Anisotropic-Defect Introduction in GaAs by Electron Irradiation

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The energy dependence of the introduction rates of the main defects created in GaAs by electron irradiations in the two crystallographic directions [111] and [$\bar{1}\bar{1}\bar{1}$] have been measured. It is demonstrated that the defects introduced are caused by displacements of As atoms and not of Ga atoms, as previously believed. We show that the observed anisotropy can be explained by an orientation dependence of the threshold energy in the range 7–11 eV.

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When a crystal is irradiated with energetic electrons, the damage results from the transmission of kinetic energy to the lattice atoms through elastic collisions.[1] When the transmitted energy to a knocked atom is larger than a threshold energy T_d, the atom is displaced from its regular site into an interstitial position and a Frenkel (vacancy-interstitial) pair is created. This notion of threshold energy for atomic displacements implies that the atom is bound to the lattice in an isotropic potential well of depth equal to T_d and that the probability of displacement is unity for a transmitted energy larger than T_d and zero if it is less. It is a first approximation, since the potential well will have a more complicated and less steep shape than a simple step function, and its depth, and hence the threshold energy, will depend on the direction in which the displaced atom is scattered.

In a compound semiconductor, a possible anisotropy of the threshold energy, and consequently of the introduction rate of a particular defect, can be used to distinguish between displacements occurring on the different sublattices.[2] Thus, the study of this anisotropy is of considerable interest in compound semiconductors, since it may allow the nature of the created defects to be determined. In this Letter, we demonstrate that the main electron-irradiation–induced defects in GaAs are due to displacements of As atoms and therefore that the previous identification[3] of Ga-displacement–related defects is incorrect.

Let us consider the case of GaAs (zinc-blende structure): For an irradiation in a [111] Ga direction it will be "hard" to displace an As atom, because a nearest-neighbor Ga atom is exactly in the forward beam direction (see Fig. 1); it will be "easy" to displace a Ga atom because the lattice is widely open in front of it. Of course, the situation is reversed in the case of an irradiation in a [111] As direction. Thus, it can reasonably be expected that the introduction rate of a defect due to the displacement of an As atom, for example, will be larger for an irradiation along a [111] As direction than along a [111] Ga direction, and conversely for a defect due to the displacement of a Ga atom.

This method, first proposed by Eisen,[2] has been used in various III-V and II-VI compounds.[4] In GaAs, Arnold and Gobeli[5] observed that the decrease of photoluminescence was larger for 420-keV electrons in a [111] As direction than in a [111] Ga direction and concluded that the nonradiative centers which are responsible for the decrease of photoluminescence originate from

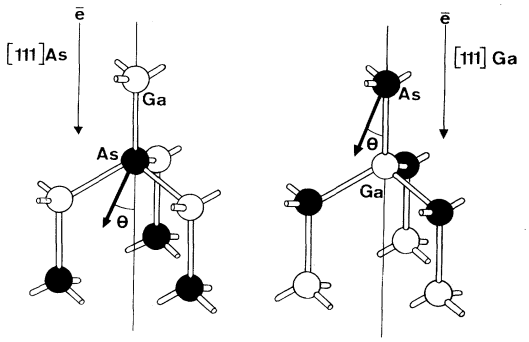

FIG. 1. Zinc-blende structure of GaAs. The [111] Ga and [111] As directions are, respectively, "hard" and "easy" directions for displacements of As atoms, and conversely for Ga atoms.

the displacement of As atoms. Lang, Logan, and Kimerling,[3] using capacitance techniques, have obtained the opposite result, namely that the defect introduction rates for 1-MeV electrons were larger in a [111] Ga direction than in a [111] As direction, and concluded that the created defects (electron traps labeled $E1$ to $E5$)[6] were due to Ga displacements.

In order to obtain convincing conclusions from such experiments, two conditions must be met. Firstly, it is necessary to investigate the defects in a region below but close to the surface of the samples. This is in order to avoid, on the one hand, surface effects (to which photoluminescence could be sensitive), and, on the other hand, too large a spreading of the incident beam at greater depths due to electronic scattering (for example, for a 0.5-MeV irradiation, the average deviation from the initial direction of the beam is about 40° at a depth of 30 μm). Secondly, the irradiations should be performed at electron energies close to the threshold T_d, for the following reason. In an elastic collision, an incident electron of kinetic energy E and mass m transmits to the recoil atom of mass M an energy T,

$$T=(2m/M)E(2+E/mc^2)\cos^2\theta, \quad (1)$$

where c is the velocity of light and θ is the scattering angle of the displaced atom with respect to the incident direction of the electrons. The maximum energy which can be transmitted corresponds, of course, to a scattering angle θ equal to zero. For electron energies close to the threshold energy, only those atoms to which the maximum energy is transmitted in the collision are displaced and their scattering angles are therefore close to zero. Clearly it is only in this last case that the displacement of an As atom will be affected by the nearest-neighbor Ga atom directly in the forward beam direction for an irradiation along the [111] Ga direction, for instance. When the energy of irradiation is larger, the knocked-on atom can be displaced with a large scattering angle. Typically for 1-MeV irradiation, the average scattering angle is 57° and the Ga atom no longer prevents the displacement of the As atom. In other words, a possible anisotropy of the defect introduction rate will only be significant for transmitted energies close to the threshold energy.

