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Dependence of the recoil energy on crystallographic directions under bombardment of a mono-crystal by slow ions

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Calculations of the recoil energy under bombardment of the surface edge (001) for the vanadium mono-crystal by K^+ ions ($E_0 = 10-50$ eV) with the initial motion trajectories lying in planes perpendicular to the plane (001) and parallel to the planes (100) and (1$\bar{1}$0), passing along the crystallographic directions [010] and [110], respectively, have been made by the method of molecular dynamics using a long-range interaction potential. Anisotropy of maximum energy transfer to one of the group of (3−5) atoms simultaneously participating in the interaction, depending on the ion motion trajectory, has been revealed. The energy spray thresholds for specified directions have been determined

Keywords: ion bombardment, single crystal, crystallographic directions, recoil energy, sputtering thresholds.

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Introduction

In papers [1,2] the energy of the effective sputtering threshold of solids was calculated via analytical formulas using the model of successive pair elastic collisions. According to M. Robinson [3], there is no satisfactory theory of threshold energies. A simple relation between the surface binding energy and the sputtering threshold energy is met only for very light and fast bombarding particles ($m \ll M$) [4]. In the case when the mass m of the bombarding particle is comparable to the mass M of the target atom, this ratio is of little value. According to Eckstein [5] the threshold energy cannot be determined directly. It can be obtained extrapolating the dependence of the sputtering ratio on the bombardment energy on low energies. In turn, sputtering dependence curves are obtained either experimentally or theoretically by calculation via analytical formulas using adjustable parameters. In this case, short-range pair interaction potentials are used. Analytical formulas are based on the energy transfer coefficient — the product of the elastic pair collisions model, which is inapplicable at low energies [6,7].

The important part of this problem is the determination of the surface binding energy of atoms in a solid body. It is determined on the basis of the energy of sublimation (cohesion) of metals [3] or on the basis of the statistical equilibrium of evaporation and condensation of metal vapors [8].

In paper [9] an attempt was made to theoretically determine the sputtering threshold energy of a metal single crystal using the results of numerical studies of the recoil energy upon its bombardment by low-energy ions ($E_0 \leq 100$ eV). The calculations were performed by the molecular dynamics method using a long-range potential within the framework of the many-particles interaction mechanism. A method for determining the threshold energy is proposed. It consists in that the threshold energy E_{thr} is determined from the calculated dependences $E_{rec\,\max}(E_0)$. (Here $E_{rec\,\max}$ are maximum values of the recoil energy obtained by one of the group of surface atoms simultaneously participating in the interaction with the ion.) It is assumed that the atom is sputtered from the surface when the surface binding energy E_{bond} is equal to or less than the recoil energy $E_{rec\,\max}$ ($E_{bond} \leq E_{rec\,\max}$).

The aim of this paper is to numerically study the process of energy transfer from a bombarding ion to atoms of BCC metal lattice depending on the crystal orientation relative to the ion beam and to determine the sputtering threshold energies depending on the crystallographic directions.

1. Target model and choice of interaction potential

The target model and the geometry of one of the initial motions of the ion relative to its surface are shown in Fig. 1, *a*. The surface face was the face (001) of the vanadium single crystal with BCC lattice. In contrast to [9], where the plane of incidence of ions perpendicular to surface face (001) coincided or was parallel to plane (100) passing along crystallographic direction [010], in these calculations the plane of incidence is rotated in azimuth by an angle of 45° and coincides or is parallel to the plane (1$\bar{1}$0) passing along crystallographic direction [110]. Before the start of motion, the ion was in one of the indicated planes at a distance $z_0 = 5$ Å from the target surface. The angle of incidence was equal to $\alpha = 55°$.

