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Energy and orientation dependence of electron-irradiation-induced defects in InP

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The concentration of several electron-irradiation-induced deep defect levels in InP has been measured by deep-level transient spectroscopy as a function of electron energy. The dominant centers exhibit a threshold at about 100 keV, which clearly points to a primary production event by electron–phosphorus-atom collision. This unambiguous determination allowed a test of the recently proposed orientation dependence technique to find the nature of the sublattice involved in the collision process for III-V compounds. A good quantitative agreement is obtained with a hard-sphere model for secondary collisions if disorientation of the beam in the sample is taken into account. Other traps exhibit higher thresholds which correspond either to indium-atom displacements or to the involvement of secondary collisions in the production event.

Electron irradiation is a convenient way to produce simple defects in semiconductors, widely used in the past.[1] However, their identification is hampered in III-V compounds by the multiplicity of possible defects. When the two lattice atoms have very different masses as for InP, the problem is simplified because at low enough energies the electrons are expected to be able to displace only the light atom. For compounds where the atoms have comparable masses like GaAs, an orientation dependence technique has been proposed to determine which is the displaced atom in the production event.[2]

We have applied both techniques to InP, where previous work[3–5] has shown that irradiation at 25 or 300 K induced many deep centers mostly stable at room temperature (RT). Electron traps were detected by deep-level transient spectroscopy (DLTS)[6] in Zn diffused p^+-n diodes [$n \simeq (2\text{–}4) \times 10^{16}\ e^-\,\mathrm{cm}^{-3}$] and hole traps in Schottky barriers on Zn doped InP [$p \simeq (0.3\text{–}6) \times 10^{16}\ h^+\,\mathrm{cm}^{-3}$]. All irradiations were performed with a Van de Graaf accelerator and a scanned beam on already mounted and tested diodes, either directly for RT irradiations, or through a 25-μm-thick steel window in the case of 15-K *in situ* irradiations. For orientation dependence measurements, several (001) epitaxial layers and bulk slices of p-type InP were oriented before diode processing by measuring the difference between the integrated intensities of (115) and ($1\bar{1}5$) Cu $K\alpha$ x-ray reflections.[7] For one sample, confirmation was obtained from chemical etching in H_2SO_4:H_2O_2:H_2O.[8]

The measured introduction rates of E_4, E_5, and E_{11} electron traps and H_2 to H_6 hole traps[5] are plotted as a function of energy in Fig. 1, normalized to 1 MeV. All curves exhibit clear thresholds, in agreement with a production by electron nucleus collision. The defects can be separated in two groups (H_2,H_3,H_4,E_5,E_{11}) and (H_5,H_6,E_4) according to the threshold energy E_t, respectively, smaller or greater than 200 keV. In principle, a comparison with theoretical models, such as the McKinley-Feshbach,[9] is possible; however, it cannot be made quantitative for 15-K irradiations because of the previously mentioned steel window which slows down the electrons and causes the beam to diverge. This effect can be estimated[1,9] to play a negligible role at high energies, i.e., 1 MeV, but not at low energies where it crucially induces error on real energy and dose. Consequently, such a quantitative comparison is made only for

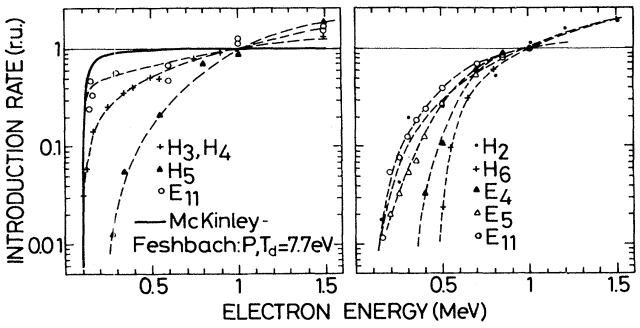

FIG. 1. Introduction rates of several electron (E_4,E_5,E_{11}) and hole traps (H_2 to H_6) induced by electron irradiation in InP as a function of electron energy, normalized to 1 MeV. Left: after direct irradiations at 300 K. Right: after irradiations at 15 K through a steel window (see text). The theoretical curve from the McKinley-Feshbach model for e^--phosphorus collisions with $T_d = 7.7$ eV is also indicated. The irradiations were performed in the [100] direction for E_4, E_5, E_{11}, H_3, H_4, and H_5 and a nonregular direction for H_2 and H_6. The dashed curves are interpolations of experimental points.

