CALCULATION OF ENERGY RELEASE FUNCTION OF FOCUSED ION BEAM IN SOLIDS

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The mathematical formulation of space-time energy release function of accelerated ions in solids is presented. Continuous focused ion beam interaction with metals is considered. The power density of deposited energy and specific energy input in a target has been calculated. A beam energy fraction expended on the collisional sputtering of target atoms has been estimated.

Today, accelerated ions are successfully used with a number of material processing technologies. Modern accelerating equipment allows generating ion beams with a wide range of particle initial energies and current densities.

However, the development of an energy efficient ion beam technology is accompanied by the control of a complicated dissipation energy process by choosing corresponding beam parameters. In the general case, there are several events of the input energy distribution. The beam energy can be expended on the atom sputtering, substance heating up, melting and evaporation. The energy dissipation structure mainly depends on a ratio between the energy release rate and energy distribution rate into a solid.

The given paper presents an approach to the mathematical description of the space-time energy release function (ERF) for the ion-solid interaction. Its calculation is a mandatory piece of the numerical simulation of thermal and erosion processes on a surface, computer modeling of the target deformation and destruction due to stress fields under the irradiation, and so on. The ERF of a continuous focused ion beam (CFIB) is considered here.

Suppose that ERF is additive that is the total amount of the energy deposited into a solid is a sum of the energy input of each ion at its stopping in the substance. Therefore, the calculation expression of the space-time energy release function W(x, r, t) in two-dimensional geometry (Fig. 1) can be presented as follows:

$$W(x,r,t) = F(r,t) \cdot Q(x,t), \quad (1)$$

where F(r, t) – the ion flux distribution along the beam radius (ion/($m^2 \cdot s$)); Q(x, t) – the distribution of linear energy losses along the target depth (J/m). In the general case, functions F(r, t) and Q(x, t) vary with time. Current and voltage oscillograms of ion sources (accelerators) contain the information about the time evolution of ion flux and ion energy.

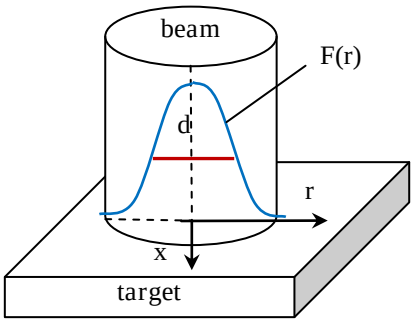

Fig. 1. Two-dimensional geometry of ion beam-target interaction

In the present work, the ion energy spread is considered as negligible for CFIB, i.e. the function of

linear energy losses on a path unit travelled by ion Q(x) is a time-independent. It realizes the calculation technique of the spatial distribution of ion energy losses with accounting nuclear and electronic stopping mechanisms [1]. This technique was developed according to the Lindhard-Scharff-Schiott theory [2].

Continuous irradiation technologies are characterized by low ion initial energies and deal with sputtering target from a solid state. CFIB parameters correspond to the following ranges: the ion initial energy E_0 = 5–100 keV; the beam diameter d = 5–1000 nm; the beam current I_b = 10 pA–30 nA [3].

Since a focused ion beam diameter is commensurable to the projected ion range, its ERF must be calculated in two-dimensional geometry. To describe ion flux density along the radius of CFIB the way from [4] is used:

$$F(r) = \frac{I_b}{e} \cdot \frac{1}{2\pi\sigma^2} \cdot \exp(-r^2 / 2\sigma^2);\ \sigma = d / \sqrt{8\ln 2}$$

where I_b – the beam current (*A*), *e* – the elementary charge (C), r – the radial coordinate, the beam center is located at r = 0 (m), d – the beam diameter, commonly defined as the full width at half maximum (Fig. 1) (m).

The duration of CFIB action equals to units–tens of seconds; increasing and falling down fronts of j(t) take inconsiderable part of irradiation duration. Therefore, suppose j(t)= const, i.e. the same number of particles fall down on a target surface per time unit.