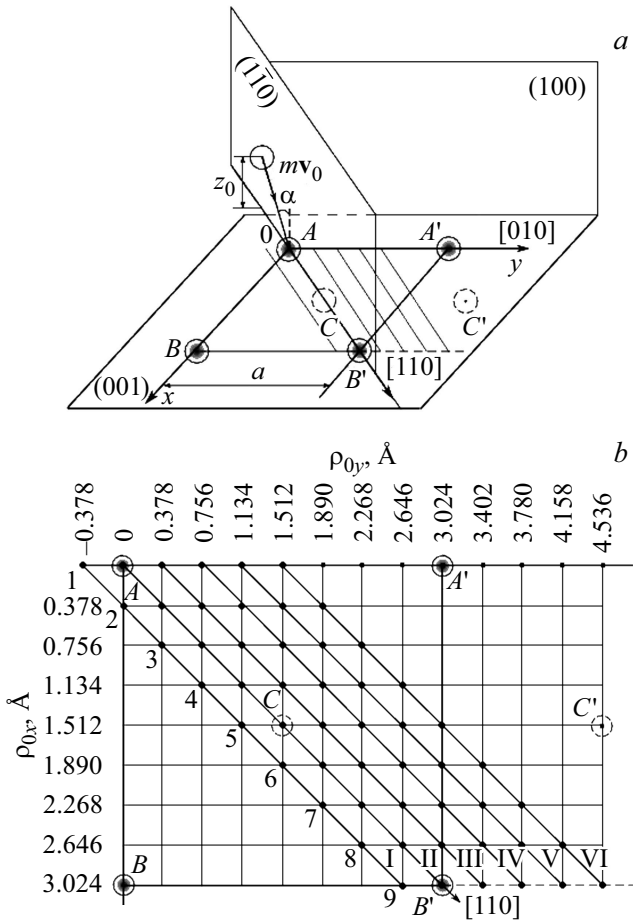

Figure 1. Target model (points 1−9 are points where the ion hits the target).

The recoil energy was calculated for different impact parameters $\rho(\rho_{0x}, \rho_{0y})$ corresponding to the points of ion incidence on the target (points 1−9). These points, like others, are the nodes of the grid with square cells 0.378×0.378 Å covering the target surface. Points 1−9 lie in the plane of incidence of the ion on the line of its intersection with the target surface (Fig. 1, *b*). Each plane of incidence has its own line (in Fig. 1, *b* these lines are indicated by Roman numerals), containing points 1−9 with the corresponding coordinates (ρ_{0x}, ρ_{0y}) and parallel to crystallographic direction [110]. The recoil energy calculations were limited only to points 1−9 because the results of calculations for all other points, i.e., nodes of the grid, due to symmetry repeat the results of calculations for points 1−9.

Depending on the value of the initial energy E_0 the calculation accuracy ranged from 0.8 to 3.8%. In particular, for $E_0 \geq 30$ eV it ranged from 0.8 to 2%, and for $E_0 \leq 25$ eV — from 1.1 to 3.8%.

The long-range interaction potential V_S [10]:

$$V_S(r) = \frac{1}{r}\left[2117.2\exp(-3.217r) + 171.2\exp(-1.423r)\right],$$

where the distance r is in [Å], the interaction energy V_S is in [eV]. Cutoff radius $r = 3$ Å.

The choice of potential and cutoff radius is determined by the calculation method and the specifics of the interaction model. Studies in [11] showed that the use of V_S potential in calculations of the K^+ ions sputtering by the vanadium target gives better agreement with experiment than in the case of other potentials use.

