Sputtering layers of different materials on tungsten surface by light ions of medium energy bombardment

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Abstract. There is an analytical formula allows to calculate the sputtering yields of heterogenous solid targets with light ions, based on the model of sputtering layered surfaces with light ions. Of particular interest is the sputtering of layers of different materials with the tungsten surface, which can be a material for the first wall of fusion reactor. The results of the calculations are in good agreement with the data of computer simulation, and show that the sputtering yields layers with a certain thickness, higher than the sputtering yields of homogeneous material layer targets ("mirror effect").

1. Introduction
In recent years more and more widely used technologies based on inhomogeneous layered surfaces. The layering of the surface could be occurred as a result of natural processes such as the adsorption of residual gases, oxidation processes, ion-enhanced diffusion and radiation-induced segregation too. This kind of layered structures set a number of tasks related to the interaction of layered materials with beams of charged particles. In particular, there is the task of sputtering layers of heterogeneity from the surface of another material is solved. Previous investigations have shown that the presence of surface heavy material with a thin layer of light material leads to a substantial increase of the sputtering yield of the material of this layer, in comparison with the coefficients of sputtering of homogeneous targets of light material ("mirror effect") [1]. In this work is solved the problem of the theoretical description of the sputtering of layered structures by light ions bombardments. The solution this problem is based on the principles of invariant embedding Chandrasekhar [2], and developed the ideas proposed to describe ion sputtering of free thin films [3, 4, 5].

2. Theoretical model
Let us consider a simple layered target with a sharp interface: a layer of thickness $x_0$ of one-component material (2) on a homogeneous semi-infinite substrate of another material (3). Let a wide beam of ions with mass $M_1$ with an energy $E_0$ is incident at an angle $\theta_0$ (angle is measured from the inner normal to the surface) on the surface of layered target. Colliding with target atoms, ions scattered on them, changing the direction of its initial movement. As result of this one part of ions move inside the target, the other part of ions move to the surface at any depth $x$. On this basis, to describe the process of sputtering of layered targets, a model is proposed based on the principles of invariant embedding [2], and includes two sputtering mechanism (Fig.1):

Mechanism 1 (sputtering by upward flow of ions) – the transmission of ions through the layers of heterogeneity of the thickness $x$, a reflection of the flow of ions from underlying layers of the target
(the layers of heterogeneity with a thickness of $x_0 - x$ and the substrate of other material), knocking out primary recoil by the reflected ion, self-sputtering of the layer thickness $x$.

Mechanism 2 (sputtering by downward flow of ions) – the transmission of the ion through the layer of thickness $x$, knocking out the primary recoil, reflection of knocked-on atoms from underlying layers of the target, or the sputtering of layered structure with a layer of heterogeneity $x_0 - x$ by knocked-on atoms, self-sputtering of the layer thickness $x$.

**Figure 1.** Schematic representation of the processes leading to the sputtering of the heterogeneity layer.

In accordance with the proposed model of sputtering of layered target, bearing in mind the principles of invariant embedding, the sputtering yield of the layers of heterogeneity can be described by the following expression:

$$Y(E_0, \theta_0, x_0) = N t_2^{(1)} \otimes R_{2/3}^{(1)} \otimes \omega \otimes S + N t_2^{(1)} \otimes \omega \otimes R_{2/3}^{(2)} + Y_S \otimes S. \quad (1)$$

In this expression, the sign $\otimes$ denotes the integration over all the common parameters, for example

$$t_2^{(1)} \otimes R_{2/3}^{(1)} \otimes \omega \otimes$$

$$\int_0^{x_0} dx \int dE_1 \int d^2 \Omega_1 \int dE_2 \int d^2 \Omega_2 \int dT \int d^2 \Omega_3 t_2^{(1)}(x, E_0, \Omega_0; E_1, \Omega_1)$$

$$R_{2/3}^{(2)}(x_0 - x, E_1, \Omega_1; E_2, \Omega_2) \omega(E_2, \Omega_2; T, \Omega_3) S(x, T, \Omega_3).$$

$N$ is the atomic density of the layer material, $t_2^{(1)}$ the transmission function of the ions (index 1) from the layer of material 2, $R_{2/3}^{(1)}$ the differential reflection function of the ions (index 1) from a layered target with a layers of heterogeneity of thickness (index 2) $x_0 - x$, $\omega$ - cross-section of energy transfer from the moving ion to the stationary atom, $S$ is a function of direct self-sputtering of material layer 2.
The differential function of the reflection of atoms of the layers of heterogeneity (index 2) from a layered target with a layer of heterogeneity of thickness (index 2) \( x_{0-x} \), \( Y_{s} \) - differential function of the backward selfsputtering of layers of heterogeneity of thickness \( x_{0-x} \).

The integration of expression (1) was carried out using the following models and approximations:
1. The model of continuous slowing down with approximation "straight-forward" to describe the transmission function \( t_{2}^{(1)} \) [6],
2. The model of power cross-section of the energy transfer from the moving ion to the stationary atom [7],
3. The pass method by integrating of the reflection functions \( R_{2/3}^{(1)} \) and \( R_{2/3}^{(2)} \),
4. Functions direct selfsputtering \( S \) and backward selfsputtering \( Y_{s} \) used according to the model [3, 4, 5].

