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# RADIATION DAMAGE DEPTH DISTRIBUTIONS IN Al AND Zn INDUCED BY Ar (400 MeV), Ne (200 MeV) AND C (112.5 MeV) ION BOMBARDMENT

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One of the most important aspects of research in the field of radiation effects is the determination of the relation between the defects induced by radiation and the associated changes in physical properties. These changes depend on the spatial distribution of radiation damage. In this paper we determine the depth distribution of the average number of displacements per atom induced by Ar (400 MeV), Ne (200 MeV) and C (112.5 MeV) ion beams.

The model applied is briefly described in the first parts. The results of our calculations are then presented in the second part of the paper.

## 1. MODEL

This section deals with the construction of a model describing the average number of displacements per atom, as a function of the penetration depth. The model is based on the fact that the behaviour of the electronic stopping cross section differs in the high and low energy regions[1]. (In the low energy region contrary to the high energy region the electronic stopping power is linear in the velocity). So, we investigate $\sigma_F(x)$ in the two regions of electronic stopping cross section separately:

$$\sigma_F(x) = \begin{cases} \sigma_F^{I}(x) & \text{at } X \leq X^*, \text{which corresponds to } E > E^*; \\ \sigma_F^{II}(x) & \text{at } X \geq X^*, \text{which corresponds to } E < E^* \text{ energy of ion.} \end{cases}$$

### 1.1. Region I. $E > E^*$

In this high energy region the average number of displacements per atom is given by integral

$$\sigma_F^{I}(E) = \int_{E_d}^{\gamma E} d\sigma(T,E) N_d(T), \qquad (1)$$

where $E$ is the ion energy, $N_d(T)$ is the average number of displacements produced by a primary of energy $T$, $d\sigma(T,E)$ is the differential cross section for the energy transfer to the primary knock on atom, $E_d$ is the energy required to displace a lattice atom, $\gamma E$ is the maximum energy which can be transferred in the collision, $\gamma = 4M_1M_2/(M_1+M_2)^2$, $M_1$, $M_2$ are the masses of the ion and target atoms, respectively.

The relationship between the incident beam energy and the path length is determined from the following. The formula connecting the linear path length with its energy is known:

$$R(E) = \int_0^E \frac{dE'}{N[S_n(E') + S_e(E')]}, \qquad (2)$$

where $N$ is the number of target atoms per unit volume, $S_n(E)$ and $S_e(E)$ are the nuclear and electronic stopping cross sections, respectively[2].

It is well known that in the high energy region the electronic interactions dominate by more than an order of magnitude, and in a first approximation the nuclear interactions can be neglected. As electronic straggling is also small, we neglect it too in this approximation.

Consequently, in the high energy region the mean path length is equal to the path length $R(E)$ as well as to the penetration depth $x(E)$.

From equation (2) we, thus obtain the function $E(x)$ and further with equation (1) the Frenkel pair cross section for the given penetration distance $x$.

### 1.2. Region II. $E < E^*$

The nuclear energy straggling of the ion becomes more important in the low energy regime. This is due to an increase of the nuclear cross sections[3] and leads to a range straggling. In this energy region $\sigma_F(x)$ is given by

$$\sigma_F^{II}(x) = \int_x^{\infty} \int_{E_d}^{\gamma E(x-x')} dx' d\sigma(E(x'-x),T) N_d(T) \frac{dR(x'-x)}{dx'} f(x'), \qquad (3)$$

where $f(x)$ is the fraction of ions in the beam with projected ranges in the neighbourhood $dx$ of $x$[4]. It is given by a Gaussian distribution:

$$f(x) = \frac{1}{\sqrt{2\pi\alpha_x^2}} \exp\left(-\frac{(x-x_m)^2}{2\alpha_x^2}\right). \qquad (4)$$

In this region the electronic stopping cross section is proportional to the square root of the energy and is given here by LSS estimates[1].