Thus, Eq. 1 for CFIB is transformed into Eq. 2:

$$W(x,r) = F(r) \cdot Q(x). \quad (2)$$

The ERF of CFIB has been obtained for 10 keV Ar+ ions falling down on Al surface (Fig. 2). We have considered a beam with the diameter of 50 nm at the current of 10 nA. A beam focusing system allows increasing ion flux density, and the same values of energy input can be reached at much less initial energies.

The maximum of CFIB energy release power density W_m is observed in the central part of a beam (at r = 0 m) on a target surface. W_m decreases with increasing distance from the beam center according to Eq. 2.

Nowadays, ion beam technologies of micro- and nanoprocessing of materials mostly operate gallium liquid metal ion sources. It is mainly thanks to the low melting temperature of this metal (29.77 ^{0}C). So, maximal energy release power density has been calculated depending on the beam current I_b for Ga+ ions in comparison with Ar+ ions (Fig.2). The amount of deposited energy linearly increases at current growth. W_m of gallium ions is slightly more than W_m of argon ions.

A considerable growth of W_m results from the reduction of the beam diameter, i.e. with increasing beam current density. The beam compression by 100 times increases the energy release power density by 4 orders (Fig. 2).

The described above approach to ERF calculation does not account energy losses on collisional

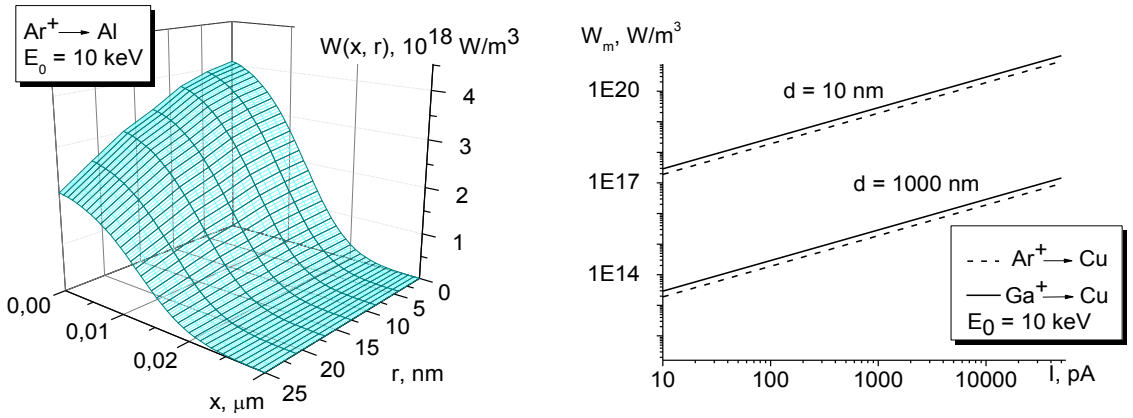

Fig. 3. The maximum of energy release power density depending on the CFIB current at the beam diameter 10–1000 nm (10 keV Ga+ (solid line) and Ar+ (dash line), target - Cu)

(physical) sputtering of surface atoms. Gallium ion mass is larger than argon ion mass (M_{Ar} = 40 amu, M_{Ga} = 69.77 amu). Energy expenditures on sputtering are expected to enhance. So, the calculation technique of energy absorption factor accounting the energy losses on collisional sputtering is given below. All the mathematical expressions conform to the SI system.

The energy absorption factor accounting the energy losses on collisional sputtering can be calculated through the expression:

$$\beta = \left(E_b - S \cdot E_1 \cdot \frac{1}{e} \int_0^{\tau} j(t)dt \right) / E_b$$

where E_b – the beam energy density (J/m^2), E_1 – the average energy of sputtered particles (J), S – the sputtering yield (atom/ion).

The variety of semi-empirical approaches to the calculation of sputtering yield and average energy of sputtered particles can be found in scientific literature. One of the ways of determining S and E_1 is set below.

