( \varepsilon_A \) is again measured from the valence band. Therefore, the charge balance equation becomes (for a system with one single acceptor state and one single donor state)

\[
n + N_A^+ + N_A^- = p + N_D^+ + N_D^- e^{(\varepsilon_A - \varepsilon_F)/kT},
\]

where \( n \) and \( p \) can also be related to \( \varepsilon_F \). The form of the charge balance equation given above can be used to obtain production rates for donors and acceptors being produced by the irradiation. The procedure is to assume that the number of donors or acceptors produced is the product of a production rate \( \phi \) and the irradiation dose \( \phi \), so that Eq. (6) becomes

\[
n + \phi r_A/1 + \frac{\varepsilon_A}{\varepsilon_A} e^{(\varepsilon_A - \varepsilon_F)/kT} = p + \phi r_D/1 + \frac{\varepsilon_D}{\varepsilon_D} e^{(\varepsilon_D - \varepsilon_F)/kT}.
\]

Similar forms of the charge balance equation can be written for systems with other combinations of donors and acceptors, including multiple charge states of the same defect.

The carrier concentrations found during irradiation need to be corrected for two factors before inclusion in the charge balance equation. The first factor is the Hall \( r \) factor, which usually varies between 1.0 and 1.3 for GaAs.

IV. RESULTS

If \( E1 \) and \( E2 \) are indeed two charge states of \( V_{Ga} \) then there are three reasonable choices for their donor or acceptor nature. The first is that of a double donor (DD) with \( E1 \) and \( E2 \) representing the \((0+/+)\) and \((+/+)\) transitions, respectively. The second possibility is that of a single donor state and a single acceptor state (SD/SA), with \( E1 \) as the \((-/-)\) transition and \( E2 \) the \((0+/+)\) transition. Finally, we must consider the double acceptor (DA) model, with the transitions \((-/-)\) and \((-/-)\) for \( E1 \) and \( E2 \), respectively. For each model, the corrected carrier concentration data were used to find the production rates for the \( E1 \) and \( E2 \) levels, as well as that of an acceptor state, arbitrarily taken to be 0.1 eV above the valence band (close to the theoretical position of the gallium vacancy, \( V_{Ga} \)). However, our results do not determine the acceptor energy except to place it well below \( E_C - 0.15 \) eV. The correct form of the charge balance equation was then used to perform a least squares fit for the production rates. As an example, if \( E1 \) and \( E2 \) represent a double acceptor, then the charge balance equation would be written
FIG. 1. The free electron concentration $n$ (circles) and ionized defect and impurity concentration $N_f$ (triangles) as a function of electron fluence $\Phi$. The solid line through the circles is a theoretical fit of $n$ vs $\Phi$ with $\tau_E$ floating, and the dotted line is for $\tau_E$ fixed at 1.5 cm$^{-1}$. The solid lines through the triangles are theoretical fits of $N_f$ vs $\Phi$ for a single shallow acceptor (SSA) and double shallow acceptor (DSA), respectively. All theoretical fits in this figure are based on $V_{A_d}$ having double donor nature with the fitting parameters given in Table I.

\[ n + \tau_E \phi / 1 + \frac{\sigma_0}{\sigma_1} e^{(\epsilon_1 - \epsilon_F)/kT} + \frac{\sigma_2}{\sigma_1} e^{(\epsilon_2 - \epsilon_F)/kT} + 2\tau_E \phi / 1 + \frac{\sigma_0}{\sigma_2} e^{(\epsilon_2 - 2\epsilon_F)/kT} + \frac{\sigma_1}{\sigma_2} e^{(\epsilon_1 - \epsilon_F)/kT} + \tau_A \phi + N_{A_d} = p + N_{D_d} \]  