the defects studied after RT irradiations H_3, H_4, H_5, and E_{11}. Qualitatively, however, E_t is related to both the ejected atom mass M and a phenomenological displacement threshold Td reflecting the chemical bond strength by the relation

$$T_d = 2\frac{m}{M}E_t\left(\frac{E_t}{mc^2}+2\right)$$

in the McKinley-Feshbach model, where m is the electron mass. Application of this formula to the dominant defects H_3, H_4, and E_{11} for which $E_t \simeq 100$ keV leads to about 2.1 and 7.7 eV for collision with In or P atoms, respectively. The former value is quite unlikely and without equivalence in other semiconductors. Clear evidence is therefore gained that these dominant irradiation-induced centers are produced by a phosphorus-atom displacement in the primary collision in agreement with early conclusions by Bauerlein[10] from a nonspectroscopic technique. A similar consequence holds for E_5 and H_2 although the threshold seems to be higher likely because of the steel window effect. This information is an important step towards defect identification since it strongly restricts the number of possibilities, the phosphorus vacancy or interstitial, or their association being, of course, prime candidates if it turns out to be intrinsic defects, as the high introduction rates seem to suggest.[5] Moreover, the very close annealing behavior of H_3, H_4, and E_{11} points to a correlated nature, unknown in detail at present.

The experimental curves for H_3, H_4, and E_{11} can, however, not be quite satisfactorily fitted with the McKinley-Feshbach model; especially an unexpected steady increase of introduction rates occurs between 300 keV and 1.5 MeV. The reason for that is not obvious. We suggest that apart from electron-phosphorus-atom collisions, other production mechanisms appear at high energies, involving In atoms through secondary In-P collisions, for instance.

The situation is less clear for the second group of centers (H_5,H_6,E_4) since several threshold energies are found, respectively, about 270, 480, and 300 keV. Although the two latter values are only approximate, it is not likely that the real ones could be as low as 270 keV, especially for H_6. This follows from a comparison with the E_{11} case where a reduction factor of 10 only is observed in the ratio of introduction rates at 270 keV and 1 MeV when irradiating through the steel window (Fig. 1).

In a binary compound like InP, these high-energy thresholds may have various origins; first the primary collision may be with the high mass atom In. Although it is not certain that displacement thresholds are equal for the two sublattices, we can take the previously determined value of 7.7 eV as a reasonable approximation, leading to a threshold energy of 310 keV, not too different from the experimental values. However, a second possibility is related to the involvement of secondary collisions for which the primary knocked-on atom must have enough residual energy to eject another one.[11] Such collisions on the phosphorus sublattice itself can lead to thresholds of $2\times(100\text{ keV}) = 200$ keV or even more if the line joining the two atoms is not collinear with the electron beam, since the energy transmitted in the electron-primary atom collision decreases with the angle of recoil. Clearly, choosing between these possibilities needs more information and is not attempted here.

A critical test of the orientation dependence technique[2] can be made here since the sublattice involved in the creation of H_3 H_4, and E_{11} is here unambiguously known. For many energies, two samples containing several diodes were simultaneously irradiated in the [111]P and [111]In directions, following the notations of Ref. 2. The resulting anisotropy curve giving the ratio of introduction rates $\eta([111]\text{P})/\eta([111]\text{In})$ at each energy is presented for H_4 in Fig. 2. The expected trend is clearly observed, irradiations in the easy [111]P direction creating more defects than in the hard one [111]In at low electron energies, while the reverse is obtained at high energies. The validity of the orientation dependence technique is thus nicely confirmed by this experiment.

A quantitative comparison with a theoretical model such as that successfully made in GaAs[12] seems, however, particularly necessary here, since the magnitude of the anisotropy is much smaller than in GaAs. For that purpose we have computed the expected anisotropy curve from a numerical simulation where the primary collision is described by the McKinley-Feshbach model and where secondary collisions with only first neighbors are allowed, and described by hard-sphere potentials. The defect is regarded as created if either a primary P atom is ejected with an energy greater than $T_d = 7.7$ eV and no secondary collision occurs, or if after a secondary collision between P and In atoms, the residual kinetic energy of the P atom is greater than Td. In the latter case, the situation where the primary atom is In is taken into account but is, in fact, found to play a negligible role on the anisotropy. With a hard-sphere radius of 1 Å comparable with the GaAs case,[12] we obtain a fairly good agreement with the experimental data at high energies, but not at low ones where a much larger anisotropy ratio is expected. Obviously, the beam disorientation in the sample must be considered here, since it is particularly important in that energy range. The Moliere theory[9] provides an estimate of the magnitude of this effect. We have therefore

