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Characteristics of flows of energetic atoms reflected from metal targets during ion bombardment

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Abstract. Particle number and energy reflection coefficients for energetic neutralized gas ions (Ar and O atoms) backscattered from metal targets during ion bombardment have been calculated using TRIM code. The energy distributions of reflected atoms are computed, too, and their dependence on the primary ion energy and the angle of ion incidence is determined. The obtained data confirm the possibility of employing energetic atoms reflection for generation of high energy neutral beams and point out to take this phenomenon into account under analysis of the ion technology for coating deposition.

1. Introduction

Gas ion bombardment of metal targets is widely used in electronic and optical industry for sputtering of metal atoms and deposition of coating onto substrates. This process is accompanied by partial reflection/backscattering of bombarding ions from the target surface [1, 2]. The reflected particles practically all are electrically neutral since the primary projectile ions are neutralized during the contact with metal surface. Besides, the primary molecular ions dissociate; so, the reflected particles are gas atoms and they may have significant part of the primary ion energy. These energetic atoms bombard the substrates, heat them and affect the microstructure of the coatings [3]. The reflection and neutralization of ions on metal surface may be used for generation of directed high-energy neutral atom beams [4–6]. Such beams are employed for sputtering of dielectrics and semiconductors [4–6].

The phenomenon of reflection/backscattering of energetic atoms from metal surface during ion bombardment was considered in literature and several computer codes have been developed for simulating this process [1, 2, 7]. It has been shown that the reflection coefficients may achieve tens of percents, especially at oblique incidence. The published information relates mainly to reflection of light (H and He) atoms [2, 7]. However from practical point of view the most interesting for sputtering technology is data on reflection of such working particles as argon and oxygen ions. The task of this work is to calculate the characteristics of energetic flows of argon and oxygen atoms reflected from different metal targets during bombardment by ions with energy in range of 0,5–5,0 keV used for sputtering. The set of light and heavy metals (from Si, Al and Ti to Ta) was chosen as the typical target set used in sputtering technology.

2. Calculation of energetic atom flows characteristics and discussion

The calculations were performed using the TRIM code (TRansport of Ions in Matter) [7]. It is based on the Monte Carlo method to follow a random walks of N_0 = 99 500 high-energy particles (the former projectile ions) in a solid target using the approximation of binary collisions of the walking particles with the target atoms. The trajectory of each projectile particle is traced as long as it does not lose its energy. Particle number and energy reflection coefficients (respectively, R_N and R_E) are used as integrated characteristics of the process. The coefficient R_N is defined as the ratio of reflected/backscattered N atoms to the number N_0 of primary atom particles bombarding the target. In the case of one-atom ions (Ar^+ or O^+) the value N_0 equals the quantity of ions. In the case of two-atom molecular ions (O^+_2) we must take N_0 as double quantity of ions because these ions dissociate and then two atoms walk within the target body as independent particles. The presence of charge at the bombarding particles does not affect R_N [2]. Table 1 and table 2 show the results of R_N and R_E calculations, where E_0 is the initial energy of the bombarding particles in terms of atoms.

Table 1. Calculation of the particle number and energy reflection coefficients for the oxygen ions (O^+) at normal incidence.

E_0, keV	Reflection coefficients, %	Material and atomic mass of the target					
		Al 26,98	Ti 47,90	Zn 65,38	Zr 91,22	Nb 92,91	Ta 180,95
0,5	R_N	5,02	12,82	20,65	22,17	23,53	36,53
	R_E	0,41	2,14	5,18	6,10	6,65	15,55
1,0	R_N	3,98	11,43	18,85	20,15	21,24	35,45
	R_E	0,33	1,99	4,74	5,58	5,98	14,81
5,0	R_N	2,44	7,74	14,36	16,22	16,50	31,06
	R_E	0,21	1,33	3,65	4,35	4,55	12,82

Table 2. Calculation of the particle number and energy reflection coefficients for the argon ions (Ar^+) at normal incidence.

E_0, keV	Reflection coefficients, %	Material and atomic mass of the target					
		Al 26,98	Ti 47,90	Zn 65,38	Zr 91,22	Nb 92,91	Ta 180,95
0,5	R_N	0,0834	2,90	9,25	12,73	13,53	28,40
	R_E	0,0014	0,12	0,74	1,57	1,79	7,98
1,0	R_N	0,0724	2,66	7,91	1,52	12,41	26,87
	R_E	0,0010	0,11	0,60	1,45	1,65	7,28
5,0	R_N	0,0673	1,75	5,07	8,77	9,25	22,08
	R_E	0,0010	0,08	0,44	1,12	1,23	6,15

As one can see, the R_N is from several percent to tens percent (subject to the target material), which is a very large value. The lighter bombarding ions, the less energy E_0 and the heavier target atoms, the bigger R_N is (see coefficients for Al, Ti and Ta). The backscattering from the silicon target was very small and it is not presented in the tables. Energy reflection coefficient R_E also lies in the range from several percent to tens percent, but it is several times smaller than the R_N.