2. Results and discussion

Fig. 2 shows the curves of the maximum recoil energy $E_{rec\,max}$ obtained by one of the group (3−5) of vanadium crystal atoms participating simultaneously in collision with ion K^+ vs. the impact parameter ρ for different lines I−VI (incidence planes) and different bombardment energies E_0. It follows from the calculated dependences $E_{rec\,\max}(\rho)$ that the maximum recoil energy decreases as the ion moves away from the atoms, and the largest maximum recoil energy E_n falls on the line II (points 1−3) (the plane of incidence (1$\bar{1}$0)) passing through a series of atoms in crystallographic direction [110]. The shift of the maximum of the dependence curves $E_{rec\,\max}(\rho)$ to the region of action of one atom closest to the ion with the energy E_0 increasing is due to the mechanism of multiparticles interaction, when with the bombardment energy increasing (the ion speed increasing), its role decreases, since the influence of other atoms decreases (their contribution to the recoil energy decreases) due to the collision time decreasing [11]. For this reason, the choice of a long-range potential is important. For comparison, the Table shows the values of the relative maximum recoil energies $E_{rec\,\max}/E_0$, obtained within the framework of the multiparticle mechanism, and E_{front}/E_0, calculated using the model of pair elastic collisions in a frontal collision of the ion with the target atom. It can be seen that as E_0 increases, the ratio $E_{rec\,\max}/E_0$ increases, approaching the value E_{front}/E_0, where E_{front} is recoil energy at the central impact. This indicates that as the bombardment energy increases, the role of multiparticle interactions decreases, while the role of pair interactions increases. It can be supposed that for sufficiently large values of $E_{rec\,\max}/E_0$ the ratio will be equal to E_{front}/E_0,

Maximum relative recoil energies calculated within the framework of many-particles interaction and by the model of pair elastic collisions

E_0, eV	Multiparticle interactions $E_{rec\,\max}/E_0$	pair collisions E_{front}/E_0
15	0.66	0.98
30	0.67	0.98
40	0.725	0.98
50	0.75	0.98