The mutual continuation of the two regions is determined by the condition

$$\sigma_F^{I}(x^*) = \sigma_F^{II}(x^*). \qquad (5)$$

## 2. CALCULATIONS AND RESULTS

The differential projectile-target cross section was chosen to be represented by:

a) the Rutherford differential cross section

$$d\sigma = \pi \frac{M_1}{M_2} \frac{(Z_1 Z_2 e^2)^2}{E} \frac{dT}{T^2}, \qquad (6)$$

b) the Lindhard differential cross section

$$d\sigma = \pi a^2 \frac{dt}{2t^{3/2}} f(t^{3/2}), \qquad (7)$$

where $t = \epsilon^2 T/\gamma E$, $\epsilon = M_2 Ea/(M_1 + M_2) Z_1 Z_2 e^2$, $a = 0.8853\, a_0 (Z_1^{2/3} + Z_2^{2/3})^{-1/3}$

$Z_1$, $Z_2$ are the atomic numbers of the scattered and recoiling particles, respectively, $a_0$ is the Bohr radius, $e$ is the electron charge $f(t^{1/2}) = \lambda t^{1/6}[1 + (2\lambda^{2/3})^{2/3}]^{-3/2}$, $\lambda = 1.309$.

The average number of displacements, $N_d$ was calculated

a) by the Kinchin-Pease damage function[6]

$$N_d = \begin{cases} 0 & 0 < E < E_d \\ 1 & E_d < E < 2E_d \\ E/2E & 2E_d < E < E_1 \\ E_1/2E_d & E_1 < E < \infty, \end{cases} \qquad (8)$$

where $E_1 = M_2 \epsilon_0 / 16 m$, $M_1$, $m$ are the masses of primary knock-on atom and electron, respectively, and $\epsilon_0$ is the Fermi energy,

b) by the modified Kinchin-Pease expression[7]

$$N_d = \frac{\kappa \hat{E}}{2E_d}, \qquad (9)$$

$E \quad \epsilon \to 0 \quad M_1 = M_2$

where $\kappa = 0.8$, $\hat{E} = \hat{E}/[1 + k g(\epsilon)]$, $g(\epsilon) = 3.4008\epsilon^{1/6} + 0.40244\epsilon^{3/4} + \epsilon$,

$k = 0.1337\, Z_1^{1/6} (Z_1/M_1)^{1/2}$, $\epsilon = M_2 Ea/(M_1 + M_2) Z_1 Z_2 e^2$.

T

$Z_2 \quad M_2$

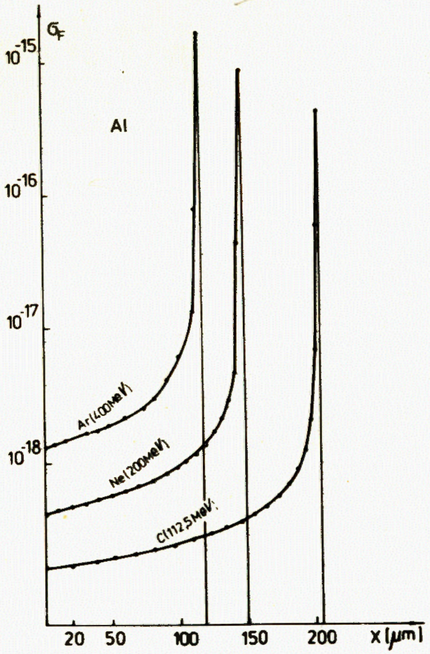

Fig.1. Depth distributions of displacements per atom induced by Ar (400 MeV), Ne (200 MeV), C (112.5 MeV) ions bombardment in target Al. The calculations were made by model LMKP.

