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THRESHOLD ENERGY DETERMINATION IN THICK SEMICONDUCTOR SAMPLES (*)

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Résumé. — On décrit un calcul de la section de capture σ pour le déplacement atomique par des électrons énergétiques en fonction de la pénétration x . On donne les courbes de $\sigma(x)$, calculées pour différentes valeurs de l'énergie du seuil de déplacement, dans le cas du silicium. On détermine ensuite les profils de concentration de défauts introduits dans le silicium par irradiation avec des électrons d'énergies variées en utilisant des mesures de capacité-tension sur des diodes Schottky or-silicium. La mesure des taux de création à profondeur nulle donne une valeur de l'énergie de seuil égale à $20,5 \pm 1$ eV.

Abstract. — A description of the calculation of the cross-section for the atomic displacement σ by energetic electrons, versus penetration depth x , is given. Curves of $\sigma(x)$ computed for various values of the threshold energy for displacement are given in the case of silicon. The profiles of the concentration of the defects introduced by electron irradiation of various energies in silicon is determined from capacitance-voltage measurements on gold-silicon Schottky diodes. The measurement of the defect creation rates at zero depth gives 20.5 ± 1 eV for the threshold energy.

1. Introduction. — The cross-section for atomic displacement in a solid by energetic particles is the product of the probability that a given recoil energy produces a displacement times the differential cross-section that an atom has that recoil energy. In a first approximation a step-function displacement probability — such that any recoil energy smaller than the threshold energy T_d is ineffective in displacing an atom while any energy greater than T_d has unit probability of displacing an atom — is considered.

The knowledge of this quantity T_d is important, not only from a fundamental point of view (it gives an idea on the bonding energy in a crystal) but also because it is necessary in practice to calculate defect creation rates. Only qualitative evaluation of T_d has been given [1] and the calculation of defect creation rates is based only on experimentally determined values of T_d . Unfortunately, these values have been obtained with only a very poor accuracy in semiconductors (for instance the values given in the literature range from 9 to 20 eV for silicon [4-8], and from 12.7 to 23 eV for germanium [6], [8-13]). There are three

reasons for this : 1) the actual displacement probability function is not a step-function and depends upon the crystalline orientation ; 2) the experimental determination has to be performed in very thin samples in order to minimize the electronic energy losses and for such thicknesses surface effects can become preponderant (for instance, in silicon for which the energy loss is on the order of 10^7 eV cm⁻¹, a 10 % accuracy on T_d necessitates, if the threshold energy value is around 20 eV, a sample thickness of 2×10^{-3} cm, which is difficult to realize) ; 3) for reasons which are not clearly understood, T_d seems to depend upon a number of parameters [3] such as the temperature, the Fermi level, etc...

It is therefore interesting to be able to measure T_d in thick samples. Of course, due to multiple scattering of the electron beam, there is a spread in the incident beam direction and the value of T_d which is then obtained is averaged over all the possible electron scattering angles. Actually the theory of multiple scattering — such as the Molière's theory [14, 15] — shows that the characteristic angle θ which defines the scattering distribution (Gaussian) function (θ is the angle for which the amplitude of the distribution is one half of the maximum) varies rapidly with the penetration depth at low enough energy, i. e. for energies close

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to the electron energy corresponding to T_d , which are used to measure T_d (for instance (see Fig. 1) at 200 keV, the energy corresponding to $T_d \simeq 20$ eV in silicon, $\theta = 50$ degrees at 25 μm depth and $\theta = 75$ degrees at

FIG. 1. — Variation of the characteristic angle θ with penetration depth for electrons of various energies in silicon.

50 μm depth). Under such conditions, in a lattice such as a cubic or a diamond lattice, practically all the directions of irradiation, compared to the crystallographic orientations, are included in an attempt to measure T_d and the threshold energy to be considered is indeed an isotropic threshold energy averaged over all the orientations. It is usually such an *average threshold energy* which is interesting to know in practice.

The usual way of determining T_d is to fit the variation of the defect creation rate as a function of incident electron energy with the variation of the normalized cross-section σ for displacement calculated for various values of T_d . As mentioned above, such a method necessitates the measurement of the defect creation rate in very thin samples, since σ varies rapidly with the penetration depth x of the incident electrons. The aim of this paper is to describe a possible method of measuring T_d in thick semiconductor samples. It consists in the use of the variation with depth x of the concentration C of the defects introduced, i. e. of the profile $C(x)$, and in the comparison of the slopes of $C(x)$ and $\sigma(x)$ for small x . The measurement of $C(0)$ by extrapolation of $C(x)$, allows the determination of T_d in the equivalent of an infinitely thin sample ; such determination permits the study of the variation of T_d with the orientation of the irradiating beam compared to the crystallographic orientations.

