Model of sputtering of binary homogeneous targets by light ions bombardment

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Abstract. An analytical model of the sputtering of binary homogeneous targets by light ions bombardment has been developed, an analytical formula has been obtained, which makes it possible to calculate the total and partial sputtering coefficients of a binary (multicomponent) target by light ions bombardment. The calculation results are in good agreement with the experimental data. The patterns of preferential sputtering of two-component materials at low energies of bombarding ions are revealed.

1. Introduction
Sputtering of multicomponent materials with light ions is of interest both from the point of view of applied research and from the theoretical side of the description of the phenomenon. A distinctive feature of the sputtering of multicomponent materials by ion flows is the fact that when bombarding alloys the target components are sputtered with different intensities (the sputtering coefficients of the components are different) [1, 2]. As a consequence of this phenomenon (as well as other related processes: implantation, ion mixing, etc.), the concentration of components in the surface layers of the target changes (the targets become non-uniform), which, in turn, affects the sputtering intensity. In this regard, the theoretical description of the phenomenon of dispersion of multicomponent materials is a multitasking problem. The theory of the sputtering of multicomponent materials by P. Sigmund, based on solving the Boltzmann kinetic equation, although it has a limited scope (not applicable to sputtering with light ions of medium energies), is still the main one in calculating the sputtering coefficients and associated effects (preferential sputtering) [1, 2]. This paper proposes a model of sputtering homogeneous two-component materials with light ions, based on an approach tested for the case of sputtering one-component homogeneous targets [3], in which it is assumed that target atoms are sputtered due to two mechanisms: sputtering with a descending ion flow and sputtering with an ascending ion flow. This model approach is easily transformed under the description of sputtering of inhomogeneous targets [4], which allows us to investigate more realistic targets.

2. Theoretical model
Let us consider a homogeneous semi-infinite two-component target $A_qB_b$ (where $q$ is the stoichiometric coefficient of the element $A$ of mass $M_1$ in the compound, $b$ is the stoichiometric coefficient of element $B$ of mass $M_2$ in the compound), on the surface of which a wide beam of light ions (mass $M_0$) incidents at the surface with energy $E_0$. We confine ourselves to the case of low doses of radiation, which makes it possible to consider the target to be uniform in depth, and the composition of the target does not change throughout the sputtering time.
In the theoretical description of the process of sputtering two-component materials, the following models and approximations were used:

1) Moving particles do not interact with each other;
2) The interaction of moving particles with fixed atoms of the target is described in the model of pair collisions;
3) The elementary process of interaction is described by two independent channels: elastic (both the direction of movement of the particle and its energy change) and the inelastic (the moving particle loses energy, but does not change its direction of movement) [5];
4) The elastic interaction cross section is described by power dependence;
5) Stopping of fast ions in a multicomponent compound is described as stopping in a single component material consisting of atoms with an effective charge and mass

\[ Z_{ef} = \sum_{i=1}^{n} c_i Z_i, \quad M_{ef} = \sum_{i=1}^{n} c_i M_i \]  

\[ (i=1, \ldots, n) \]  

where \( c_i \) is the relative concentration of the \( i \)-th component in the compound. Since the sputtering of target atoms is determined by the energy transferred by them from the incident ion (energy lost by ions due to elastic collisions with target atoms), we believe that an ion transfers in a unit volume the energy to an atom with an effective charge \( Z_{ef} \), which is redistributed between the target components \( A \) and \( B \) according to their relative concentration in the compound. The energy attributable to each atom of the compound should not exceed the maximum possible energy transferred during elastic interactions of ion-atom - \( \gamma_i E_0 \) (\( \gamma_i \) is the kinematic factor, \( \gamma_i = 4M_0 M_i / (M_0 + M_i)^2 \), \( M_0 \) is the ion mass, \( M_i \) is the mass of the atom).

6) When describing atoms leaving the target, the model of a flat surface potential barrier is used. The energy of the surface bond of atoms of the \( i \)-th component in the compound \( U_i \) is calculated by the formula:

\[ U_i = \frac{U_{0i} \sum_{j=1, j \neq i}^{n} c_j U_{0j}}{1 + \sum_{j=1, j \neq i}^{n} c_j} \]  

where \( U_{0i} \) is the binding energy of atoms of the \( i \)-component in the single component material.

The model describing atom sputtering with light ions is based on the assumption (based on the principles of invariant embedding applied to the sputtering description [3]) that there are two fast ion fluxes in the target at depth \( x \): one is directed mainly inland of the target, the other is due to scattering ions directed towards the surface. At a depth of \( x \), two flows of initially knocked-out atoms can be distinguished: one is directed mainly deeper into the target, the other towards the surface. On this basis, it can be assumed that the sputtering of two-component materials (as well as single-component targets) is described by two mechanisms [3,4]: 1) sputtering by a downward flow of ions, 2) sputtering by an upward flow of ions. Each mechanism is represented as a sequence of the following processes leading to the sputtering of the \( i \)-th component of the target (Fig. 1):

Mechanism 1 - the transmission of a flow of ions of a layer of thickness \( x \); knocking out primary recoil atoms in the direction towards the bottom of the target; the reflection of the initially knocked-off atoms of components \( A \) and \( B \) from the underlying material layers, or sputtering of the underlying atoms of the material; emission of primary and secondary knocked-out atoms moving at a depth \( x \) to the surface.

Mechanism 2 - the transmission of a flow of ions of a layer of thickness \( x \); reflection of the ion flux from the underlying material layers; knock-out by ions moving to the surface of primary recoil atoms at a depth \( x \); emission of ejected atoms moving from depth \( x \) to the surface.
Figure 1. Schematic representation of the processes leading to the sputtering of binary homogeneous target.

