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# Sputtering of carbide films from the surface of the metal by helium ions bombardment

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The paper investigates the dependence of the sputtering yields by light ions bombardment of the surface layers of titanium and tungsten, modified with carbon, on the thickness of the layer. The theoretical study was conducted on the basis of a sputtering model (previously adapted to describe the sputtering of two-component targets and layered-inhomogeneous surfaces), based on two sputtering mechanisms, which allows to analyze the obtained dependencies. Theoretical calculations of the total yields sputtering by helium ions bombardment of the surface layers of titanium and tungsten modified with carbon are given in comparison with the results of computer simulation obtained using the SRIM-2013pro program.

**Keywords:** modified surface, ion bombardment, sputtering, light ions, layered surface, metal carbide, sputtering yield, partial sputtering yield.

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## Introduction

The increasing use of materials with a carbon-modified surface layer, including in plasma installations, poses the problem of the interaction of charged particle fluxes with such surfaces. In particular, there is a problem of theoretical description of sputtering of such inhomogeneous surfaces. Often used for calculations of sputtering yields of homogeneous materials, sputtering theories [1–3], which allow obtaining sufficiently accurate results, cannot be applied to the case of sputtering of layered structures. Previously, a light ion sputtering model was proposed based on the method outlined in Chandrasekhar's work [4]. According to this model, sputtering can be represented as the result of both upward and downward ion fluxes, which can be highlighted within the bombarded target. Using a model based on two sputtering mechanisms made it possible to describe quite accurately the sputtering not only of homogeneous single-component materials, but also of two-component homogeneous materials and layered targets [5]. Application of the model based on two sputtering mechanisms allows to correctly describe sputtering of different structural materials, and also to explain the effects that can be observed in this case [6]. In the present work, this model is adapted to the case of sputtering of surface carbon-modified titanium and tungsten layers with helium ions.

## 1. Theoretical model

To theoretically describe the sputtering of a carbon-modified titanium or tungsten surface by bombardment with light helium ions, we used the model of a layered heterogeneous target with a sharp interface. According to this model, a homogeneous layer of titanium carbide TiC (or tungsten carbide WC) ($M_1$ — mass of titanium (tungsten) atom, $M_2$ — mass of carbon atom) of thickness $x_0$ is placed on the uniform titanium (or tungsten) substrate of great thickness. The target is bombarded by a wide beam of light helium ions of mass $M_0$ and energy $E_0$, directed at an angle of $\theta_0$ toward the target (the angle is counted from the internal normal to the surface). To exclude accounting for possible changes in the component composition of the target during sputtering, we will assume that the irradiation dose is small.

The model of sputtering of titanium (tungsten) carbide films from the surface of titanium (tungsten) by helium ions is based on the statement that two ion flows can be distinguished in the target at depth x: one directed mainly inside the target, the other, as a result of scattering of ions on atoms, is directed to the surface. Following the method outlined in [4], the collisions of the downward and upward flux ions with the target atoms result in two flows of initially knocked-out atoms at depth x: one directed mainly deep into the target, the other — toward the surface. As a consequence, it is assumed that the sputtering of each layer component can be represented as a sequence of processes initiated by upward and downward ion fluxes independently (two sputtering mechanisms). This approach does not assume the joint solution of integral equations describing separately the fluxes of ions and knocked-out atoms, but rather writes an integral expression that includes functions describing both the flux of ions and the flux of atoms, whose values are determined by independent methods. Thus, the sputtering of layered two-component materials by light ions is described by two mechanisms. A graphical representation of the sequence of processes leading to the sputtering of the

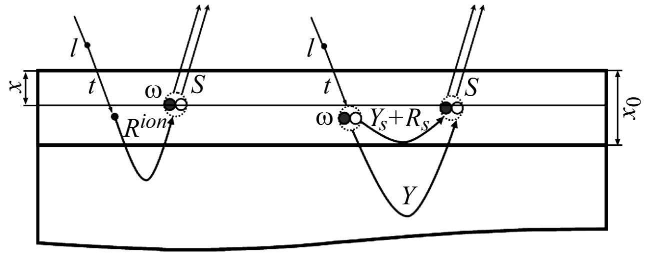

**Figure 1.** Graphical representation of the processes leading to sputtering of a target with a carbon-modified layer on the surface.

