Effects of crystal structure of surface relief in sputtering

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The work is motivated by the fact that for ions with energy E_0 > 1 keV, the sputtering yields of some metals obtained in calculations for an amorphous target with a smooth surface differ significantly from the experimental ones. This may be due to both the crystallinity of the target and the ion-induced surface relief. In this work, the sputtering yields of amorphous and crystalline targets bombarded with 0.1-100 keV Ar ions were calculated using computer simulation. Calculations for nickel and tungsten irradiated with 30 keV Ar ions were performed with and without taking into account the surface relief.

INTRODUCTION

Sputtering of solids by ion bombardment has been studied for a long time, but many aspects of this phenomenon are still insufficiently clarified. Theoretically, irradiated targets are often considered amorphous. In fact, not all materials are or become such during ion bombardment. The expected differences in the sputtering yields of amorphous and polycrystalline materials have been mentioned in the literature, but research in this area is extremely limited. It was shown in [1] that at $E_0 > 1$ keV, the sputtering yield of a polycrystalline Pt target significantly exceeds the sputtering yield of a similar amorphous target, whereas at low energies, the yields practically coincide. A stronger sputtering of a polycrystalline W target compared to its amorphous counterpart was noted in [2]. Differences in the values of the sputtering yield Y were explained [1,2] by sputtering due to linear collision sequences.

This paper continues the discussion of this topic.

CALCULATION METHOD

The OKSANA program was used in the calculations, which makes it possible to simulate the sputtering of crystalline and amorphous targets in the binary collision approximation. The elastic interaction of particles is determined by the potentials ZBL, Kr-C, Lenz-Jensen and Zinoviev [3], and electronic stopping is taken as a combination of local and nonlocal energy losses. The surface binding energy E_S is equal to the heat of sublimation U_0. The surface potential barrier is considered planar.

An amorphous target is modeled by the rotation of a crystalline atomic block, the rotation procedure is performed for each new incident particle and then repeated from collision to collision. To trace the transition from a polycrystal to an amorphous target, the rotation of the block after each collision is carried out with a probability w, which can vary from 0 (polycrystal) to 1 (amorphous target). At $0 < w < 1$, this procedure makes it possible to simulate a target that contains both disordered and crystalline grains (crystallites). The parameter w is related to the average size of the crystallite $\langle L \rangle$ by a simple relation: $\langle L \rangle \sim R_n / w$, where R_n is the distance between the nearest atoms of the crystal.

The direction of the bombardment is set in a rectangular coordinate system, the Z axis of which is directed inside the target. According to experimental data [4], the relief has a tooth-like shape and is described in the X-Z plane by a two-dimensional function with a period of $2x$ and a height of z. The same relief shape is set in the Y-Z plane. Thus, the surface of the target is a set of pyramids. It was taken into account that the pyramids are randomly distributed over the surface. The results presented below were obtained at $x = y = 30$ nm. Increasing x and y does not change the results, but increases the counting time. The change in the shape of the relief during ion bombardment is not taken into account, i.e. a stationary sputtering regime is simulated. A local planar barrier with height $E_S = U_0$ is used. The bulk binding energy E_B atom varies. When calculating the trajectories, it was taken into account that atoms knocked out of the target, as well as scattered bombarding ions, can reach the walls of neighboring surface structures and cause their sputtering.

For amorphous Ni irradiated with 30 keV Ar ions, examples of ion trajectories are shown in Fig. 1.