On this basis, the description of the sputtering phenomenon of the i-component of a two-component target will be carried out as sputtering of a single-component homogeneous target consisting of atoms with \( Z_i \) taking into account the flat surface potential \( U_i \).

In accordance with the proposed model, taking into account the principles of invariant embedding, the partial sputtering coefficient of component \( i \), defined as the average number of atoms of component \( i \) emitted from the target surface per incident ion, can be described by the following expression:

\[
Y_i(E_0, \theta_0) = N_i t \otimes R_{i0}^{\text{ion}} \otimes \omega \otimes S_i + N_i t \otimes \omega \otimes [R_s + Y_s] \otimes S_i
\]  

(3)

In this expression, the \( \otimes \) sign denotes integration over all common parameters, \( N_i \) is the atomic density of the \( i \)-th component, \( t \) is the ion transmission function by a target layer of thickness \( x \), \( R_{i0} \) is the differential function of ion reflection from the target, \( \omega \) is the cross section for energy transfer from a moving ion to a stationary atom , \( S_i \) is the function of direct (on the chamber) self-sputtering of a layer of material with thickness \( x \), \( R_s \) is the differential self-reflection function of the target atoms, \( Y_s \) is the differential function of the reverse self-sputtering of the target.

The integration of expression (3) 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 [5],
2. The pass method by integrating of the reflection functions [6],
3. Functions direct self-sputtering \( S \) and backward self-sputtering \( Y_s \) used according to the model [7].

As a result of the integration of expression (3), a formula is obtained which makes it possible to calculate the partial sputtering coefficients of the \( i \)-th component of the target material by light ions:

\[
Y_i(E_0, \theta_0) = \frac{1}{8\zeta_{0,1}^{m} \gamma} \left\{ R_{i0}^{\text{ion}}(E', \theta)S_i(E^*(E')) \left[ 1 - \left( \frac{u_i}{\gamma_i E^*(E')} \right)^{1-m} \right] \right\} + S_i(E^*) \phi \left( \frac{E_i^*}{\gamma_i E^*}, \theta_0 \right)
\]

(4)

where \( E' = E_0 \left( 1 - \frac{3}{4C_0 N_0 (1+p) R_0^2 \cos \theta_0} \right), C_0 \) is a constant in the power scattering cross section [1] \((C_0 = 1.808089 \text{ Å}^2)\); \( N_0 \) is the concentration of atoms in the target material; \( \gamma_0 \) is the kinematic factor of elastic interaction “ion-atom with \( Z_i \)” \((\gamma_0 = 4M_1 M_2 / (M_1 + M_2)^2)\); \( R_{i0}^{\text{ion}}(E_0, \theta_0) \) is the total coefficient of reflection of ions; \( p \) is a dimensionless quantity determined by the range of ions in the material: \( p = 2G_0 R_0 R_p \cos \theta_0 / 3l_{tr} \), \( R_0 \) – total range of the ions in the material (2). \( R_p \) – projective range of ions in
the material, \( l_t \) – transport range of ions in the material; \( S_n \) - nuclear stopping cross-section \[8\]; \( E^* \) the average energy of ions reflected from a target: 
\[
E^* = E_0 \cdot \frac{R_{E}^{(1)}(E_0, \theta_0)}{R_{N}^{(1)}(E_0, \theta_0)} \cdot R_{E}^{(1)}(E_0, \theta_0, x_0)
\]
reflection coefficient of energy of ions from the target; \( E_{th} \) - threshold energy selfsputtering \[9\]; \( m \) – the exponent in the power cross-section approximation, \( \psi \) - the function that determines selfsputtering of atoms, which is approximated by the expression \[4\]: 
\[
\psi(y) = 0.18694 \left(1 - y^{2/3}\right) \cdot \left(1 - y\right)^2.
\]

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

\[
Y(E_0, \theta_0) = \sum_{i=1}^{2} Y_i(E_0, \theta_0)
\]

The results of calculations according to the formula (4) of the partial sputtering coefficients for two-component targets are shown in Fig.2.

**Figure 2.** The partial sputtering coefficients of the compound TiB\(_2\) by helium ions (He\(^+\)) (normal incidence) depending on the ion energy: 
1 - the sputtering coefficient Ti, calculated by the formula (4); 
2 - sputtering coefficient, calculated by the formula (4); 
3 — Ti sputtering coefficient, experimental data \[10\]; 4 - B sputtering coefficient, experimental data \[10\].

In fig. 2 shows the results of calculations of the partial sputtering coefficients of a TiB\(_2\) compound by helium ions (He\(^+\)) as a function of the ion energy. The results of the calculations are given in comparison with the experimental data \[10\], there is a preferential sputtering of the lighter component of the compound, which is confirmed by the experimental data.

**3. Conclusions**

On the basis of the proposed sputtering model for two-component targets with light ions, a rather simple calculation formula was obtained for the partial sputtering coefficients of the components. The analysis of the resulting formula, as well as the results of the calculations, allow us to draw the following conclusions:
1. The less bound component is sputtered more efficiently, which is determined by the surface binding energy of the component $U_i$. When sputtering low-energy ions, the surface will be depleted by the less bound component.

2. The lighter component is sputtered more intensely, and a situation similar to the preferential sputtering of the less bound component is possible.

3. The threshold sputtering energy (of each component) for the sputtering mechanism by the upward flow of ions is different from the threshold sputtering energy by the downward flow of ions. The analysis shows that the threshold sputtering energy is higher for the downward flow of ions, which means that the threshold sputtering energy for atoms of the $i$-th component is determined by the threshold sputtering energy for the upward flow of ions.

In the future, it is supposed to develop a model of the case of sputtering inhomogeneous two-component targets with light ions.

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