$i$th component of the upper layer of the target is shown in Fig. 1.

The left part of Fig. 1 shows the processes that lead to sputtering of the $i$th component of the upper layer of the target as a result of collisions of the upward flux of ions with the atoms of the titanium carbide (tungsten) layer:

- The upward ion flux at depth x is the result of ions passing through a metal carbide layer of thickness $x$ (described by the differential transmission function $t$ of the target layer of thickness $x$ [7]) and the reflection of ions from underlying target layers (determined by the differential ion reflection function $R_{ion}$ from a layered heterogeneous target with heterogeneity layer thickness $x_0 - x$ [8]);
- when upstream ions collide with atoms, a primary recoil atom with an effective charge $Z_{\text{eff}}$ (described by the energy transfer cross section $\omega$ from the moving ion to the stationary atom [1]) is knocked out of the two-component heterogeneity layer;
- the atom escape from the target surface is determined by the emission of knocked-out atoms of the binary heterogeneity layer moving from depth x to the surface, which is considered within the model [9] using a differential function $S_i$ direct (on the shot) self-sputtering of the component $i$ material layer.

The right part of Fig. 1 shows the processes leading to sputtering of the $i$th component of the upper layer of the target as a result of collisions of the downward flux of ions with the atoms of the metal carbide layer:

- in this mechanism, the downward flux of ions, i.e., the flux of ions passing through a metal carbide layer of thickness $x$, knocks out primary recoil atoms with an effective charge $Z_{\text{eff}}$ from the two-component heterogeneity layer toward the depth of the target;
- further, the knocked-out atoms of the components of the two-component heterogeneity layer may reflect off the underlying layers of the target (described by the differential function of the self-reflection of target layer atoms $R_s$) or participate in the sputtering of the underlying target atoms (including the substrate atoms), which is defined by the differential function of the backward self-sputtering of the $Y_s$ [9] layer and the differential function of the sputtering of the substrate material $Y$;
- the atom escape from the surface of the target is seen as the emission of primary and secondary knocked-out atoms moving from depth $x$ to the surface.

When describing the emission of atoms from the surface of a metal carbide (two-component material), it is taken into account that only atoms with an energy greater than the surface binding energy of the atoms of the $i$th component in the compound $U_i$ (flat surface potential barrier model) can leave the target surface, which is calculated by the formula [2]:

$$U_i=\Big(U_{0i}+\sum_{j=1,j\neq i}^{n}c_jU_{0j}\Big)\Big/\Big(1+\sum_{j=1,j\neq i}^{n}c_j\Big), \qquad (1)$$

where $U_{0i}$ — the binding energy of the atoms of the $i$th component in a single-component material, $c_i$ — the relative concentration of the $i$th component in the compound.

On the basis of the proposed model, taking into account a number of approximations [5], we obtained an analytical formula that allows us to calculate the partial sputtering coefficients of the $i$th component of the metal carbide layer by light ions:

$$\begin{aligned}Y_i(E_0,\theta_0,x_0)&=\frac{1}{8C_0U_i}\frac{1}{1+p}\left[\frac{\gamma_i}{\gamma_0}\right]^{1-m}\\&\times\Bigg\{R_N^{ion}(E',\theta,x_0)S_n(E^*(E'))\\&\times\left[1-\left(\frac{U_i}{\gamma_iE^*(E')}\right)^{1-m}\right]+S_n(E')\psi\left(\frac{E^S_{th}}{\gamma_iE'},\theta_0\right)\\&\times(1+\delta_{1i}3\mathrm{E}_3(C_0Nx_0))\Bigg\}\cdot[1-4\mathrm{E}_4(C_0Nx_0]. \qquad (2)\end{aligned}$$