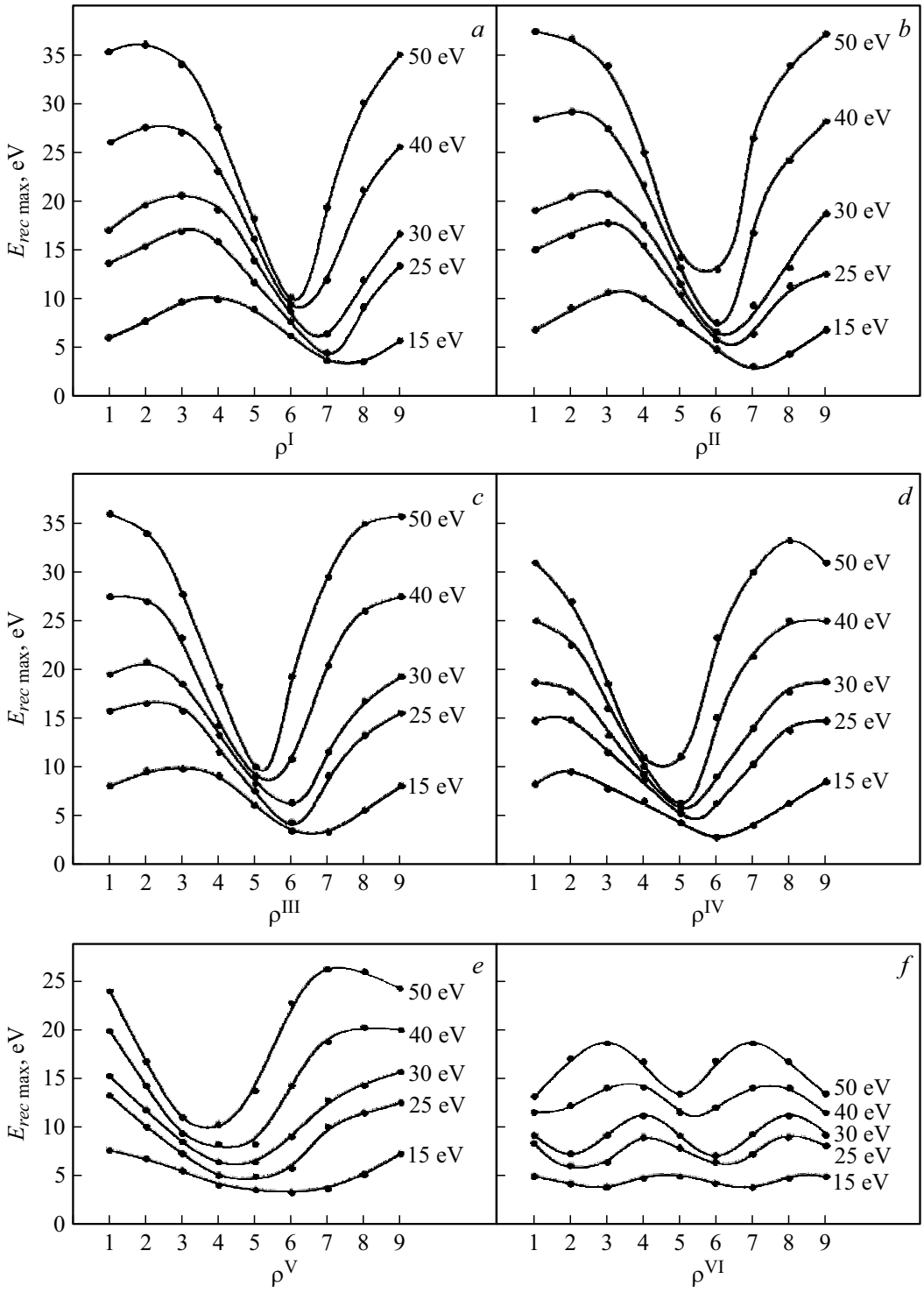

Figure 2. Curves of the maximum recoil energy received by one atom from a group of atoms of a vanadium single crystal, simultaneously participating in collision with ion K^+ vs. impact parameter (points 1–9) for different lines I–VI and different bombardment energies.

and the maximum of $E_{rec\,\max}(\rho)$ will take the position corresponding to the position of the atom in the crystal lattice $\rho(\rho_{0x}, \rho_{0y}) = 0$.

Fig. 3 shows the total recoil energy $E_{rec\,\Sigma}$ obtained by the entire group (3–5) of crystal atoms simultaneously participating in the interaction with the bombarding ion vs. the impact parameter ρ for different lines I–VI and different energies E_0. It can be seen that as the plane of incidence of the ion moves away from the crystallographic plane $(1\bar{1}0)$, „smoothing“ of curves $E_{rec\,\Sigma}(\rho)$ occurs, and the recoil energy becomes minimum. This is due to the mechanism of the ion interaction with atoms.