Integration of the expression (1) gets a formula that allows calculating sputtering yields of the material of the upper layer of heterogeneity of layered targets by light ions bombardment:

\[
Y(E_{0}, \theta_{0}, x_{0}) = \frac{1}{8C_{0}U} \left[ \frac{1}{p-1} \left[ R_{N2/3}^{(1)}(E_{0}, \theta_{0}, x_{0}) \cdot S_{n}(E') \cdot \left[ 1 - \left( \frac{U}{pE'} \right)^{1-m} \right] \right] \right.
+ \left. S_{n}(E_{0}) \psi(E_{th}^{s}/\gamma E_{0}, \theta_{0}) \right] \cdot \left[ 1 - 4E_{4}(C_{0}N_{x_{0}}) \right].
\]

(2)

Here \( U \) is the surface binding energy of atoms in the layer [7]; \( C_{0} \) - constant in a power cross-section approximation [7] \( (C_{0}=1.808089 \text{ Å}^{2}) \); \( E_{4}(C_{0}N_{x_{0}}) \) - integral exponent; \( \gamma \) is the kinematic factor \( (\gamma = 4M_{1}M_{2}/(M_{1} + M_{2})^{2}) \); the coefficient of reflection of ions from layered surfaces; \( p \) is the dimensionless quantity determined by the range of the ions in the material (2):

\[
p = 2C_{0}R_{0}R_{p}cos\theta_{0}/3l_{tr} ,
\]

\( R_{p} \) - projective range of ions in the material (2), \( l_{tr} \) - transport range of ions in the material (2); \( S_{n}(\ ) \) - nuclear stopping cross-section [8]; \( E' \) the average energy of ions reflected from a layered structure: \( E' = E_{0} \cdot R_{N2/3}^{(1)}(E_{0}, \theta_{0})/R_{N2/3}^{(1)}(E_{0}, \theta_{0}), R_{N2/3}^{(1)}(E_{0}, \theta_{0}, x_{0}) \) - reflection coefficient of energy of ions from the layered surface; \( E_{th}^{s} \) - threshold energy selfsputtering [9]; \( m \) – the exponent in the power cross-section approximation, \( \psi \) - the function that determines selfsputtering of atoms of layer heterogeneity, which is approximated by the expression:

\[
\psi(\gamma) = 0.18694 \left[ 1 - \gamma^{2/3} \right] \cdot \left[ 1 - \gamma \right]^{2}.
\]

3. Results of calculations
The results of calculations by formula (2) of the sputtering yields of carbon films with tungsten surface by helium ions shows that there is a significant increase (“mirror effect” [1]) of the sputtering yield a certain thickness of the layer of light material from the surface of the heavy substrate (Fig. 2) compared with the sputtering yield of homogeneous targets from the material of the layer heterogeneity. This effect is confirmed by computer simulation (program SRIM-2013pro (http://www.srim.org/)) and was previously studied experimentally in [1] for other combinations of materials of the layer and the substrate. The results show that starting from a certain thickness of the layer of heterogeneities (in this case, 120-150 Å) the heavy substrate will not affect on the value of the sputtering yield of the layer heterogeneity.
Figure 2. The coefficient of sputtering the carbon film (C) from the surface of tungsten (W) with hydrogen ions (H\textsuperscript{+}) (normal incidence), depending on the thickness of the carbon film: 1 - calculation by formula (2), hydrogen ion energy 1000 eV, 2 - computer simulation results SRIM-2013pro, the energy of hydrogen ions is 1000 eV, 3 is calculation by formula (2), the energy of hydrogen ions is 5000 eV, 4 is the results of computer simulation of SRIM-2013pro, the energy of hydrogen ions is 5000 eV.

The sputtering of the layer of heavier material (aluminum) from the substrate of tungsten shows on figure 3. The “mirror effect” is not so pronounced in this case.
Figure 3. The coefficient of sputtering the aluminum film (Al) from the surface of tungsten (W) with deuteron ions (D⁺) (normal incidence), depending on the thickness of the aluminum film: 1 - calculation by formula (2), deuteron ion energy 1000 eV, 2 - computer simulation results SRIM-2013pro, the energy of deuteron ions is 1000 eV, 3 is calculation by formula (2), the energy of deuteron ions is 5000 eV, 4 is the results of computer simulation of SRIM-2013pro, the energy of deuteron ions is 5000 eV.

4. Conclusions
The proposed model allows to explain the observed in the experiment "the mirror effect" - a significant increase of the sputtering yield of the certain thickness layer heterogeneity of a light material from the surface of the heavy substrate compared with the sputtering yield of homogeneous targets from the material of the layer heterogeneity. Namely, the presence of substrate of heavy material significantly increases the flux of reflected ions [10], and as a consequence, the increase of the upward flow of knocked out the atoms of the layer heterogeneity.

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