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Comment to the paper by A.I. Tolmachev and L. Forlano „Depemdence of the sputtering yield on the angle of ion incidence on the target surface“ (2022, V. 92. Issue 5. P. 660−664)

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A criitical analysis of the approach applied by A.I. Tolmachev and L. Forlano (ZhTF, 92 (5), 660 (2022)) to solving the problem of ion sputtering of solids is presented.

Keywords: sputtering, angular dependence of the sputtering yield, computer simulation, program PAOLA, program SRIM, transport equation, binary collisions.

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The sputtering of solids in the range of angles of ion incidence from 0 (normal incidence) to 90° (limiting sliding incidence) was studied in [1]. The work includes theoretical analysis based on the numerical solution of the transport equation and computer simulation using the PAOLA program based on the model of binary elastic collisions. The results are presented in the form of dependencies $Y(\theta_0)/Y(0^\circ)$, where Y is the sputtering yield and θ_0 is the angle of incidence. It is shown that Y increases with an increase of θ_0 to a certain maximum value, and then decreases to $Y(90^\circ)$. The obtained values $Y(90^\circ)/Y(0^\circ)$ are within 0.5−5. A qualitative consistency with the calculations using the SRIM program [2] and a discrepancy with the calculations by the OKSANA program [3] were found. OKSANA gave values of $Y = 0$ in the case of sliding bombardment of flat surfaces of amorphous Si and Ge targets with 1 keV Ar and Xe ions. It is concluded that the discrepancy may be attributable to the „inaccurate interpretation of the first collision of ion entering the target“ [1].

The absence of sputtering during sliding bombardment of flat surfaces was noted in many works. For amorphous targets, this result was obtained in calculations using the programs MARLOWE [4], TRIM.SP [5], ACAT [6], TRIDYN [7], SDTrimSP [8], IMSIL [9,10], etc. Calculations were performed for H, Ar, Ga, Xe ions and various targets (Si, Ni, Cu, Ag, Ta) in the ion energy range 1−30 keV. The absence of sputtering at large angles θ_0 is associated with the complete reflection of ions from the surface as a result of a series of correlated collisions with atoms of the upper layer like in case of scattering by a surface chain of atoms [11,12]. This is illustrated by Fig. 1 showing the trajectories of ions when scattered by a chain of atoms and a three-dimensional amorphous target. The spread of trajectories (b) is associated with a different position of the target atoms for each new incident ion. The absence of scattering at large angles, as in the case of reflection from the chain (a), is explained by the mutual shading of atoms located near the surface, as a result of which collisions at small impact parameters do not occur at low impact parameters. This complicates the transfer energy to the target atoms, which gives zero values of Y.

In the PAOLA program [1], random numbers R_1, R_2 and R_3 are generated before each collision in the range from 0 to 1. These numbers determine the particle path between collisions $\lambda = \lambda_0 \ln(1/R_1)$, the polar scattering angle ω in the center of mass system

$$\cos\omega = \frac{2(1+\varepsilon)R_2 - 1}{1 + 2R_2\varepsilon} \qquad (1)$$

and the azimuthal scattering angle $\varphi = 2\pi R_3$, where λ_0 — average free path length and ε — reduced energy. As follows from (1), at $R_2 = 0$, the scattering angle is $\omega = 180^\circ$, which corresponds to a head-on collision in which the energy transfer to the target atom is maximal. With a random sample of scattering angles, such hard collisions can also occur at the initial section of the ion trajectory, initiating sputtering even at angles θ_0 close to 90°, which was observed in [1]. This result is a consequence of the fact that the model used in the work [1] does not take into account the possibility of correlated collisions associated with mutual shading of atoms and playing an important role at sliding angles of incidence. It should also be noted that for $R_1 = 1$, the value is $\lambda = 0$, which contradicts the presence of a short-range order in the arrangement of solid atoms.

As for SRIM [2], this program assumes that the starting points of the ion trajectories lie directly on the surface of the target, so the scattering of ions when approaching the surface, as described above, is not considered at all. This

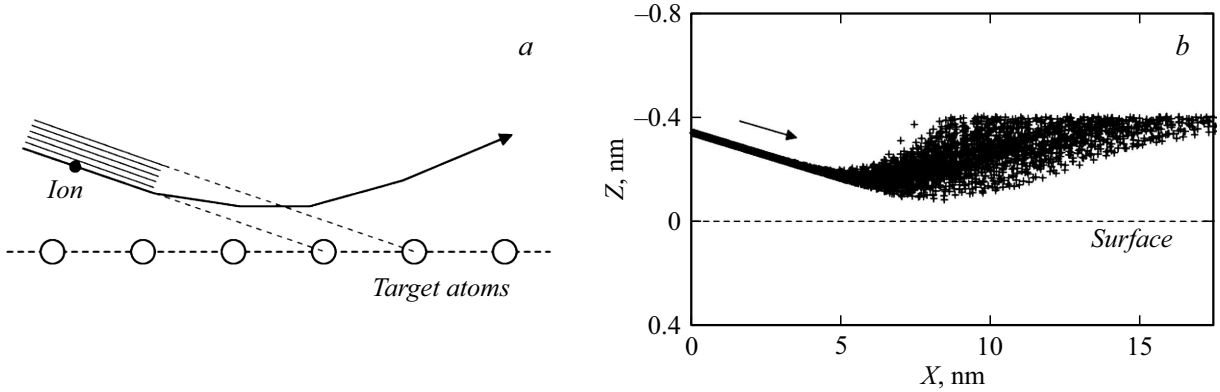

Figure 1. *a* — scheme of ion scattering by a chain of atoms; *b* — trajectories of Ar ions with an energy of 1 keV scattered by the surface of amorphous Ge at an angle of incidence of 88° (calculation by the OKSANA program using the Thomas-Fermi-Moliere potential with the Lindhard screening length). The trajectories are given in projection onto the plane of incidence.

was shown by the analysis of the ion trajectories generated by the SRIM program carried out in [3]. Ignoring the scattering of ions when approaching the surface leads to non-zero values of Y at $\theta_0 \approx 90°$, i.e. when the ions move almost parallel to the surface. This result of SRIM calculations is called in [13] „clearly non-physical".

The sputtering yield at large angles of incidence can increase dramatically when taking into account the surface roughness (for example, [9,14]), as well as the attraction of incident particles by the surface (for example, in the case of self-sputtering [15]), however, the relevant discussion is beyond the scope of this comment.

Thus, the trajectory calculation algorithm used in the PAOLA program [1] distorts the collision pattern as the ion approaches the surface, does not take into account the effect of correlated particle collisions associated with the mutual shading of atoms, and, as a result, leads to the conclusion of non-zero sputtering coefficients at angles of incidence close to 90°. The coincidence of the simulation results using the PAOLA program and the numerical solution of the Chandrasekhar integral equation noted in [1] indicates that these disadvantages also occur in the case of the description of sputtering based on the transfer equation.

Conflict of interest

The author declares that he has no conflict of interest.

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