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Research paper

Modeling of Fast Neutral Atoms Flow Generation in Channel Rays of Glow Discharge

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Abstract

A physical-kinetic approach has been used for modeling of fast neutral atoms flow generation in the channel rays of abnormal glow discharge. The fast atoms are generated due to charge exchange of ions accelerated by voltage drop on the cathode layer of positive space charge. The limits of applicability of the created model and the range of operating parameters of the fast atom source are established for the Ar (gas) – Ta (cathode) pair. The work is directed towards implementation of the beam processing of dielectric optical nanostructured metamaterials with help of fast neutral atoms.

Keywords: *nanostructured metamaterial, model, atom, technology*

1. Introduction

In many technological processes with dielectric and poorly conductive materials, in particular, for physical sputtering and physical-chemical oxidation or nitriding of materials for optics and optoelectronics, it is effective to use high-energy beams of neutral atomic particles [1-3]. Unlike processing with ions, the electrical charge on the workpiece surface does not accumulate and there are no complications related to this. Thus, such processes are useful for the development and industrial use of beam technology for the production of dielectric nanostructured optical metamaterials [4, 5].

The known fast neutral atoms sources usually consist of an ion generating gas-discharge chamber, an ion accelerator and a neutralizer of ions with a gas or metal target [1-3]. At the same time, it is known that a glow discharge in the abnormal mode (AGD) or in a non-self-sustained form with an ion behind-anode source generates so-called channel rays of particles passing from the discharge gap into the space below the cathode through cathode holes [6]. The channel rays are formed by fast particles that are generated and accelerated in the cathode layer of voltage drop. These rays contain both ions and fast neutral particles (usually atoms). The latter are formed as a result of charge exchange of accelerated ions during interaction with neutral gas molecules. The former ions save their energy and vector of velocity but they move as neutral particles after charge exchange. Thus, the AGD cathode layer can be used as a source, an accelerator and a neutralizer of ions and, in general, as a source of fast neutral particles.

The ion component of the channel rays will be intercepted by the cathode, and the walls of the holes in the cathode serve as a collimator for the passing particles. Advantages of such a source are the relative simplicity of the design and the possibility of obtaining a very homogeneous flow of neutral atoms (neutrals) of large cross section.

When designing the source, it is necessary to estimate the magnitude of the flow of neutrals contained in the channel rays. Herein, it is necessary to take into account the peculiarities of physicalkinetic processes in the cathode layer, first of all the fact that the motion of ions in a strong electrical field and low-pressure gas occurs in the nonequilibrium with the field, when the ion energy is determined not by the local field (as in the regime of mobility at elevated pressure) but by the passed potential difference between charge exchanges. The aim of the work is to construct a mathematical model of the channel rays source on the physical kinetic principles to determine the conditions for obtaining the maximum value of the neutral atoms fraction in the channel rays and to calculate the energy (velocity) of the atoms as well as the fast neutral atoms flow in typical operating modes.

Figure 1 depicts the structure of the fast neutral atoms source on the channel rays. The plasma region is either the negative glow region of AGD or the auxiliary discharge plasma. The plasma boundary can be free or fixed by a fine-structured anode grid. The cathode performs the function of an accelerating electrode for ions (both for plasma ones and after charge exchange). The holes in the cathode can be overlapped with a fine-structured grid.

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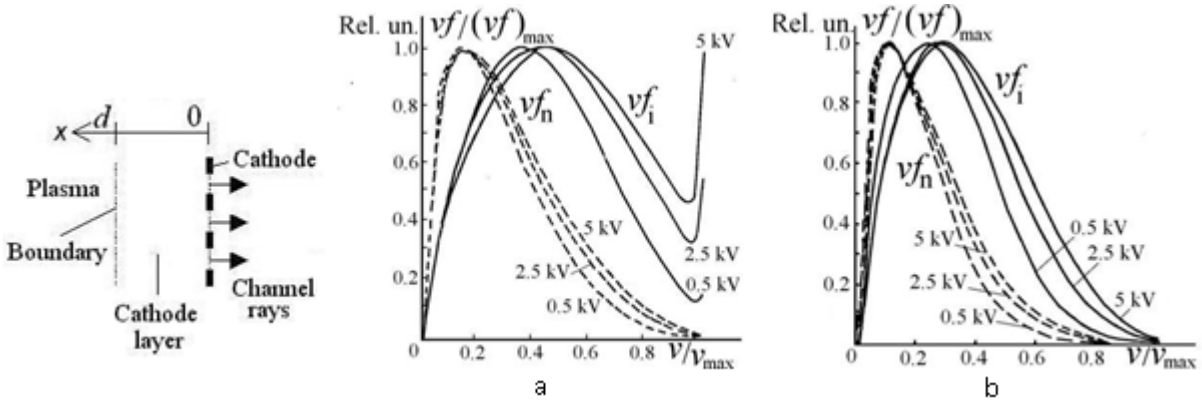