(9)

where $\epsilon_1 = 1.424 - 0.15 = 1.274$ eV would be the energy at 296 K necessary to bring an electron from the valence band onto the neutral $V_{A_d}$, making it $V^{+}_{A_d}$, and $\epsilon_2 = 1.274 + (1.424 - 0.045) = 2.653$ eV would be the energy of the two-electron system after a second electron was added, making $V^{++}_{A_d}$. The relevant degeneracies would be $g_0 = 6$, $g_1 = 15$, and $g_2 = 20$, since the $V^0_{A_d}$, $V^{+}_{A_d}$, and $V^{++}_{A_d}$ states have 1, 2, and 3 electrons, respectively, in a six-fold degenerate $T_2$ state. Also, in Eq. (9), $\tau_E$ would be the production rate of both $E1$ and $E2$ (each a transition related to $V_{A_d}$), $\tau_A$ the production rate of the acceptor (assumed to be at $E_F + 0.1$ eV), and $N_{D_d}$ and $N_{A_d}$ the donor (Si) and acceptor (C) concentrations, respectively, of the material before irradiation.

The data, shown in Figs. 1-3, were fitted to Eq. (9) (or the analogs for the DD and SD/SA cases) either by allowing both $\tau_E$ and $\tau_A$ to float or by holding $\tau_E$ at 1.5 cm$^{-1}$ (approximately the literature value) and floating only $\tau_A$. In each figure, the solid line through the $n$ vs $\Phi$ points represents the best fit for both $\tau_E$ and $\tau_A$ floating, while the dashed line is for fixed $\tau_E=1.5$ cm$^{-1}$ and only $\tau_A$ floating. The best fit parameters as well as a sum of squares (SSQ) are given in Table I. Here we have assumed that $\tau_A$ represents a single acceptor; for the double acceptor case, $\tau_A$ must be divided by 2. As can be seen in the figures and from the SSQ values, all of the dashed lines ($\tau_E=1.5$ cm$^{-1}$) give poor fits, and all of the solid lines good fits, with the SD/SA fit having the lowest SSQ of the three possibilities. Further information may be obtained by analyzing the mobility data $\mu$ vs $\phi$. From the $n$ vs $\phi$ fits, we can

![Graph](image-url)

FIG. 2. Symbols same as in Fig. 1, but all theoretical fits based on $V_{A_d}$ having single donor/single acceptor nature with the fitting parameters given in Table I.

![Graph](image-url)

FIG. 3. Symbols same as in Fig. 1, but all theoretical fits based on $V_{A_d}$ having double acceptor nature with the fitting parameters given in Table I.

\[ \text{TABLE I. Fitting parameters used in Figs. 1-3. The SSQ is a relative measure of the goodness of fit.} \]

<table>
<thead>
<tr>
<th>Figure</th>
<th>Case</th>
<th>Solid lines $\tau_E$</th>
<th>Solid lines $\sigma_{A_d}$</th>
<th>Dashed lines $\tau_E$</th>
<th>Dashed lines $\sigma_{A_d}$</th>
<th>SSQ</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>double donor</td>
<td>0.38</td>
<td>1.80</td>
<td>0.0264</td>
<td>1.50</td>
<td>2.33</td>
</tr>
<tr>
<td>2</td>
<td>single donor</td>
<td>0.55</td>
<td>1.37</td>
<td>0.0138</td>
<td>1.50</td>
<td>1.19</td>
</tr>
<tr>
<td>3</td>
<td>double acceptor</td>
<td>0.63</td>
<td>0.85</td>
<td>0.0744</td>
<td>1.50</td>
<td>0.06</td>
</tr>
</tbody>
</table>

