An influence of ion and sputtered atom flows inhomogeneity on time evolution of the target surface relief in glow discharge

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Abstract. A mathematical model of ion and sputtered atom transport in the vicinity of the target with a periodical surface relief in glow discharge in pure gas is developed. Under the assumption that the relief amplitude is small, analytical expressions for their flows are found by the perturbation method and an equation describing the relief amplitude time evolution is derived. It is shown that intensity of sputtering exceeds intensity of sputtered material redeposition at the relief tops, and relief smoothing always takes place in the process of homogeneous target treatment in glow discharge in pure gas.

1. Introduction

Under material processing in glow discharge plasma, the ion flow at the target surface is generally supposed to be homogeneous. In reality, on targets with structural or compositional inhomogeneity a surface relief is formed in the course of time [1]. This can result in ion flow focusing at the relief tops due to electrical field line bending followed by their more intensive sputtering [2,3]. On the other hand, the back flow of sputtered material from plasma to the target surface can be higher at the relief tops as well. The combined effect of the both processes on relief evolution was not investigated before.

In this work, the ion and sputtered atom flows at the target with a periodical surface relief in glow discharge in pure gas are calculated and an influence of their inhomogeneities on relief evolution is studied.

2. Mathematical model

Let the discharge be maintained between the target with a surface relief defined by equation

\[
z_c = z_0 + h_c \cos kx
\]

and the flat electrode \(z = L_0\), where \(k = 2\pi/L_c\), \(h_c\) and \(L_c\) are the relief amplitude and period, respectively (see figure 1). The target is bombarded by ions accelerated in the discharge cathode layer of width \(d_c\), which results in its sputtering. Sputtered atoms become thermalized after several collisions with background gas atoms, then move in the diffusion mode, and some of them return back to the target and are re-deposited at its surface [4-6].

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Figure 1. Schematic of discharge geometry.

If the sputtered atom mean path length $\lambda$ between collisions with gas atoms is much less than the discharge volume dimensions, i.e.

$$\lambda << l_c, \lambda << (L_0 - z_0), \lambda << d_e,$$

then charged particle transport in the cathode sheath of glow discharge in pure gas is described by the system of equations for the electron and ion flow densities $\vec{j}_e$ and $\vec{j}_i$, the ion number density $n_i$ and the electric field potential $\varphi$ [7]:

$$\text{div} \vec{j}_e = \alpha_i j_e, \quad \text{div} \vec{j}_i = \alpha_i j_e, \quad \vec{j}_i = -\mu_i n_i \nabla \varphi, \quad \Delta \varphi = -\frac{e}{\varepsilon_0} n_i$$

(2)

with boundary conditions

$$j_i(x, d_e) = 0, \quad j_e(x, z_c) = \gamma_j j_i(x, z_c), \quad \varphi(x, z_c) = 0, \quad \varphi(x, d_e) = U_c,$$

(3)

where $\mu_i$ is the ion mobility, $\alpha_i$ is the coefficient of gas ionization by electrons, $\gamma$ is the ion-electron secondary emission rate of the target material, $U_c$ is the cathode voltage drop, $e$ is value of the electron charge and $\varepsilon_0$ is the dielectric constant.

Distribution of the thermalized sputtered atom number density $n_a$ in the discharge volume satisfies the diffusion equation [4,5]

$$\Delta n_a = -f(x, z)/D$$

(4)

with boundary conditions

$$n_a(x, z_c) = 0, \quad n_a(x, L_0) = 0,$$

(5)

where $D$ is the diffusion coefficient of sputtered atoms in the gas, $f(x, z)$ is the source function of thermalized sputtered atoms.

If the target surface relief amplitude is small ($h_c << l_c$), such that the condition

$$kh_c << 1$$

(6)

is fulfilled, then discharge distortions caused by it are also small, and an approximate solution of equations (2) and (4) with boundary conditions (3) and (5) can be found with the perturbation method [8].

3. Ion flow at the target

Distributions of the $z$-component of the electron and ion flow densities as well as the sputtered material number density and the electrical field potential in the discharge cathode sheath can be written in the form
\[ j_{iz} = j_{iz0}(z) + j_{iz1}(z) \cos kx, \quad j_{iz} = j_{iz0}(z) + j_{iz1}(z) \cos kx, \]
\[ n_1 = n_{i0}(z) + n_{i1}(z) \cos kx, \quad \varphi = \varphi_{i0}(z) + \varphi_{i1}(z) \cos kx \]

with amplitude of the second terms being much less than the first terms under condition (6).

Substituting expressions (7) in (2) and (3) and taking into account zero-order and first-order values only, it can be found under the condition \( c < d_c \) [9] that at the target surface (in plane \( z = z_0 \))

\[ j_{i0}(z_0) = kh_c j_{i0}(z_0). \]

Therefore, it follows from expression (7) for \( j_{iz} \):

\[ j_{il}(x) = j_{iz}(x, z_0) = -j_{i0} - j_{i0}kh_c \cos kx, \]

where \( j_{i0} = J_0/e(1+\gamma) \), \( J_0 \) is the discharge current density.

Expression (8) shows that focusing of the ion flow at the relief tops (at \( x = 2\pi m \), where \( m \) is an integer) proportional to the relief amplitude \( h_c \) exists, which results in their more intensive sputtering.

### 4. Sputtered atom flow at the target

The flow density of atoms sputtered by ions from the target surface is defined by the expression

\[ j_{as}(x) = -Y_{ic}(x), \]

which can be written as follows

\[ j_{as}(x) = Y_{j0} + Y_{j0}kh_c \cos kx, \]

where \( Y \) is the energy-averaged ion sputtering rate of the target material.