The increase of the ion incidence angle φ leads to significant increase of R_N (see figure 1) due to less penetration depth of the projectile particle into the target body at oblique incidence and, hence, greater chance for the particle to return back to the target surface and to go out from the target. The less the way of the particle inside of the target, the less the loss of particle energy and the higher the energy of the backscattered atom are. Thus, the reflected atoms have greater energies at oblique ion incidence than at normal incidence (φ = 0°). The latter is clearly demonstrated by figure 2 and figure 3, which depict the energy distributions of oxygen atoms, which are reflected/backscattered from the targets of titanium and tantalum.

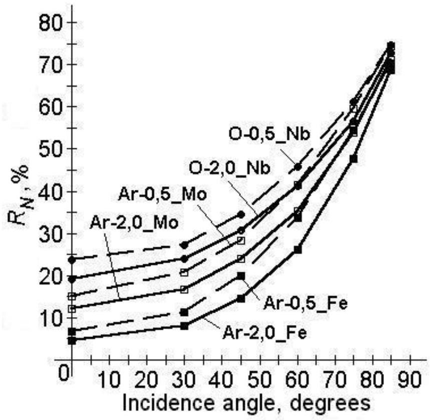
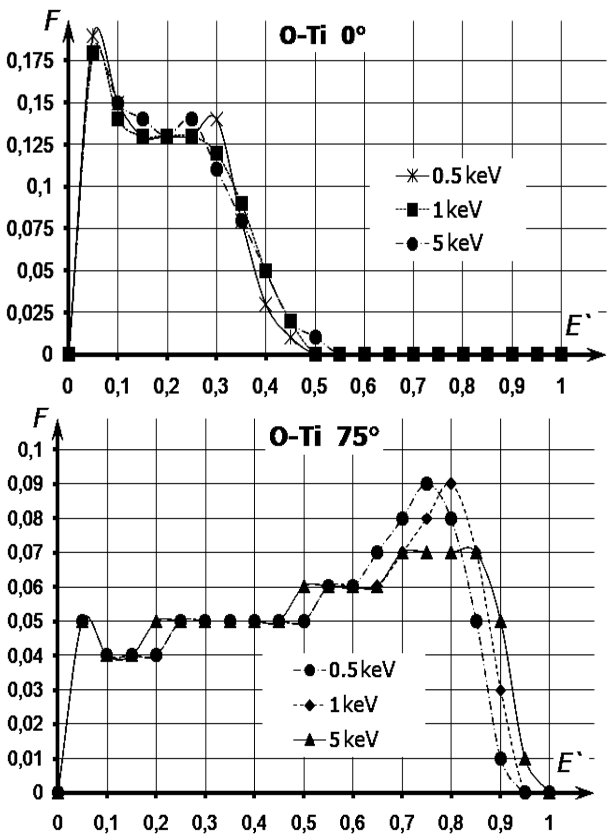


Figure 1. Dependences of particle number reflection coefficient R_N on incidence angle φ for O^+ and Ar^+ ions with initial energy E_0 of 0.5 keV and 2 keV. Target materials are Fe, Mo and Nb.



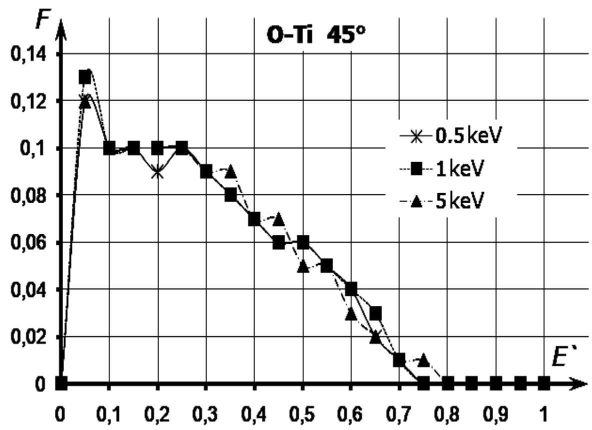


Figure 2. Energy distributions of oxygen atoms reflected from the titanium target at different incidence angles. $E' = E/E_0$.