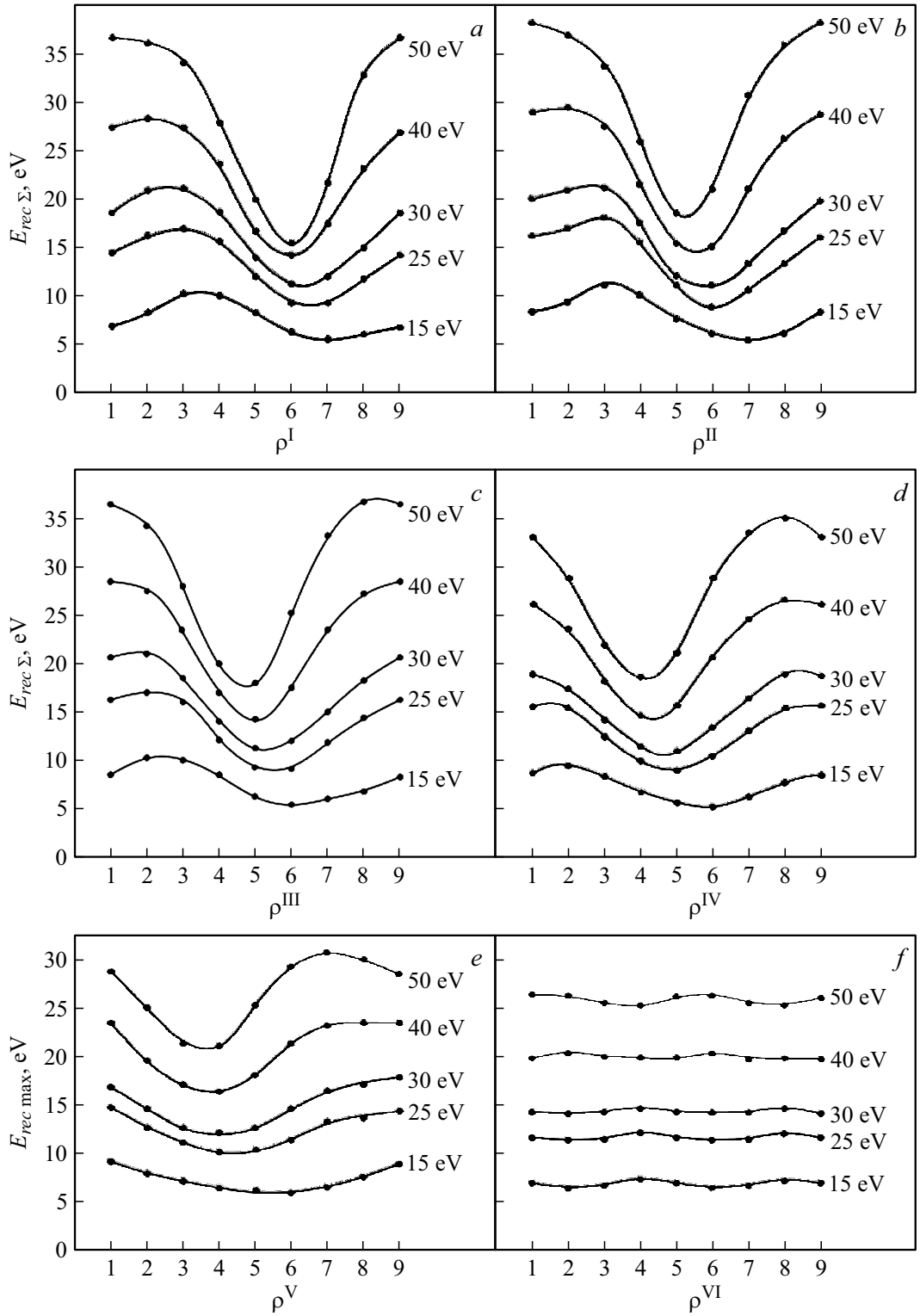

Figure 3. Curves of the total recoil energy received by the entire group of atoms of a vanadium single crystal, simultaneously participating in collision with ion K^+ vs. impact parameter for different lines I–VI and different bombardment energies.

Thus, the proposed study method makes it possible to determine the places on the target surface with maximum and minimum energy transfer from a ion to an atom, and thereby predict „centers“ of possible sputtering, and for multicomponent targets — the possibility of their selective sputtering.

Fig. 4 shows the highest energy E_n of all possible maximum values of the recoil energy $E_{rec\,\max}$ transferred to

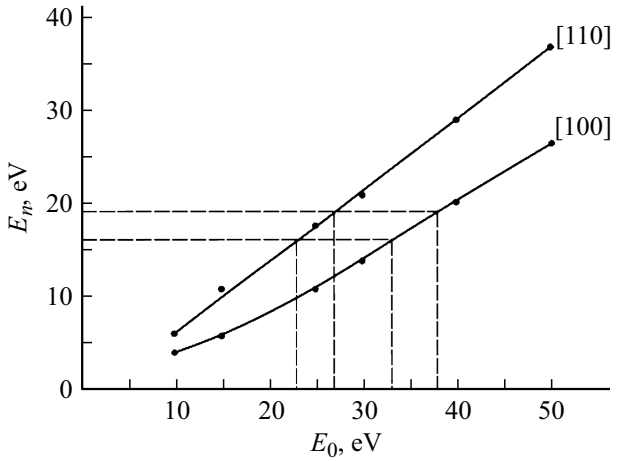

Figure 4. Highest energy of all possible maximum recoil energies received by atom vs. the bombardment energy for different crystallographic directions.