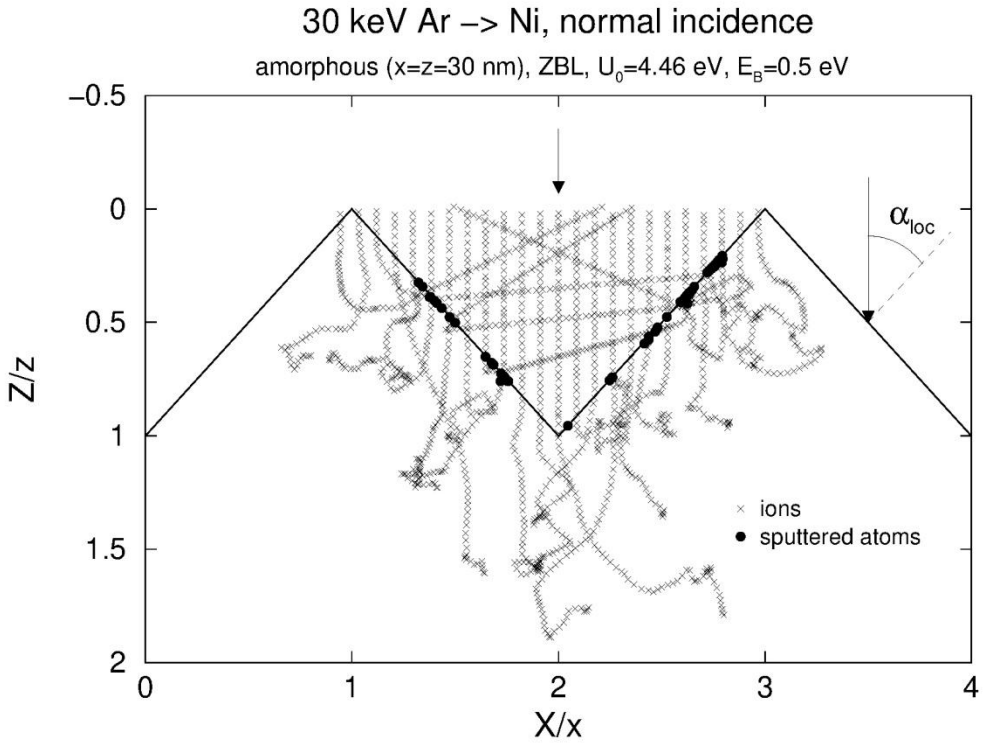


Fig.1. Trajectories of 30 keV Ar ions under bombardment of a ridged Ni surface (x = z = 30 nm). Calculation using the ZBL potential. Circles are the initial positions of sputtered atoms. The trajectories of the particles are given in projection onto the X-Z plane. α_{loc} is the local angle of incidence.