The source function of thermalized sputtered atoms \( f(x, z) \) can be found using the approximation of their continuous slowing down in the gas [4]:

\[ f(x, z) = \int dx \int d\Omega \psi(x', e, \theta) \delta(z - z_0) - R(e) \cos \theta, \]

where \( \psi(x', e, \theta) = j_{s0}(x')F(e)\cos \theta / \pi \), \( F(e) = 2U_s/(e + U_s)^3 \), \( x' = x + R(e) \sin \theta \cos \varphi \), \( R(e) \) is the mean thermalization path length of sputtered atoms with initial energy \( e \), \( U_s \) is the target material binding energy, \( \delta(z) \) is the Dirac function and \( d\Omega = \sin \theta d\theta d\varphi \) is the solid angle element.

From expressions (10) and (11) we obtain after integration

\[ f(x, z) = f_0(z) + f_1(z) \cos kx, \]

where

\[ f_0(z) = Y_{j00} \frac{2R_s^2}{(z^2 + R_s^2)}, \quad f_1(z) = Y_{j00} \frac{R_s^2}{z^2 + R_s^2} k^3 h_c K_2 \left( k \sqrt{z^2 + R_s^2} \right), \]

\( R_s = R(U_s) \) is the mean thermalization path length of sputtered atoms with initial energy \( U_s \) and \( K_2(x) \) is the second-type modified Bessel function.

Solution of the diffusion equation (4) with boundary conditions (5) taking into account the source function form (12) can be represented as

\[ n_s = n_{s0}(z) + n_{s1}(z) \cos kx. \]

Substituting expressions for \( n_{s0}(z) \) and \( n_{s1}(z) \) found from (4) and (5) into the expression for the flow density of thermalized sputtered atoms at the target surface

\[ j_{as}(x) = -D \frac{dn_s}{dz}(x, z_0) = -D \left[ \frac{dn_{s0}}{dz}(z_0) + \frac{dn_{s1}}{dz}(z_0) \cos kx \right], \]

and supposing that the surface relief period \( l_c \) is much less than characteristic discharge dimensions \( L \) and \( R_s \), i.e. \( kL >> 1 \) and \( kR_s >> 1 \), we obtain

\[ j_{as}(x) = -\alpha Y_{j0} - \alpha Y_{j0}kh_c \cos kx, \]

where \( \alpha = 1 - (kr_c / kL) \arctan(kL / kr_c) \) gives the fraction of sputtered material re-deposited at the target surface, \( L = L_0 - z_0 \). Expression (15) shows that more sputtered material is re-deposited at the relief tops than at the other relief parts. This can be explained by sputtered atom flow line bending at
the relief tops similar to electric field line bending (because the sputtered atom number density and the electrical field potential are both described by Poisson-type differential equations).

The total sputtered material flow density at the target surface is

\[ j_{sc}(x) = j_{ac}(x) + j_{ar}(x) = (1 - \alpha) Y_{j0} + (1 - \alpha) Y_{j0} k h_{c} \cos kx. \]  

(16)

As under condition (6) it is positive for all \( x \) values, target surface etching takes place at all its points.

5. Time evolution of the target surface relief

Time variation of target surface \( z \) - coordinate due to ion sputtering and sputtered material re-deposition is described by the equation

\[ \frac{dz_{c}}{dt} = - \frac{M_{s}}{N} j_{sc}(x), \]  

(17)

where \( N \) and \( M_{s} \) are the target material density and atomic mass, respectively.

Assuming that the sputtering rate of the target is periodically varying along its surface,

\[ Y = Y_{0} - Y_{i} \cos kx, \]  

(18)

and substituting the target surface coordinate \( z_{c} = z_{0} + h_{c} \cos kx \) and expressions (16), (18) in (17), an equation for the relief amplitude can be derived

\[ \frac{dh_{c}}{dt} = \frac{1}{\tau_{f}} (h_{t} - h_{c}), \]  

(19)

where

\[ \tau_{f} = \frac{N}{M_{s} Y_{0} j_{0} k (1 - \alpha)}, \quad h_{t} = \frac{Y_{i}}{Y_{0} k (1 - \alpha)}. \]  

(20)

Its solution has the form

\[ h_{c} = h_{t} + (h_{0} - h_{t}) \exp \left( -t / \tau_{f} \right), \]  

(21)

where \( h_{0} \) is an amplitude initial value.

It follows from expression (21) that an equilibrium relief with amplitude \( h_{t} \) is formed at the target surface during time of the order of \( \tau_{f} \). For instance, under copper sputtering in argon discharge at voltage 1000 V, gas pressure 100 Pa, \( Y_{0} j_{0} = 4.53 \times 10^{20} \text{m}^{2} \text{s}^{-1} \), \( \alpha = 0.935 \) [10] it can be obtained from (20) for \( Y_{i} / Y_{0} = 0.1 \), \( l_{c} = 10^{-3} \text{m} \) that \( \tau_{f} = 4.6 \times 10^{5} \text{s} \), \( h_{t} = 2.5 \times 10^{-4} \text{m} \). In case of \( Y_{i} = 0 \) the relief amplitude \( h_{c} \) as well as ion and sputtered atom flow non-uniformities decrease with time and vanish in the equilibrium state. Thus, under homogeneous target etching in pure gas glow discharge, intensity of sputtering exceeds intensity of sputtered material re-deposition at the relief tops, and target surface relief smoothing takes place.

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