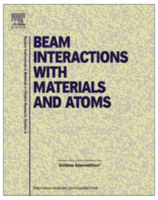
Nuclear Instruments and Methods in Physics Research B 315 (2013) 261–264

Contents lists available at SciVerse ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb



Erosion yield of metal surface under ion pulsed irradiation

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ARTICLE INFO

Article history:
Received 28 November 2012
Received in revised form 18 March 2013
Accepted 4 April 2013
Available online 18 April 2013

Keywords:
Erosion yield
Ion pulsed irradiation
Sputtering
Evaporation
Computer simulation

ABSTRACT

The paper is devoted to the study of erosion processes on a metal surface (Ag, Ni, Cu, W) under argon ion bombardment. The erosion yields including the sputtered and evaporated particles have been calculated for a wide range of the initial ion energy (1–1000 keV). They are revealed to reach the values from units to 10^4 atom/ion under a pulsed ion beam with the power density of 10^2–10^{10} W/cm^2. The ion beam and target parameters are shown to influence on the erosion intensity.

1. Introduction

Accelerated charged particle beams and plasma flows are successfully used for modifying material properties. The irradiation effect is defined by the great number of physical–chemical processes. One of them is an erosion of an irradiated surface due to sputtering and evaporation of a target.

Erosion processes have various physical nature and evolution depending on energy flux density, type of particles (ions, or electrons), and their initial energy. Some of the ion-beam technologies are based on the study of substance removal kinetics and its dependence on irradiation conditions.

The main technological mechanisms of surface erosion are collisional (physical) sputtering of atoms through the kinetic energy transfer from a falling ion to a target atom, and substance evaporation due to transferring beam particles energy into the internal energy of a target substance. The contributions of these processes to the emitted atom flow are different; it is changed depending on irradiation parameters.

The results of numerical modeling of substance evaporation kinetics for high-power pulsed charged particle irradiation were presented in [1]. But, the contribution of collisional sputtering to the atom removal did not take into consideration due to high ion energies (hundreds of keV) and high power density (10^6–10^9 W/cm^2). However, to calculate erosion coefficients properly, particularly, in the case of low ion energies (less than 100 keV) and low power density (10^2–10^5 W/cm^2), the ion energy losses on elastic collisions with target atoms and their following sputtering should be taken into consideration. The present paper is devoted to the numerical investigation of erosion processes on a metal surface (Ag, Ni, Cu, W) under pulsed irradiation with 1–1000 keV argon ions.

2. Computer simulation of erosion processes on a solid surface under ion pulsed irradiation

The effectiveness of a removing target substance process is characterized by an erosion yield. It is an averaged amount of emitted atoms per one falling charged particle. Here, processes of sputtering and evaporation are considered to be irrespective of each other, so the erosion yield is calculated according to the expression:

$$Y = \frac{\frac{S}{e}\int_0^{\tau} j(t)dt + n\int_0^{t_f} V_f(t)dt}{\frac{1}{e}\int_0^{\tau} j(t)dt}, \tag{1}$$

where S – sputtering yield (atom/ion), τ – irradiation duration (s), t_f – evaporation duration (s), $j(t)$ – current density in an impulse function (A/m^2), n – atomic density of a target material (m^{-3}); V_f – evaporation rate (m/s), e – the electron's charge (C).

Thus, correct calculation of a solid surface erosion yield for the wide range of the ion initial energies includes the determination of sputtering yield S and evaporation rate V_f.

2.1. Sputtering yield calculation

To calculate sputtering yield, the formula obtained by means of a statistical model [2,3] has been used:

$$S = B \cdot \frac{\pi}{4 \cdot 10^8 \cdot Q_n^2} \cdot \left(\frac{0.0075}{\pi U_0}\right)^{\frac{4}{3}} \cdot \left(\frac{1}{0.0012 \cdot n}\right)^{\frac{2}{3}} \cdot \chi^2 \tag{2}$$

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http://dx.doi.org/10.1016/j.nimb.2013.04.012

Here, B – the fraction of displaced atoms actually emitted from a surface due to sputtering [2]; Q_n – the average value of the linear nuclear energy losses of a bombarding ion (eV/m); U_0 – the heat of atomization (sublimation energy, eV), which is close to the sublimation energy; n – the atomic density of a target material (m^{-3}); and $\chi = \frac{1.2 \cdot \beta \cdot E_n^{\frac{1}{3}}}{1.2 + 0.8 \cdot \beta \cdot E_n^{\frac{2}{3}}}$.

The value of E_n is the sum of ion nuclear energy losses (eV); and $\beta = (0.5 \times 10^{-14}/Q_n) \cdot (0.016 \cdot 10^{30} \cdot \mathrm{U}_0 \pi \cdot n)^{\frac{1}{3}}$ ($eV^{\frac{2}{3}}$)

The values of Q_n and E_n have been calculated according to Lindhard-Scharff-Schiott theory [4].

The formula (2) supposes that the intersected affected area in the surface volume is proportional to the sputtering yield [3]. As is shown in [2,3], the calculations with the help of (2) are in good agreement with the theoretical and experimental results of other authors.