Capacitance experiments are well adapted for the measurement of the orientation dependence of the introduction rates and threshold energies, since they enable the defect concentration to be measured in a depth of order 1 μm, where the direction of the incident electrons can be assumed to be still preserved. It is the purpose of this Letter to present the results of the determination by deep-level transient-spectroscopy (DLTS) technique[6] of the anisotropy of defect introduction rates in GaAs. This experiment has been performed using bulk n-type Czochralski-grown GaAs. Aluminum Schottky diodes have been evaporated on mechanochemically, then chemically polished Ga(111) and As(111) wafers. The dopant concentration before irradiation was 6×10^{16} cm^{-3}. The experimental setup of our DLTS spectrometer has been described elsewhere.[7] A detailed study of each diode has been performed before irradiation. This bulk material contains two electron traps which are similar to the traps labeled EL2 and EL6 by Martin, Mitonneau, and Mircea.[8] The concentrations of these traps were, respectively, 6×10^{15} and 2×10^{15} cm^{-3}. Electron irradiations were performed at 300 K using a Van de Graaff accelerator. The electron beam was scanned over a large area compared to that of the samples in order to ensure a uniform dose. The electron flux was of the order 0.5 μA cm^{-2} and the doses were chosen in such a way that the concentration of the introduced defects was in all cases less than 10% of the dopant concentration. For a given energy, two samples were irradiated simultaneously, one oriented in a [111] Ga direction, the other in a [111] As direction, so that they received rigorously the same dose at the same energy.

The DLTS spectra recorded after irradiation exhibit the well-known $E1$, $E2$, and $E3$ traps.[6] The $E4$ and $E5$ traps are probably present, but are masked by the EL2 trap originally present. Because the $E3$ and EL6 traps have comparable emission rates, they cannot be resolved in the DLTS spectra. The concentration of the $E3$ trap (of the order of that of the EL6 trap) has been obtained by subtracting spectra after and before irradiation, carefully recorded in exactly the same conditions of diode polarization, refilling pulse duration, and emission rate window. This procedure is justified by the fact that the irradiation has introduced only negligible changes in the static electrical characteristics of the diodes.

We have plotted in Fig. 2 the "anisotropy ratios" as a function of the electron energy for the traps $E1$, $E2$, and $E3$. The anisotropy ratio is defined as the ratio of the introduction rates along the [111] As and [111] Ga directions, of a given deep trap at a given energy. It can be seen that for

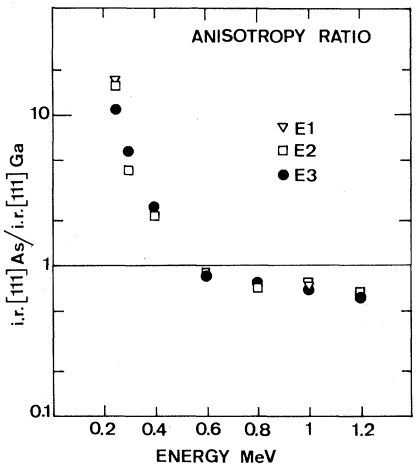

FIG. 2. Orientation dependence of the introduction rates of the $E1$, $E2$, and $E3$ levels, as a function of the energy of irradiation. The anisotropy ratio is defined as the ratio of introduction rates along [111] As and [111] Ga directions.

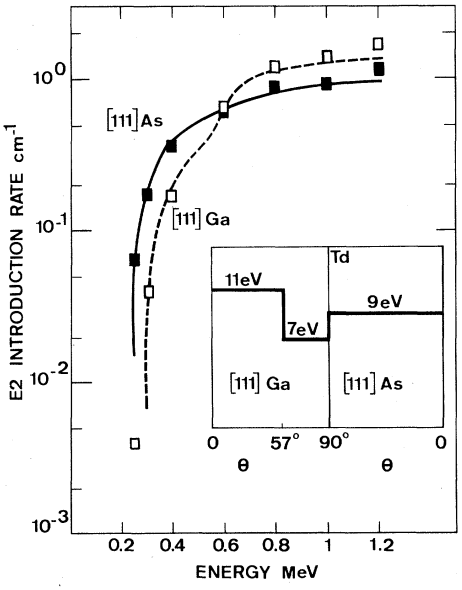

FIG. 3. Introduction rates of the $E2$ level in the two opposite directions [111] As and [111] Ga. Solid and dashed lines are calculations of the cross section for displacement of As atoms, respectively, in the [111] As and [111] Ga directions. These cross sections have been calculated using the orientation dependence for the threshold energy shown in the inset. The normalization constant to fit the data is the same for the two curves.

energies above 0.6 MeV, the introduction rates are larger for an irradiation along the [111] Ga direction than along the [111] As direction, in qualitative agreement with the results of Lang, Logan, and Kimerling.[3] However, for low energies the situation is reversed: At 0.25 MeV, for instance, the introduction rates are more than ten times larger for all three traps for an irradiation along the [111] As direction than along the [111] Ga direction. With the help of the arguments developed above, we can therefore conclude that the main deep traps introduced by electron irradiation in GaAs are due to displacements of As atoms, and not, as proposed by Lang, Logan, and Kimerling,[3] of Ga atoms.