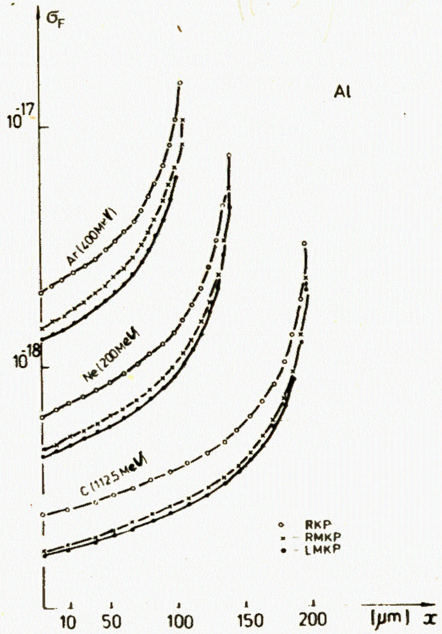

Fig.2. Depth distributions of displacements per atom induced by Ar (400 MeV), Ne (200 MeV), C (112.5 MeV) ion bombardment in target Al. The calculations were made by models RKP, RMKP, LMKP.

In calculating the integral (2) the handbook[8] has been used. Figures 1-4 show the results of the calculations. In the figures $\sigma_F^{RKP}$ is the displacements per atom using the Rutherford differential cross section (6) and the Kinchin-Pease damage function (8). In the calculations of $\sigma_F^{RMKP}$ and $\sigma_F^{LMKP}$ the modified Kinchin-Pease damage function (9) was used with Rutherford's and Lindhard's differential scattering cross sections, respectively.

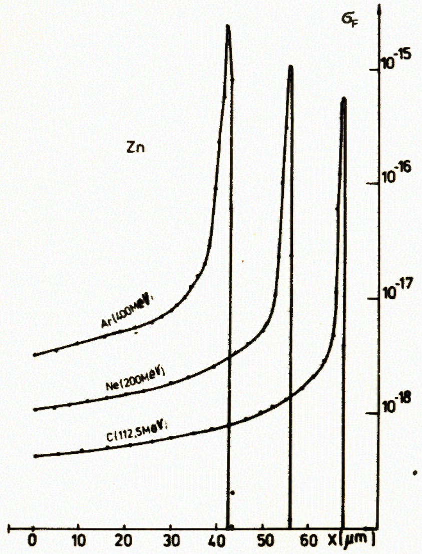

Fig.3. Depth distributions of displacement per atom induced by Ar (400 MeV), Ne (200 MeV), C (112.5 MeV) ion bombardment in target Zn. The calculations were made by model LMKP.

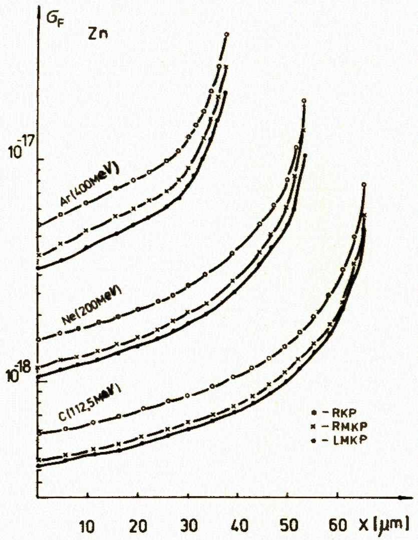

Fig.4. Depth distributions of displacement per atom induced by Ar (400 MeV), Ne (200 MeV), C (112.5 MeV) ion bombardment in target Zn. The calculations were made by models RKP, RMKP, LMKP.

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Бардош Д., Федянин В.К., Гавриленко Г.М. E17-83-303
О распределении радиационных дефектов в Aℓ и Zn, образованных при облучении ионами Ar /400 МэВ/, Ne /200 МэВ/, C /112,5 МэВ/

Рассчитано число выбитых ионов материала Aℓ и Zn, приходящихся на единичный поток ионов Ar /400 МэВ/, Ne /200 МэВ/, C /112,5 МэВ/ в зависимости от глубины их проникновения в материал.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Bardos G., Fedyanin V.K., Gavrilenko G.M. E17-83-303
Radiation Damage Depth Distributions in Aℓ and Zn
Induced by Ar /400 MeV/, Ne /200 MeV/
and C /112.5 MeV/ Ion Bombardment

A method for the approximate calculation of damage depth distributions induced by ion bombardment has been described and results are presented for Ar /400 MeV/, Ne /200 MeV/ and C /112.5 MeV/ ion projects in Aℓ and Zn substrates.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Pr arch. Dubna 1983