In the second section the principle of the calculation of $\sigma(x)$ is given and results are presented for various electron energies and various threshold energies. In the third section an experimental technique for the determination of the defect profile $C(x)$ is described together with some results obtained. These results are discussed and compared with the calculation in a fourth section

in order to verify the validity of the method proposed and its limitations.

2. Calculation of $\sigma(x)$. — The variation of the cross-section for atomic displacement σ versus the penetration depth x of the electrons of incident energy E is obtained from the knowledge of the variation of the cross-section with the energy $\sigma(E)$ and of the variation of the energy with the penetration depth $E(x)$. The differential cross-section for Coulomb scattering, $d\sigma(T)$, i. e. the cross-section for the transmission of an energy in the range T and $T + dT$, is given by the Rutherford formula modified to account for the fact that the electrons are relativistic [16]. The exact formula, derived by Mott [18, 19], being the sum of two conditionally convergent infinite series is quite complex and the approximation given by McKinley-Feshbach [20] can be used with elements for which $Z < 40$. We have taken the conventional sharp displacement threshold model. When the primary displaced atom is sufficiently energetic to produce additional displaced atoms, we invoke the Kinchin and Pease cascade model [21] which gives the average number of displacements $\nu(T)$ produced by a primary knock-on of energy T as $\nu(T) = T/2 T_d$ when $T \geq 2 T_d$ and $\nu(T) = 1$ when $T_d < T < 2 T_d$. The total cross-section is then given by :

$$\sigma(E) = \int_{T_d}^{T_m} \nu(T) \frac{d\sigma}{dT} dT$$

where the maximum transmitted energy is :

$$T_m = 2 \frac{m}{M} \frac{(E + 2 mc^2) E}{mc^2}$$

(m : electron mass, M : atomic mass, c : speed of light). A detailed description of a similar calculation can be found in reference [22].

In order to calculate $E(x)$ we choose to use the empirical range-energy relation deduced by Katz and Penfold [23] :

$$\frac{dE}{dR} = \frac{E}{R} (1.265 - 0.191 \log E)^{-1} \quad \text{for } E < 2.5$$

and :

$$\frac{dE}{dR} = 0.00189 \quad \text{for } E > 2.5$$

(E in MeV, R in mg.cm^{-2}) rather than using complicated and less accurate theoretical calculations [24, 25]. The calculation consists in the determination of the energy loss $dE(x)$ at a depth x for an increment dx , followed by the computation of σ for

$$E(x - dx) = E(x) - dE(x).$$

Results of the calculation are shown on figures 2-5 for various incident electron energy and for various threshold energies in the case of silicon ; figure 6 gives $\sigma(E)$.

FIG. 2. — Variation of the cross-section for atomic displacement at various threshold energies for 300 keV electrons.

FIG. 5. — Variation of the cross-section for atomic displacement at various threshold energies for 2 MeV electrons.

FIG. 3. — Variation of the cross-section for atomic displacement at various threshold energies for 500 keV electrons.

FIG. 6. — Cross-section for atomic displacement at various threshold energies versus incident electron energy.

FIG. 4. — Variation of the cross-section for atomic displacement at various threshold energies for 1 MeV electrons.

3. Experimental determination of $C(x)$. — The profile $C(x)$ of the defect concentration can be obtained using all the techniques which can measure a defect concentration (electrical or optical measurements, electron paramagnetic resonance, etc...) coupled with the successive removal of layers. It can also be obtained in an easier non-destructive way using the capacitance-voltage (C-V) technique as we shall illustrate in this section. We performed C-V measurements on gold-silicon Schottky diodes irradiated with various doses of 250 keV and 900 keV electrons at room temperature.

The diodes were made by evaporation of gold dots (500 μm diameter, 100 $\text{\AA}$ thick) on an epitaxial n-type layer (8 μm thick, doped with approximately 10^{16} impurities cm^{-3}) grown on a n^+ wafer to insure ohmic contact. The electrical contact was made on the gold layer with a needle positioned by a micromanipulator. The measurements were carried out at a fixed frequency of 1 MHz with a Boonton model 75-C capacitance bridge. The carrier profiles, before ($n_0(x)$) and

after $n(x)$ irradiation, were obtained by means of a computer calculation using a least mean square fit of the $1/C^2$ versus V plot. By difference between $n(x)$ and the original concentration $n_0(x)$ we get the quantity $N - N_i$ where N is the concentration of part of the defects introduced by irradiation, those which compensate the free electron concentration (i. e. those which are associated with a level situated below the electron quasi Fermi level in the depletion region) and N_i the concentration of the uncompensating ionized defects (whose level is situated above the quasi Fermi level in the depletion region) [26]. The profile of the defects introduced is therefore given by $n_0(x) - n(x)$ only when N_i is negligible, i. e. when the levels associated with the defects are below the quasi Fermi level ; this will be verified for the case considered here in the next section.