Figure 1. Structure of the fast

Figure 2. Normalized distribution functions for flows of ions and neutral atoms source.atoms at the cathode at different voltages *U* and *d* = 1 cm (a) and 2 cm (b), *p*= 6.65 Pa.

2. Modeling Method

We use a system of kinetic equations for distribution functions of the ions f_i, and of the fast neutrals f_n and the Poisson equation together with the boundary conditions for the stationary one-dimensional cathode layer of AGD. The gas ionization is not taken into account because of low *pd* (*p* is the gas pressure, *d* is the thickness of the cathode layer, see figure 1, the operation range of *pd* is at the left of the left branch of the known Paschen curve). Also the reflection of the particles from the cathode and the anode is ignored. These equations are a simplified version of the system for an ion diode, which takes into account ionization of a gas by electrons, ions and fast neutrals [7]:

$$v\frac{df_i}{dx}+\frac{eE}{\grave{I}}\frac{df_i}{dv}=2nv\delta\left(v^2\right)\int f_i\left(x,v'\right)\sigma\left(v'\right)v'dv'\text{-}nf_i\left(x,v\right)\sigma\left(v\right)v$$

$$,\quad f_i\left(0,v\right)\big|_{v>0}=0\quad,\quad f_i\left(d,v\right)=2j_{i.\mathrm{a}}\delta\left(v^2\right)/e\quad,$$

$$n=p/\mathrm{k}T=\mathrm{Const},$$

$$f_0\left(x,v\right)=n\int_x^d f_i\left(x',v\right)\sigma\left(v\right)dx'\quad,\quad f_0\left(0,v\right)\big|_{v>0}=0\quad,$$

$$f_0\left(d,v\right)=0$$

$$j_i\left(x\right)=j_i\left(d\right)=j_{i.\mathrm{a}}=e\int f_i\left(x,v'\right)v'dv'=\mathrm{Const}\quad,$$

$$\Gamma_0\left(x\right)=\int f_0\left(x,v'\right)v'dv',\ \Gamma_{0.\mathrm{K}}=\Gamma_0\left(0\right),$$

$$d^2\varphi/dx^2=\rho/\varepsilon_0,\ \varphi\left(0\right)=0,\ \varphi\left(d\right)=U,$$

$$\rho=e\int f_i\left(x,v'\right)dv',\ E=-d\varphi/dx,\ E\left(d\right)=0,$$

$$j_e\left(x\right)=j_e\left(0\right)=j_{e.\mathrm{K}}=\int\left[\gamma_i\left(v'\right)f_i\left(0,v'\right)+\gamma_0\left(v'\right)f_0\left(0,v'\right)\right]v'dv'$$

$$,\ j=j_e\left(x\right)+j_i\left(x\right)=\mathrm{Const},$$

where *x* – is the coordinate (see figure 1); *v* – particle velocity; *M* – mass of the ion; *e* – electron charge; *E* – electrical field strength; *n* – concentration of gas molecules; *T* – gas temperature; k – Boltzmann constant;δ – Dirac delta-function; σ – cross section for ion resonance charge exchange; ji – ion current density, ji.a – ion current density at the plasma boundary; Γn – fast neutrals flow density; φ – electrical potential; ε_0 – electric constant; ρ –space ion charge density; *U* – voltage drop on the cathode layer; *j*e – electron current density, *j*e.c – current density of the secondary electron emission of the cathode; i and *j*n – secondary electron emission coefficients of the cathode at bombardment by ions and neutrals, accordingly; *j* – discharge current density. The numerical calculation was performed with the "big particles" method using the algorithm [7] for the Ar (gas) – Ta (cathode) pair. The literature data [8, 9] were used for approximation of the dependencies of $\sigma(v)$, $\gamma_i(v)$ and $\gamma_n(v)$ on the velocity *v* of primary particles. Figure 2 presents the results of calculations at the entrance to the space below the cathode, where v_{max} is the maximum velocity of the ions, $v_{max}=(2eU/M)^{1/2}$.