We have plotted in Fig. 3 the introduction rate of $E2$ in the two opposite directions, as a function of the electron energy. These results are compared with theoretical curves of displacement cross sections, calculated with the McKinley-Feshbach approximation[9] (which can be shown to be equivalent to the exact Mott formulation in the case of As and Ga [1]) and normalized to fit the data. For the [111] As direction, a reasonable agreement is obtained under the assumption of an abrupt threshold energy $T_d = 9$ eV. (This value is in quantitative agreement with the value $T_d = 10$ eV found by Pons, Mooney, and Bourgoin[7] for the [110] direction.) However, the results corresponding to the [111] Ga direction cannot be fitted using one single value of the threshold.

A simple examination of Fig. 1 shows intuitively that the threshold energy for the displacement of an As atom should not depend strongly on the scattering angle θ for an irradiation along the [111] As direction, at least for low values, whereas it should in the opposite direction. For small scattering angles, a large threshold energy is expected to account for the strong core-core repulsive energy. For larger scattering angles, the first-neighbor Ga atom no longer hinders the displacement of the As atom; consequently the threshold energy must decrease with increasing scattering angles.

A good agreement with the experimental results can be obtained by taking $T_d = 11$ eV for small scattering angles and $T_d = 7$ eV for large scattering angles, as shown in the inset of Fig. 3. The introduction rate curve at low energies is sensitive to the choice of T_d for $\theta \simeq 0$, whereas at high energies it is sensitive to the choice of T_d for large θ, so the two values of 11 and 7 eV were obtained by fitting in these regimes. Likewise the transition angle of $\theta = 57°$ between the two was chosen for the best fit at intermediate energies. The abrupt transition is of course an oversimplification and is responsible for the unrealistic shape of the calculated curve in the

range 0.5–0.7 MeV.

Work is now in progress to understand the crossover between the introduction rate curves. Preliminary calculations from a simple hard-sphere model of secondary elastic collisions between the initially knocked-on atom and its four nearest neighbors show that the crossover could result from these secondary collisions and should be a general consequence of the tetrahedral symmetry of the crystal.[10] In the case of an irradiation along the [111] As direction, for instance, for large scattering angles θ, a large fraction of the initially knocked-on As atoms must interact with one of their three off-axis nearest neighbors, which should lower the global probability of effective As displacement at large energy and give the anisotropy reversal.

In conclusion, we have demonstrated that the main defects created by electron irradiation in n-type GaAs are originated by atomic displacements in the As sublattice and not in the Ga sublattice as previously suggested. We have shown that the observed anisotropy of the introduction rates could be accounted for by an orientation dependence of the threshold energy for the displacement of As atoms in the range 7–11 eV.

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[1]For a discussion of damage phenomenology, see, for example, J. W. Corbett and J. C. Bourgoin, in *Point Defects in Solids*, edited by J. H. Crawford and L. M. Slifkin (Plenum, New York, 1975), Vol. 2, Chap. 1.

[2]F. H. Eisen, Phys. Rev. 135, A1394 (1964).

[3]D. V. Lang, R. A. Logan, and L. C. Kimerling, Phys. Rev. B 15, 4874 (1977).

[4]For a review on this question, see Ref. 1.

[5]G. W. Arnold and G. Gobeli, in *Radiation Effects in Semiconductors*, edited by F. L. Vook (Plenum, New York, 1968), p. 435.

[6]D. V. Lang and L. C. Kimerling, in *Lattice Defect in Semiconductors 1974*, Institute of Physics Conference Series No. 23 (Institute of Physics, London, 1975), p. 581.

[7]D. Pons, P. M. Mooney, and J. C. Bourgoin, J. Appl. Phys. 51, 2038 (1980).

[8]G. M. Martin, A. Mitonneau, and A. Mircea, Electron. Lett. 13, 191 (1977).

[9]W. A. McKinley, Jr., and H. Feshbach, Phys. Rev. 74, 1759 (1948).

[10]Such a crossover has also been observed in InAs, the only other III-V or II-VI compound for which the anisotropy of the irradiation creation rates has been determined in a large enough range of energy: See D. J. C. Lindsay and P. C. Banbury, in *Radiation Damage and Defects in Semiconductors*, edited by J. E. Whitehouse, Institute of Physics Conference Series No. 16 (Institute of Physics, London, 1973), p. 34.