Here $C_0$ — the constant in the power section of scattering ($C_0 = 1.808089\,\text{Å}^2$); $\mathrm{E}_n(C_0N_{x0})$ — the integral exponent of degree $n$; $E'$ — the average energy of ions in the heterogeneity layer, calculated by the formula

$$E'=E_0\big(1-3/(4C_0N(1+p)R_0\cos\theta_0)\big),$$

$\delta_{1i}$ — Kronecker symbol; $N$ — concentration of atoms in the layer; $p$ — dimensionless quantity depending on the total $R_0$, projective $R_p$, and transport $l_{tr}$-ranges of ions in the material:

$$p=2C_0R_0R_p\cos\theta_0/3l_{tr},$$

$\gamma_0$ — kinematic factor in ion-atom collision with $Z_{\text{eff}}$; $R_N^{ion}(E_0,\theta_0,x_0)$, $R_E^{ion}(E_0,\theta_0,x_0)$ — number-backscattered and energy-backscattered coefficients of ions from the layered target; $S_n$ — stopping cross sections [1]; $E^*$ — average energy of ions reflected from the layered target:

$$E^*=E_0\cdot(R_E^{ion}(E_0,\theta_0,x_0)/(R_N^{ion}(E_0,\theta_0,x_0),$$

$E^S_{th}$ — threshold self-sputtering energy [10]; $m$ —the index in the power approximation of the stopping cross sections.

The degree index is calculated according to the previously approved approximation formula (for average ion energies) depending on the energy of the incoming ion (in units of Liedhardt energy $\varepsilon$ [1]):

$$m(\varepsilon) = 1 - \exp(-0.9\varepsilon^{0.22});$$

$\psi$ — function determining the self-sputtering of atoms, which is approximated by the expression [5]:

$$\psi(y) = 0.18694[1 - y^{2/3}] \cdot [1 - y]^2,$$

$$\psi(y, \theta_0) = \psi(y, 1) + (1 - \psi(y, 1))(1 - \cos\theta_0)^{1.5}.$$

The total sputtering yields of the target are calculated as the sum of the partial sputtering coefficients of the layer components:

$$Y(E_0, \theta_0, x_0) = \sum_{i=1}^{2} Y_i(E_0, \theta_0, x_0).$$

The results of calculations of the total coefficients of helium ion sputtering of titanium and tungsten carbide layers of different thicknesses of the surface of the corresponding metal are shown in Figs. 2 and 3.

## 2. Calculation results

The dependence of the total sputtering coefficients on the thickness of the layer of carbon-modified titanium and tungsten from the surface of the corresponding metal by helium ions was studied based on the above-described model. It should be noted that previously this model [5] and its simplified version [6] have been used to analyze the sputtering of layered heterogeneous single-component materials. These studies have shown that when sputtering light layers of heterogeneity from the surface of a heavy substrate, there is a mirror effect — a significant increase in the sputtering coefficient of layer material at a certain thickness compared to that of a homogeneous target of layer material [6].

In Fig. 2, the results of calculating the sputtering coefficients of TiC layers from the surface of pure titanium by helium ions ($He^+$) as a function of titanium carbide layer thickness (normal incident ions with energy 1 keV) are compared with the results of computer simulation using SRIM-2013pro program (http://www.srim.org/). There is good agreement between the calculated values and the results of computer modeling. It should be noted that there is a significant increase in the sputtering coefficient at a certain layer thickness compared to the sputtering coefficient of a homogeneous two-component target, as in the case of sputtering of layered heterogeneous single-component materials [5].

The results of calculating the coefficients of sputtering of WC layers from the surface of pure tungsten by helium ions ($He^+$) depending on the thickness of the tungsten carbide layer (normal incident ions with energy 1 keV) are presented in Fig. 3 in comparison with the results of computer simulation with the SRIM-2013pro program (http://www.srim.org/).