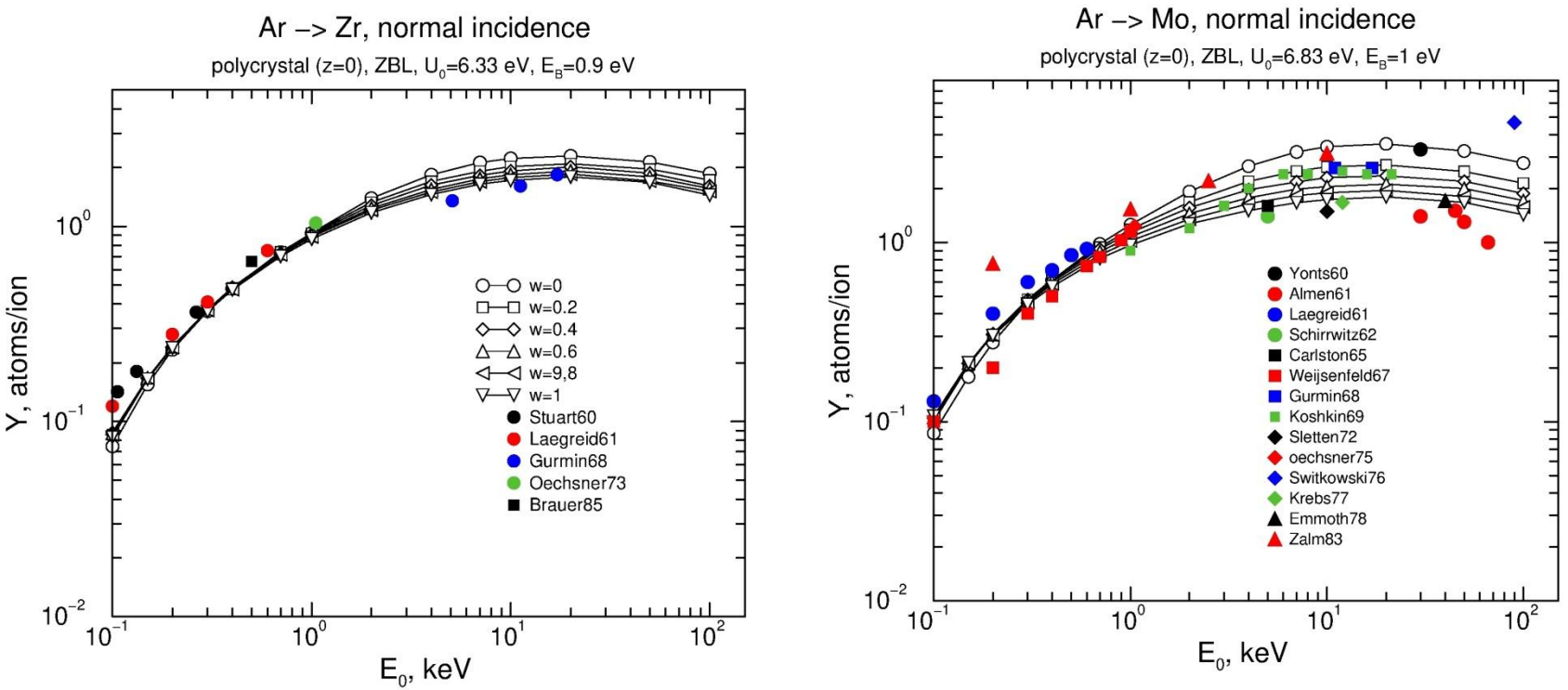


Fig. 2. Sputtering yields of Zr and Mo targets with a flat surface (z = 0), depending on the energy of Ar ions for the values of w in the range from 0 (polycrystal with large grains) to 1 (amorphous target). The points are experimental data from different authors. Note the increase in the sputtering yield when going from an amorphous to a polycrystalline target at E_0 > 1 keV.

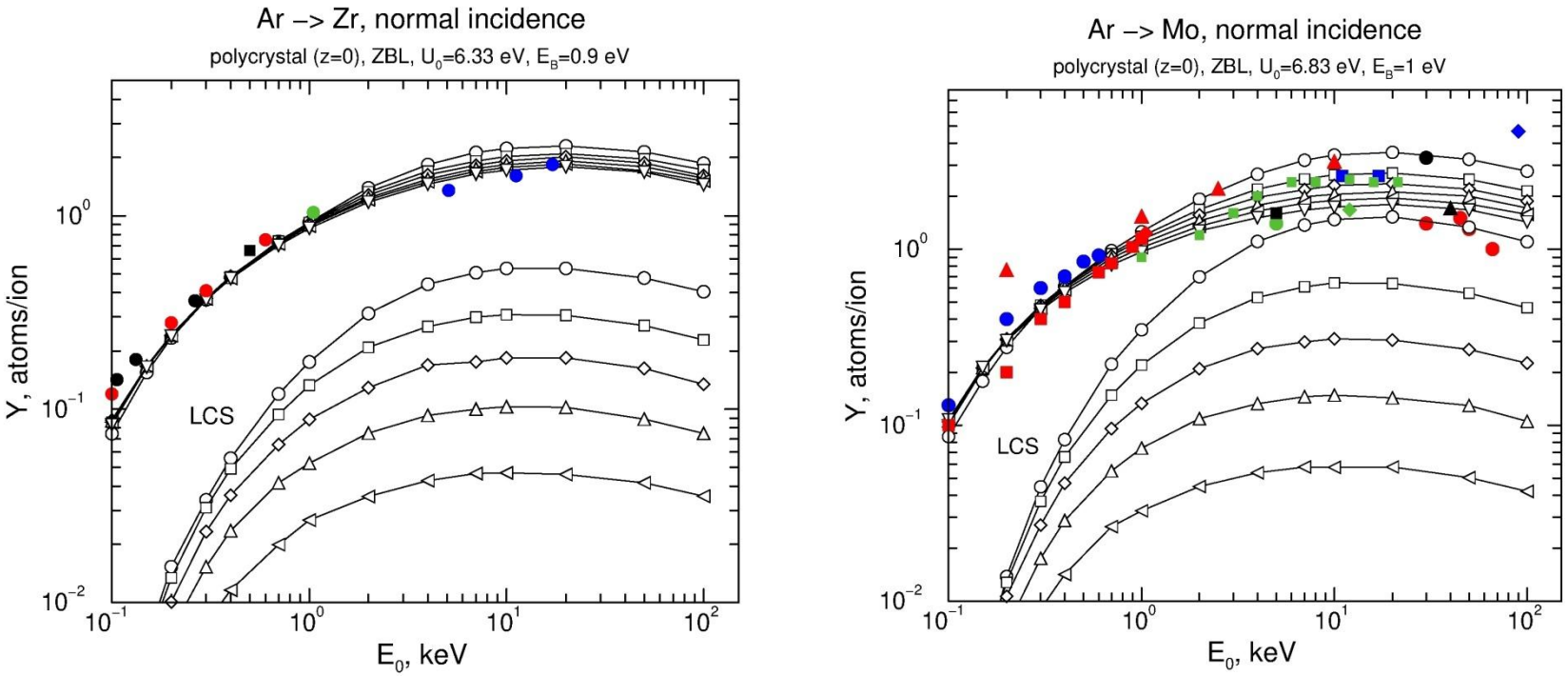


Fig.3. The same as in Fig.2, but indicating the contribution of linear collision sequences (LCS) to sputtering. Chains of collisions with a length of two or more interatomic distances were taken into account. The difference in results is mainly due to the fact that zirconium has a hexagonal lattice, which does not contribute too much to the formation of LCS. Molybdenum has a bulk-centered lattice, which is more favorable in this regard.