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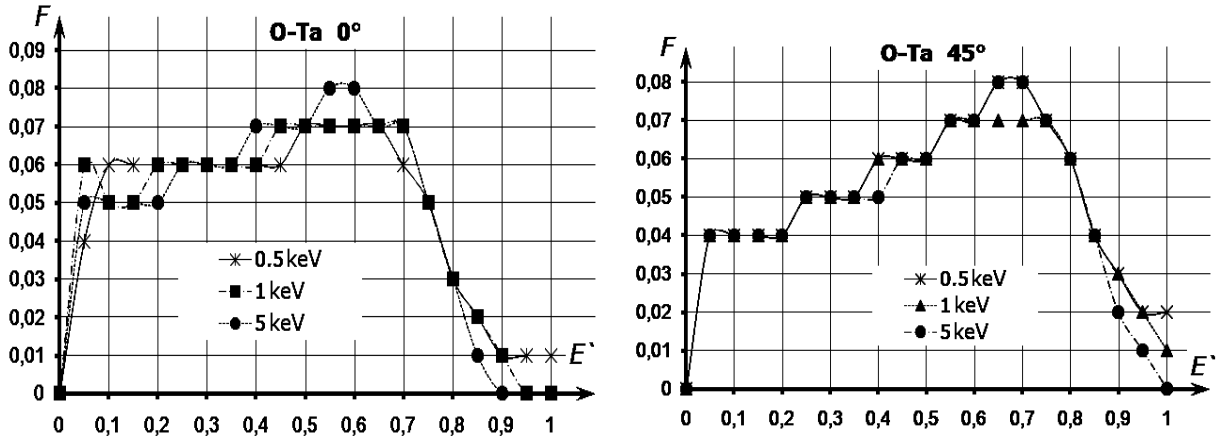

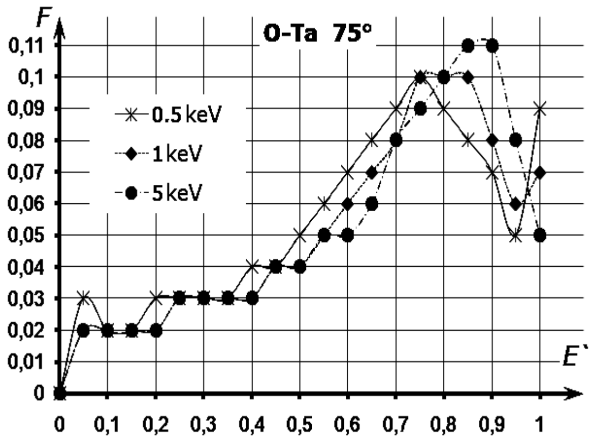

Figure 3. Energy distributions of oxygen atoms reflected from the tantalum target at different incidence angles. $E' = E/E_0$.

Figure 2 and figure 3 present the results of the calculation of energy distributions of the reflected atoms for three values of the bombarding ion energy (0,5, 1 and 5 keV) and three values of the incidence angle (0, 45 and 75 degrees). Results are presented as a polygon. Here, $E' = E/E_0$ is relative energy of the reflected atoms and F was defined as the ratio of number of atoms having an energy in the range of $[E' – 0{,}05, E']$ to the total amount of the reflected atoms N. The entire range of possible energies was divided into 20 parts, so that the sum of 20 discrete values of F is equal to 1.

As one can see, the general form of distributions of reflected atoms on the relative energy is not strongly dependent on the value of the initial energy E_0 of the bombarding ions in the range of 0,5–5,0 keV. However, the increase of incidence angle φ strongly influences on the energy distributions. If $\varphi \sim 0°$ the distributions have a squared shape, when $\varphi = 75°$ their shape becomes triangular-like with a large number of atoms with $E' \sim 0{,}7–1{,}0$. Atoms flows, which are reflected from the target with big atomic mass, contain many high-energy particles. This is particularly valuable for producing beams of energetic neutral atoms from ion beams by ion neutralization of on the metal surface [4–6].

3. Conclusions

Thus, the results of calculations show the significant flows of energetic Ar and O atoms reflected/backscattered from the metal target are generated in the sputtering process with participation of both the heavy argon ions and the lighter oxygen ions. Energy of reflected atoms, which is transferred to the substrate surface, may significantly affect the formation and characteristics of the deposited coatings; in particular, it may strongly affect the refractive index profile during deposition of gradient optical coatings [8]. So, it is necessary to take into account the reflection of energetic atoms and transfer of their energy to substrates under analysis of coating deposition conditions. The obtained data on the reflection of energetic gas neutralized particles can also be used during design of sources of neutral atom beams with neutralizing the primary ion beams on the metal surface. The use of heavy metals is more preferable for building the neutralizers.

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