At ion initial energies much more than the sputtering threshold energy ($E_0 >> E_{th}$), the average energy of sputtered particles E_1 is calculated through the Falcone formula [5]:

$$E_1 = 2U_0 \cdot (\ln \omega - 3/2),$$

where U_0 – the surface binding energy, usually taken to be equal to the sublimation energy (J), $\omega = E_0/E_{th}$, E_0– the initial ion energy (J),E_{th} – the sputtering threshold energy (J).

To determine S, the Sigmund formula for ions with E_0>1 keV was used [6]:

$$S = 4.2 \cdot 10^{18}\ (m^{-2}) \cdot \frac{\alpha(M_2/M_1) \cdot S_n(E_0)}{U_0}$$

where α – the dimensionless function of the mass ration between the target mass M_2 and the ion mass M_1, calculated with the Matsunami expression [7], $S_n(E_0)$ – the nuclear stopping power of target substance $(J \cdot m^2)$.

To determine $S_n(E_0)$ according to the Linhard-Scharff-Schiott theory [2], the required set of formulae is given below (for the case of $10^{-4} \le \varepsilon \le 10^2$):

$$\varepsilon = E_0 \frac{a_T 4\pi\varepsilon_0}{Z_1 Z_2 e^2} \cdot \frac{M_2}{(M_1 + M_2)};$$

$$S_n(E_0) = \frac{a_T Z_1 Z_2 e^2 M_1}{\varepsilon_0 \cdot (M_1 + M_2)} \cdot S_n(\varepsilon);\ S_n(\varepsilon) = \frac{1.7\varepsilon^{1/2} \ln(\varepsilon + 2.718)}{1 + 6.8\varepsilon + 3.4\varepsilon^{3/2}} \quad (9)$$

where ε – the dimensionless reduced energy; $\varepsilon_0 = 8.85 \cdot 10^{-12}$ – the dielectric constant (F/m), $a_T = 0.4683 \cdot 10^{-9} \cdot (Z_1^{2/3} + Z_2^{2/3})^{-1/2}$ - the Lindhard screening parameter (m); $Z_1$and Z_2 are the atomic number for the ion and target atoms.

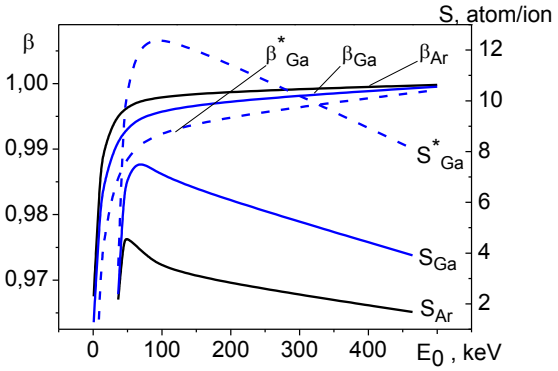

Fig. 4. The energy absorption factor and sputtering yield depending on the initial energy of Ar+ and Ga+ ions falling down on copper surface
(—— – the present paper result;
- - - - – the result obtained with [8])

The sputtering yield S and energy absorption factor β have been calculated depending on the ion initial energy in the range of 1–1000 keV. The results have been obtained for Ar+ and Ga+ ions incident on copper target with the maximal current density of 100 A/cm^2 (Fig. 4).

In the whole energy range, β is close to one, the amount of energy expended on sputtering does not exceed 4 %. The similar result of S calculation has been obtained for Ga+ ions with the calculator tool [8] (dash line in Fig. 4).

Hence, almost all the kinetic energy of falling ions is transformed into the substance internal energy. Energy losses on collisional sputtering are not considerable component in the energy dissipation structure, but to get the precious result they should be accounted.

The depth profile of energy release power density of accelerated ions in metal surface layer has a step-shape. The energy input depth is proportional to the ion projected range. Owing to focusing system, the ion flux density increases and the energy release power density reaches values ~ 10^{21}W/m^3 at lower initial energies (tens of keV vs. hundreds of keV).The ion beam energy losses on collisional (physical) sputtering of a target are equal to units of percent.

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