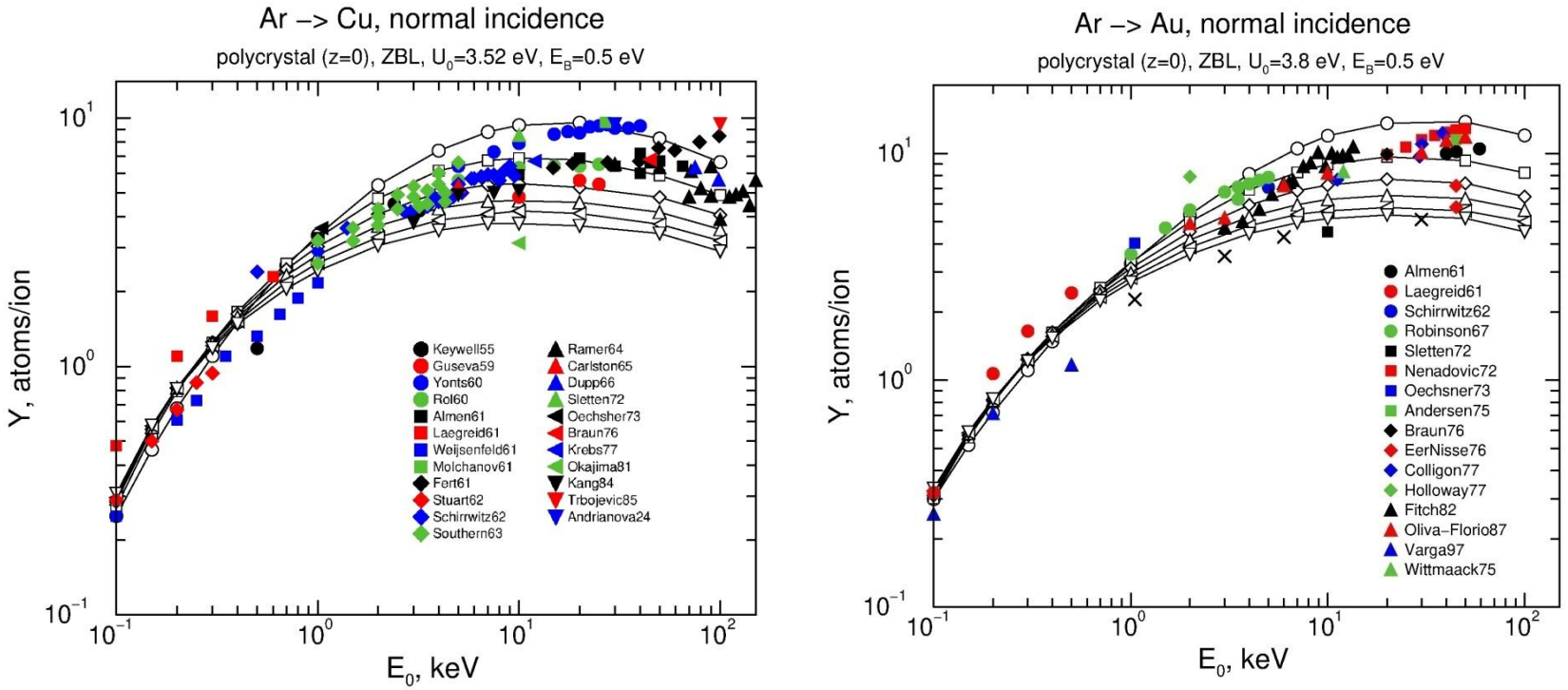
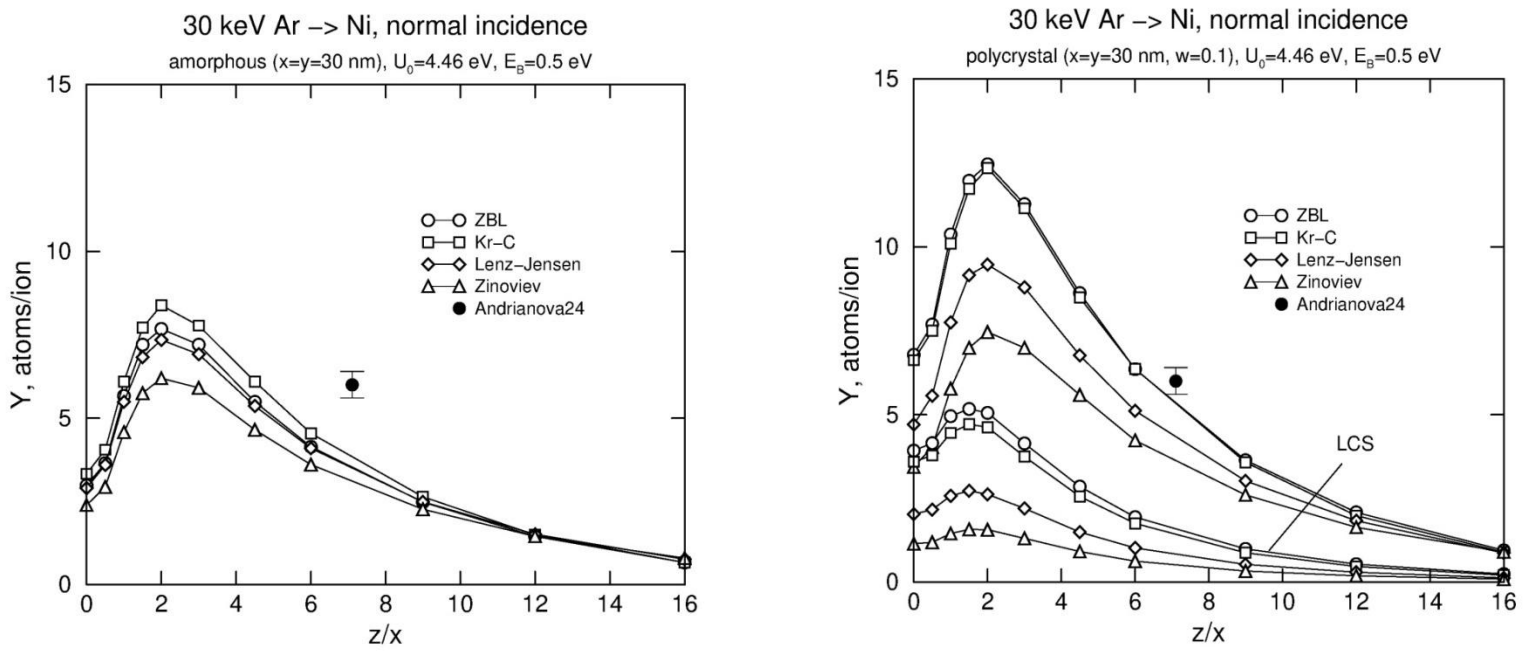