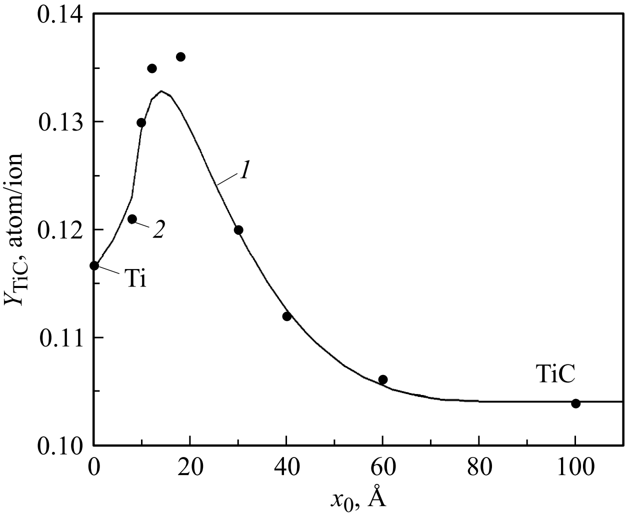

**Figure 2.** Results of calculating the sputtering coefficients of TiC layer from Ti surface by helium ions as a function of TiC layer thickness: *1* — calculation according to the formula, *2* — results of SRIM-2013pro computer simulation.

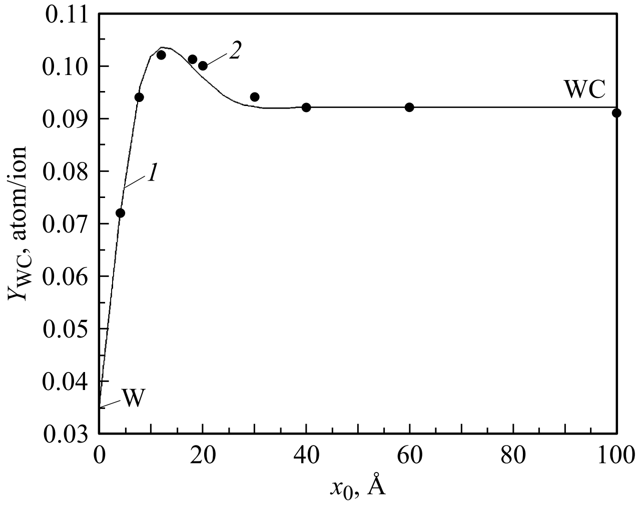

**Figure 3.** Results of calculating the sputtering coefficients of WC layer from the surface of W by helium ions as a function of WC layer thickness: *1* — calculation according to the formula, *2* — results of SRIM-2013pro computer simulation.

The analysis of the presented results shows that at a thickness of the carbon-modified metal layer of 10–20 Å there is a significant increase in the layer sputtering yield compared to the sputtering yield of a thick metal carbide target. This effect is observed both in the case of carbon-modified titanium surface sputtering and in the case of carbon-modified tungsten surface sputtering.

The existence of a maximum on the dependence of the sputtering coefficient of the heterogeneity layer on the layer thickness can be explained within the framework of the sputtering model used. On the one hand, both sputtering mechanisms indicate an increase in the average number of knocked-out atoms of the layer as the layer thickness increases (due to an increase in the number of atoms with which ion collisions and subsequent secondary atom collisions can occur) to a value at several average depths of sputtering atom formation [11]. On the other hand, the upward ion flux is determined by the reflection of the ions from the layered structure and, in our case (a layer of light material on heavy material), it decreases with layer thickness [8]. Thus, two oppositely directed factors act in the mechanism of sputtering by an upward flow of ions, which determine the presence of a maximum in the dependence of the sputtering coefficient on the thickness of the layer.

## Conclusion

The above-mentioned „mirror effect“ [6] in sputtering metal carbide films of a certain thickness from the metal surface is due to the fact that the effective mass of the upper sputtered layer is less than the mass of atoms of the homogeneous substrate. Therefore, the upward flux of ions in a layered target is greater than in a target consisting of layer material. As a consequence of this — the sputtering coefficient is also larger. It can also be noticed that when the thickness of the carbide compound layer tends to zero, the sputtering coefficient is determined by the value of the sputtering coefficient of the substrate material. If the metal carbide layers are thick enough, the sputtering coefficient is determined by the value of the sputtering coefficient of the target consisting only of metal carbide.

### Conflict of interest

The author declares that he has no conflict of interest.

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