2.2. Evaporation model

The V_f calculation has been implemented with a two-phase evaporation model with a Knudsen layer [1,5]. It describes solid surface evaporation under a moderate intensive charged particle beam; and, owing to weak interaction of vapor molecules, the target substance vapor is considered to be an ideal gas. The area, which is near the condensed phase, is called Knudsen layer. It has the size of an order of several mean free paths that are mean travels of particles between two successive collisions. Knudsen layer is characterized by other temperature $\bar{T}$ and density $\bar{\rho}$:

$$\bar{T} = 0.65 \cdot T_0, \bar{\rho} = 0.31 \cdot \hat{\rho}. \tag{3}$$

Here, $\hat{\rho}$ – the density of saturated vapor (kg/m^3), T_0 – the temperature of a target surface (K).

$$\hat{\rho} = m \cdot \left(\frac{m \cdot k \cdot \theta^2}{2\pi \cdot \hbar^2 \cdot T_0} \right)^{\frac{3}{2}} \cdot \exp\left(-\frac{E_v}{kT_0} - 1 \right) \tag{4}$$

where m – the target atom mass (kg); k – the Boltzmann's constant (J/K), θ – the Debye temperature (K), E_v – the target lattice binding energy (J), $\hbar$ – the reduced Planck's constant (J/Hz).

Being having calculated the vapor mass rate on the interface $\bar{u} = (5kT/3m)^{\frac{1}{2}}$ (m/s), we can determine the target substance evaporation rate:

$$V_f = \frac{\bar{u} \cdot \bar{\rho}}{\bar{\rho} - \rho}, \tag{5}$$

where ρ – the target material density (kg/m^3).

The given approach correctness is approved by good agreement of calculated results with experimental data. Fig. 1 shows the comparison of calculated evaporated layer thickness with experimentally measured crater depth on a metal surface impacted by high-power pulsed proton-carbon ion beam (40% of H$^+$ and 60% of C$^+$, the impulse duration τ = 120 ns, the maximal current density in the impulse J = 1.2 kA/cm^2, the initial ion energy E_0 = 660 keV) [6]. The evaporated layer was calculated without accounting the contribution of sputtering because of high intensity of a beam. Here, the irradiation result is characterized by very intensive evaporation of a target material, so sputtering has not a considerable atom yield in comparison with evaporation.

The difference between calculated (theoretical) and experimental data is less than 15%. This confirms the calculated results validity.

To calculate the substance evaporation rate, the equation of energy balance on a target surface should be solved with taking into account energy losses on collisional sputtering and phase transitions.

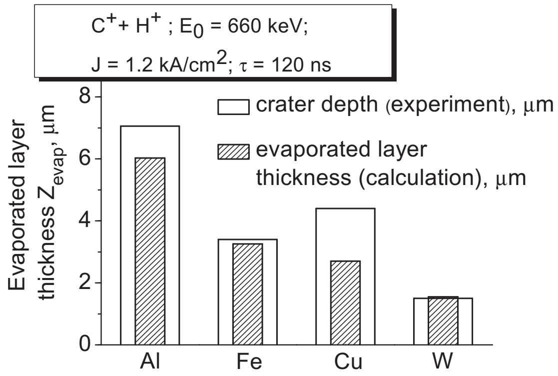

Fig. 1. Comparison of calculated evaporated thickness layer with experimentally measured data of crater depth [6] caused on a target surface due irradiation.

2.3. Model of surface erosion under ion impulse irradiation

The model includes main beam energy dissipation channels: energy expenditures on removing atoms due to collisional sputtering, heat losses on phase transitions (melting and evaporation), energy absorption by a vapor phase. This allows using the model to study erosion impact of accelerated ions in a wide range of power density (10^2–10^9 W/cm^2), and to predict its results.

The calculation of erosion yields is based on solving the energy balance equation [1,5]:

$$\frac{\partial E(x,t)}{\partial t} - V_r(t) \frac{\partial E(x,t)}{\partial x} = a \frac{\partial^2 E(x,t)}{\partial x^2} + W(x,t), \tag{6}$$

Here, $E(x,t)$ – the target substance internal energy (J/m^3), $V_r(t) = \frac{S}{n} \cdot \frac{j(t)}{e} + V_f$ – the rate of atoms removal from an irradiated surface (m/s), a – the temperature conductivity coefficient of a target material (m^2/s), $W(x,t)$– the energy release function (W/m^3).

The x-axis is directed perpendicularly to the irradiated surface inward the target. Initial and boundary conditions are prescribed as follows:

$$E(x,0) = c \cdot \rho \cdot T_0, \tag{7}$$

$$\frac{\lambda}{c\rho} \frac{\partial E(0,t)}{\partial x} = \rho \cdot V_f \cdot \Delta H + \alpha \cdot \sigma \cdot [T(0,t)^4 - T_0^4], \tag{8}$$

$$\frac{\lambda}{c\rho} \frac{\partial E(l,t)}{\partial x} = -\alpha \cdot \sigma \cdot [T(l,t)^4 - T_0^4], \tag{9}$$

Here, λ, c, ρ – the heat conductivity, heat capacity and density of a target material, T_0 – the initial magnitude of a target temperature, ΔH – the difference between the solid and gas-phase enthalpies, α – the thermal emissivity of a target, σ – Stefan–Boltzmann constant, l – target thickness, $T(0,t)$ and $T(l,t)$ – the surface and back side temperature of a target, respectively.

The presented above boundary conditions take into account the thermal emission of both sides of a target. Heat transfer on the surface includes accounting substance vapor appearing.

The equation (6) is the heat conductivity equation written via the substance internal energy. This equation form allows taking into account energy expenditures on melting. For that purpose, the temperature is described as a function of substance internal energy (Fig. 2), and it is determined through the following expressions:

$$T(x,t) = \begin{cases} \frac{E(x,t)}{c\rho}, & E(x,t) < E_1; \\ T_m + \frac{E(x,t) - E_2}{c\rho}, & E(x,t) > E_2; \\ T_m, & E_1 \leqslant E(x,t) \leqslant E_2. \end{cases} \tag{10}$$