*Values assuming that $\tau_A$ represents a single acceptor. If $A$ is really a double acceptor, then the $\tau_A$ values should be divided by 2.
determine the charged fractions of \( V_{\text{As}} \) and the acceptor at a particular \( \phi \), sum these fractions to determine the total ionized concentration \( N_I \) (remembering to weight the various fractions by \( Z^2 \), where \( Z \) is the charge), and compare this \( N_I \) with that found from a Boltzmann equation analysis of the experimental \( \mu \) value at the same \( \phi \). For each case (DD, SD/SA, DA) we have determined \( N_I \) vs \( \phi \) under two different assumptions: (1) the shallow acceptor created by the irradiation is singly charged (SSA); and (2) it is doubly charged (DSA). It is possible that this acceptor could even be triply charged, as has been suggested for the defect \( V_{\text{Ga}} \), but we did not include this possibility in the figures. The best fit of \( N_I \) vs \( \phi \) is also for the SD/SA case, with the assumption that the irradiation acceptor \( A \) is doubly charged. Thus, both the \( n \) vs \( \phi \) and \( N_I \) vs \( \phi \) curves can be explained if \( E1 \) is the (\(-/-\)) transition, and \( E2 \) the (0/+) transition of a \( V_{\text{As}} \)-related defect, having a production rate of 0.6 cm\(^{-1}\), and \( A \) is a doubly charged acceptor, with a production rate of 0.7 cm\(^{-1}\). The good fits for the SD/SA case do not of course totally exclude the other cases because all of the \( n \) vs \( \phi \) fits were reasonably good, and the \( \mu \) vs \( \phi \) data could be influenced by irradiation-induced inhomogeneity.

V. DISCUSSION

The SD/SA case seems to give the best fits to both the \( n \) vs \( \phi \) and \( N_I \) vs \( \phi \) data, although not overwhelmingly so. However, there are additional negative factors regarding the other two cases. For example, the (+/+ +) transition of the DD case might be expected to have an energy much larger than \( E_C - 0.15 \) eV, since the electron must come from the deep \( A_1 \) state which is usually assigned an energy quite close to the valence band.\(^7\) Also, the AA case is doubtful on the basis of the capture cross section of \( E1 \), \( 2 \times 10^{-15} \) cm\(^{-2}\), which seems much too large for a (\(-/-\)) transition, in which an electron is being captured on an already negative center. It is somewhat disturbing, however, that the \( \tau_{\gamma} \)'s for all three cases are well below the values of 1.5–2.0 cm\(^{-1}\) measured by earlier DLTS and Hall effect measurements.\(^5\) The same holds for the value of \( \tau_{\phi} \), which was found to be about 4 cm\(^{-1}\) for a single shallow acceptor (or 2 cm\(^{-1}\) for a double shallow acceptor) in a Hall effect study.\(^5\) The answer could lie in the fact that most of these earlier studies were performed on much purer GaAs samples (\( n \approx 10^{14} \text{ to } 10^{15} \) cm\(^{-3}\)) compared with the \( 10^{17} \) cm\(^{-3}\) samples being considered here. Indeed, electron loss rates \( \Delta n/\Delta \phi \) of 0.5–5.0 cm\(^{-1}\) have been reported in the literature,\(^5\) and some of this variation may arise from differences in materials although measurement conditions, such as beam current density, could also be important. It is tempting to normalize our \( \tau_{\phi} \) value of 0.55 cm\(^{-1}\) to the accepted value of 1.5 cm\(^{-1}\), which would then bring \( \tau_{\phi} \) to 1.9 cm\(^{-1}\), close to the previously measured value; however, we can find no obvious justification for this procedure. In spite of our lower values of \( \tau_{\phi} \) and \( \tau_{\gamma} \), one central point should not be missed, namely, that the acceptor center \( A \) (represented by \( \tau_{\phi} \)) is being produced at a higher rate than that of \( E1 \) and \( E2 \), which were previously thought to be the dominant electron irradiation centers. This was also the central message of an earlier Hall effect study in which it was suggested that \( A \) may be related to Ga sublattice damage,\(^5\) although the production of \( V_{\text{As}} \) with the subsequent hopping transition \( V_{\text{As}} \rightarrow V_{\text{Ga}} \text{GaAs} \) cannot be ruled out.\(^6\)

In summary, we have shown that an acceptor well below \( E_C \)–0.15 eV is being produced at a high rate in degenerate, n-type GaAs. By fitting \( n \) vs \( \phi \) and \( N_I \) vs \( \phi \) to statistical models, it appears most likely that \( E1 \) is the (\(-/-\)) transition and \( E2 \) the (0/+) transition of \( V_{\text{As}} \), and that the irradiation acceptor is doubly charged. However, these conclusions are not absolute, and the final model must await further studies.

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\(^1\)J. C. Bourgoin and H. J. van Baakeland, J. Appl. Phys. 64, R65 (1988).