Fig. 4. Sputtering yields of Cu and Au targets with a flat surface as a function of the ion energy at different values of *w*. × – TRIM.SP. It follows from the figure that in the energy range $E_0 > 1$ keV, the amorphous target model is poorly suited for describing the sputtering of these materials.



(a) (b)

Fig. 5. Sputtering yields of amorphous (a) and polycrystalline Ni targets (b), calculated taking into account the tooth-like surface relief, as a function of the aspect ratio *z*/*x*. The filled circle: experiment [4]. Higher yields for polycrystalline targets are associated with the LCS contribution. It can be seen that the sputter yields for a smooth (*z*/*x* = 0) and tooth-like surface (*z*/*x* = 7.1) are close. It follows from the figure that the main reason for the high values of *Y* measured experimentally [4] is the crystallinity of the target, rather than the roughness of its surface. Similar results were obtained for tungsten.

CONCLUSIONS

Sputtering of a large set of amorphous and polycrystalline targets (Ni, Cu, Zr, Mo, Ag, Au, W, Al, Fe, Ti, V, Cr, Be, Ta, etc.) by 0.1-100 keV Ar ions was calculated using the OKSANA program. As in the case of Pt sputtering [1], the sputtering yields of polycrystals in the energy range above 1 keV exceed the sputtering yield of similar amorphous targets. This is the result of sputtering due to linear collision sequences, the contribution of which is closely related to the type of the corresponding crystal lattice. The best agreement with the experiment was obtained using the ZBL and Kr-C potentials.

Литература

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