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ANALITICAL CALCULATION OF THE VACANCY DISTRIBUTION AND THE SEMICONDUCTOR AMORPHIZATION DOSE DURING ION IMPLANTATION

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In recent years the theoretical calculations of the vacancy distribution and semiconductor amorphization dose have been carried out (e.g. see an exellent paper [I] and references to it). The calculations were mainly performed by means of the numerical integration. The ion-atom interaction was described by the power low potential. The electronic stopping was disregarded.

The purpose of the present paper is to study in detail some aspects of analitical calculation of the problem.

We have used an approximated energy relation of the reduced dimentionless nuclear stopping power based on the Thomas - Fermi interatomic potential [2]:

$$\left(\frac{d\varepsilon}{d\rho}\right)_n = \frac{c\,\varepsilon^{1/2}}{d+\varepsilon} \qquad (1)$$

In the same units the electronic stopping power is represented by Lindhard - Scharff model [3]:

$$\left(\frac{d\varepsilon}{d\rho}\right)_e = k\,\varepsilon^{1/2} \qquad (2).$$

We have taken into account the usual displacement collision assumptions [4] including that the displacement threshold energy is transferred to the crystalline lattice.

To the 10-500 keV energies the vacancy distribution along the ion path may with good approximation be corresponded to the energy nuclear loss distribution. Thus

$$\frac{dV}{d\rho} = \frac{\partial e}{3\varepsilon_d}\cdot\frac{c\,\varepsilon^{1/2}}{d+\varepsilon}, \qquad (3)$$

where $\partial e = \frac{Z_1}{2\sqrt{2}}\cdot\frac{(Z_1^{2/3}+Z_2^{2/3})^{1/2}}{Z_2^{4/3}}\cdot\frac{M_1+M_2}{M_2}$,

c=0.23 and d=0.1 if $\varepsilon < 0.1$,
c=0.45 and d=0.3 if $\varepsilon \geq 0.1$.

The distribution is seen to have a maximum appearing when the ion energy falls to $\varepsilon = d = 0.3$. The fig.1 shows the vacancy distribution along the phosphorous ion path in silicon at the initial energies E_o being equal to 40 (1), 100 (2) and 200 (3) keV.

Using equation (3) and the range along the path – energy relation given by [2] we have obtained the correlation between the maximum vacancy distribution and the average range along the ion path in the dimentionless form:

$$\frac{\rho_d}{\rho_0} = 1 - \frac{\sqrt{d} - \frac{c/k}{\sqrt{c/k+d}}\,\mathrm{arctg}\sqrt{\frac{d}{c/k+d}}}{\sqrt{\varepsilon_0} - \frac{c/k}{\sqrt{c/k+d}}\,\mathrm{arctg}\sqrt{\frac{\varepsilon_0}{c/k+d}}} \qquad (4)$$

By means of the equation (4) we may establish that the maximum ρ_d lays at the ion-implanted surface if the initial energy $\varepsilon_0 = 0.3$. At the energies $\varepsilon_0 < 0.3$ the vacancy concentration at the surface is always more than that in the bulk of the crystal. When the energy $\varepsilon_0 \geq 0.3$ the ρ_d / ρ_0 correlation grows with the energy and tends to I (see fig.I): $\rho_d / \rho_0 = 0.57$ (40 keV), 0.8I (I00 keV) and 0.9I (200 keV). The surface vacancy concentration is simultaneously decreasing.

From (3) we obtain directly the radiation damage function ν (table I) when integrating.

$$\nu = \frac{\varkappa\, \varepsilon_n}{3\, \varepsilon_d} \,, \qquad (5)$$

where $\varepsilon_n = \frac{c}{k} \ln\left(1 + \frac{\varepsilon_0}{c/k+d}\right)$ – the dimentionless energy lost on the elastic collisions.

From ref. [I] the crystal amorphization is over as an each atom is displaced. Analitically the amorphization dose may be written:

$$N_a = \frac{N_i}{d\nu/dR} \,, \qquad (6)$$

where N_i – the intrinsic crystal atom concentration.

Using (3) we may rewrite (6) for the case of the surface dose:

$$N_{as} = \frac{3\,\varepsilon_d\,(d+\varepsilon_0)}{c\,\varkappa\sqrt{\varepsilon_0}\,\pi a^2 \gamma} \,, \qquad (7)$$

where a – the Thomas-Fermi screening radius,

$\gamma = 4M_1M_2/(M_1+M_2)^2$.

Table I. The radiation damage function of silicon.

E_0, keV	ν, vacancies/ion		
	II_B^+	$3I_P^+$	$I2I_{Sb}^+$
I0	I58	I96	208
40	435	7I9	832
I00	723	I570	2020
200	960	2630	3930

We may conclude that the ion energy dependence of N_{as} is the same as that of the surface vacancy distribution. Table 2 compares calculated by (7) and experimentally obtained [5] values of N_{as} of 40keV ions P^+, Ga^+ and Sb^+ in silicon and In^+ in germanium.

Table 2. Comparison between theoretical and experimental surface amorphization doses

	N_{as}, ions/cm^2			
	P^+	Ga^+	Sb^+	In^+
By(7)	4.5×10^{14}	1.7×10^{14}	1.1×10^{14}	7.5×10^{13}
By[5]	$\sim 4 \times 10^{14}$	$\sim 2 \times 10^{14}$	$\sim 1 \times 10^{14}$	$\sim 8 \times 10^{13}$

The good date open possibility for the accurate simple analitical calculations of the vacancy distribution and the semiconductor amorphization dose for various cases of ion implantation.

References

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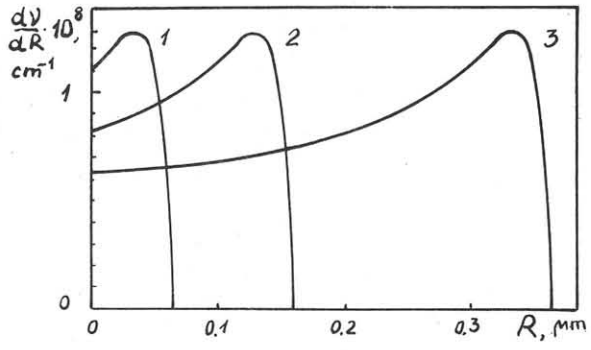

Fig. I