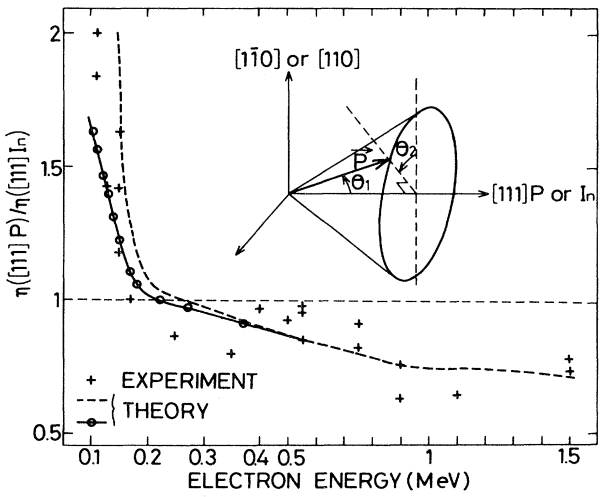

FIG. 2. Ratio of introduction rates of H_4 for irradiations performed in the [111]P and [111]In direction (crosses). The solid and dashed curves are theoretical from the model described in the text with electron beam disorientation included (open circles: computed points) or without, respectively. Inset: definition of angles θ_1 and θ_2 used for the calculations in the latter case. $\vec{P}$ is the momentum of an electron deviated from the original [11] direction after multiple scattering in the sample.

computed a new theoretical anisotropy curve where the introduction rates are numerically averaged on the various possible momentum directions of the electrons for an angularly broadened beam:

$$\eta_{\text{avg}}(E)=\frac{\int_0^{2\pi/3} d\theta_2 \int_0^{\pi/2} \eta(E,\theta_1,\theta_2) f_{\text{Mol}}(\theta_1)\sin\theta_1 d\theta_1}{\int_0^{2\pi/3} d\theta_2 \int_0^{\pi/2} f_{\text{Mol}}(\theta_1)\sin\theta_1 d\theta_1} .$$

Here, the angles θ_1 and θ_2 define the electron momentum direction with respect to the sample crystal axes (see Fig. 2); E is the electron energy and $f_{\text{Mol}}=\exp-[\theta_1/\theta_W(E)]^2$ gives the angular distribution of the broadened beam. Integration in θ_2 is limited to an interval of $2\pi/3$ by rotation symmetry around the [111] axis. In calculating $\theta_W(E)$ from the Moliere expression,[9] we have replaced the Schottky metallization by an InP layer inducing an equivalent disorientation. Since only secondary collisions with first neighbors are considered, there is an additional cylindrical symmetry when irradiations are performed in the [111]In direction, so that $\eta(E,\theta_1,\theta_2)=\eta(E,\theta_1)$, and the expression further simplifies to

$$\eta_{\text{avg}}(E)=\frac{\int_0^{\pi/2} \eta(E,\theta_1) f_{\text{Mol}}(\theta_1)\sin\theta_1 d\theta_1}{\int_0^{\pi/2} f_{\text{Mol}}(\theta_1)\sin\theta_1 d\theta_1} .$$

The final curve is satisfactorily fitted to the experimental data as shown in Fig. 2, with, in particular, a maximum anisotropy ratio much closer to the experimental value of $\simeq 2$, which directly confirms the importance of disorientation effects in such experiments. The residual discrepancy originates both from experimental uncertainties and from the incorrect form of f_{Mol} at very low energies (i.e., strong disorientation).

In summary, we have shown that most of the irradiation-induced deep centers in InP are created by displacements of a phosphorus atom, among which the dominant ones H_3, H_4, and E_{11}. This determination is fully consistent with that deduced from the dependence of the H_4 introduction rate on irradiation direction [111]P or [111]In. The validity of the latter technique to identify the sublattice involved in the primary collision is thus clearly confirmed in materials with the zinc-blende structure. Finally, a few centers E_4, H_5, and H_6 are either created by indium-atom displacements or result from secondary atom-atom collisions.

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