the atom vs. the bombardment energy for crystallographic direction [110]. In the same Figure, as a comparison, the $E_n(E_0)$ dependence for same face (001) is shown, but when the ion moves in plane (100) coinciding with crystallographic direction [010] [9]. It can be seen that the dependence curve $E_0(E_n)$ for direction [110] goes higher than for direction [010], i.e., there is an anisotropy of the maximum recoil energy when the ion moves in planes coinciding with different crystallographic directions.

3. Surface binding energy

Assuming that sputtering starts when $E_n \geq E_{bond}$, one can find from the $E_n(E_0)$ dependence curve (Fig. 4) the sputtering threshold energy of face (001) of the vanadium single crystal for different crystallographic directions if the energy E_{bond} is known. To determine the value of E_{bond} we use the fact that for metallic crystals the surface binding energy is additive, and when it is found, the interaction of the nearest first and second neighbors [8] is taken into account. (For low-index faces there is interaction between nearest neighbors only.) The total value of the surface binding energy is determined by the number of first and second nearest neighbors, which correspond to the energy ε_1 and $\varepsilon_2 < 0.1\varepsilon_1$ per atom, respectively. In a „semi-crystalline“ position (state) of the surface for BCC crystal, it is, according to [8], $E_{bond} = 3\varepsilon_1 + 6\varepsilon_2$, where „three“ and „six“ indicate the number of first and second neighbors respectively. The selected state of the surface differs from all others in that it corresponds to a statistical equilibrium between direct evaporation and direct condensation of atoms of metal single crystals.

Taking the energy ε_1, equal to the sublimation (cohesion) energy of the metal for vanadium $\varepsilon_1 = 5.3\,\text{eV/at}$, the surface binding energy will be equal to $E_{bond} = \big(15.9 + (< 3.18)\big)\,\text{eV}$, i.e., it lies within $15.9 < E_{bond} < 19.08\,\text{eV}$. Therefore, according to Fig. 4 the sputtering threshold of face (001) V for direction [010] lies within $33.2 < E_{thr} < 38\,\text{eV}$, and for direction [110] it lies within $23 < E_{thr} < 27\,\text{eV}$. Thus, the anisotropy of the maximum recoil energy in the collision leads to the anisotropy of the sputtering threshold energy of the metal single crystal. In paper [12] the calculated binding energies for individual faces of single crystals of some metals range from 3.8 to 12 eV/at.

Note that the numerical studies of the ion interaction with the surface refer to the ideal surface of the single crystal. In fact, the real surface is not ideal [13]. Various steps and atoms with broken bonds are possible on it. Therefore, for the „rough“ surface the number of nearest neighbors will be less than those accepted in the present calculations, and, consequently, the threshold energy found in the study may turn out to be less than the calculated value. Apparently, for the minimum value of the sputtering threshold energy E_{thr} in the case of $K^+(Ar^+) \to V$ one should take the value $E_{thr} = 12.5\,\text{eV}$ [9] corresponding to the minimum binding energy $E_{bond} = 5.3\,\text{eV}$. However, the comparison of the thresholds of vanadium sputtering by ions K^+ (or Ar^+) calculated in this paper with the experimental data $E_{thr} = 23\,\text{eV}$ given in [14], indicates a satisfactory agreement between the calculation and the experiment.

Conclusion

The presented results of computer calculations of energy transfer during the bombardment of the crystal surface with slow ions and the proposed method for determining the sputtering energy thresholds of metal single crystals make it possible to make predictions about the properties of the surface and its modification during sputtering. Surface areas with broken atomic bonds or the absence of stoichiometry in the case of alloys may turn out to be areas with low sputtering thresholds and, consequently, — sputtering „centers“.

Conflict of interest

The authors declare that they have no conflict of interest.

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