The direct I-V characteristics of the diodes show that, for biases greater than 0.1 V, they follow the usual thermionic emission theory ; the value of the gold-silicon barrier height obtained from the I-V characteristics are in good agreement with the values found in

the literature [27]. Before irradiation the C-V plots lead to a linear variation of $1/C^2$ versus V , corresponding to approximately constant carrier profiles

$$n_0(x) = 3 \times 10^{15} \text{ cm}^{-3}.$$

The evolution of the C-V characteristics with the electron dose at 250 keV and 900 keV are given in figures 7 and 8 respectively ; the corresponding profiles are given in figures 9 and 10. Figure 11 is a plot of the apparent defect concentration ($N - N_i$) at constant depth (0-1 μm) for these energies ; it provides a defect introduction rate (at $x = 0$) of $3 \times 10^{-3} \text{ cm}^{-1}$ at 250 keV and of $1.7 \times 10^{-2} \text{ cm}^{-1}$ at 900 keV.

FIG. 7. — Evolution of the capacitance versus voltage characteristics with the dose of irradiation at 250 keV.

FIG. 8. — Evolution of the capacitance versus voltage characteristics with the dose of irradiation at 900 keV.

FIG. 9. — Evolution of the carrier profile with the dose of irradiation at 250 keV.

FIG. 10. — Evolution of the carrier profile with the dose of irradiation at 500 keV.

FIG. 11. — Variation of the defect concentration at 1 μm depth with the dose of irradiation at 250 and 900 keV.

4. Discussion. — Electron irradiation at room temperature creates several types of defects (such as E- and A-centres, divacancies) in various concentrations ;

depending upon the positions of the levels associated with these defects they compensate the free electron concentration (N) or not (N_i). In oxygen free silicon, such as we used, an electron energy below 1 MeV results in the creation of a concentration of E-centres very large compared to the concentration of other types of defects [28-29] and, in practice we can consider that we are dealing with only one type of defect (the threshold energy for divacancy creation being twice the value of the threshold energy for vacancy-interstitial pair creation, the cross-section for divacancy formation is negligible compared to the cross-section for vacancy-interstitial pair formation below 1 MeV). Since the E-centre is known [28-29] to be associated with an acceptor level at about 0.4 eV below the conduction band, i.e. well below the quasi Fermi level, the assumption $N \gg N_i$ that is: $N(x) = n_0(x) - n(x)$ applies. Verification of this assumption can be found in the fact that the defect introduction rate measured at 900 keV is in correct agreement with the defect introduction rate measured by resistivity measurements [30] in similarly doped silicon samples irradiated at room temperature.

As a result of the doping level and the small value of the reverse voltage which can be applied on the diodes used, the defect profile has only been determined in the

FIG. 12. — Ratio R of the cross-sections for atomic displacement at 900 and 250 keV versus the threshold energy T_d .

range 1-3 μm . In such a short range the variation of $\sigma(x)$ with T_d is not strong enough to allow the determination of T_d through the comparison of the $C(x)$ and $\sigma(x)$ profiles. Schottky diodes of better quality should be used.

But T_d can be determined from the ratio R of the defect introduction rates at 200 and 900 keV measured at $x = 0$ (the nature of the defects created at 200 and 900 keV being the same). The value of R corresponds to $T_d = 20.5$ eV on the curve (Fig. 12) giving the calculated ratio of the cross-sections for displacement at 900 and 250 keV, versus T_d . Considering the accuracy of the determination of the defect introduction rates, T_d is obtained within ± 1 eV.

5. Conclusion. — The value of T_d we determine using the method proposed compares favorably with previously published results [4-8]. Such a method is in principle more accurate than the conventional ones, used up to now, since the defect creation rate taken is the defect creation rate at a given depth x , instead of the defect creation rate integrated over all the thickness of the sample. The method has the advantage of being independent upon the thickness of the sample and, in particular, T_d can be determined at $x = 0$, which allows a correct study of T_d versus orientation.

Of course the C-V technique has its own limitations (in the carrier concentration of the samples studied and in the nature of the defects created — they have to be associated with levels deeper than the quasi Fermi level) — but it can be widely used in all semiconductors (including diamond [31]). The interpretation of the results obtained is based on the fact that the compensating centers which decrease $n(x)$ are the defects introduced by the irradiation; it therefore assumes that deep centers are not introduced during irradiation by other means (such as by diffusion [32]). Such assumption is reasonable in case of room temperature irradiation with the low doses which are used.

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