3. Results and Analysis

One can see, the most probable velocities are of the order of 20–40 % for ions and of 10–15 % for fast neutral atoms relatively v_{max}. At *d* = 1 cm, some of the ions were not charge exchanged on the path to the cathode, but practically all ions made at least one charge exchange at *d*> 1 cm and *p* = 6.65 Pa. When *U* increases, the velocity spectra become enriched with faster particles due to the decreasing σ(*v*). The fact that fast particles have velocities in a wide range of values confirms the validity of the use of the kinetic approach. The results of the calculation of the distribution functions are consistent with the experimental data [10] and our experimental data when we used these functions for calculation of the sputtering of Ta cathode in AGD.

Table 1 shows the results of the particle flow parameters calculations. Comparison with real systems may be done using the measured *U*, *p*, *d* and current density *j* (the latter determines the value of ji.a).

Table 1. Fast neutrals source parameters at different *U, p and d.*

U, kV		2.5			5.0	
p, Pa			1.33			
d, cm	1.0	2.0	3.0	1.0	2.0	3.0
j, мА/cm^2	1.100	0.247	0.098	3.466	0.779	0.316
$J_{i.a}$, мА/cm^2	0.945	0.210	0.085	2.714	0.610	0.247
$e\Gamma_{n.c}$, мА/cm^2	0.905	0.423	0.266	2.286	1.078	0.681
$e\Gamma_{n.c}/j_{i.a}$, rel.un.	0.957	2.014	3.129	0.842	1.767	2.757
p, Pa			3,325			
d, cm	1.0	2.0	3.0*	1.0	2.0	3.0*
j, мА/cm^2	0.929	0.188	0.071	2.971	0.609	0.232

$j_{i.a}$, мА/cm^2	0.800	0.162	0.061	2.327	0.477	0.182
$e\Gamma_{o.к}$, мА/cm^2	2.049	0.899	0.540	5.240	2.329	1.411
$e\Gamma_{n.c}/j_{i.a}$, rel.un	2.561	5.549	8.852	2.252	4.882	7.753
p, Pa			6,65			

d, cm	1.0	2.0*	3.0*	1.0	2.0*	3.0*
j, мА/cm^2	0.753	0.142	0.052	2.436	0.462	0.169
$j_{i.a}$, мА/cm^2	0.648	0.122	0.050	1.908	0.362	0.133
$e\Gamma_{o.к}$, мА/cm^2	3.596	1.487	0.864	9.316	3.907	2.287
$e\Gamma_{n.c}/j_{i.a}$, rel.un	5.549	12.19	17.28	4.882	10.79	17.20

As it can be seen, the total current density j is not much larger than ^{j}i.a, which indicates a small value of je.c and the possibility of estimating ^{j}i.a by the experimental value of j. In fact, γ_i for ions with energy of 5 keV is only 0.28, and the mean values γ_i and γ_n are even smaller. This fact, together with the fact that $U \sim 0.5...5$ kV, allowed not to take into account the space charge of electrons and ionization. The values of d* with the asterisk correspond to the values of pd, at which the plasma boundary may shift towards to the cathode of AGD or an independent self-sustained glow discharge may occur in the gas gap with width d* between electrodes. Such phenomenon leads to decrease of the parameters $e\Gamma_{n.c}/j_{i.a}$ relatively those depicted in table 1. Thus, the regimes with $pd = pd$* are boundary ones for applying the results of these calculations. The values of d* for given p and U were determined from the experimental Paschen curves given in [11].

The parameter $e\Gamma_{n.c}/j_{i.a}$ characterizes the efficiency of generating the fast neutral atoms flow in the canal rays. As pd increases, the parameter $e\Gamma_{n.c}/j_{i.a}$ increases. Its value in the discharge modes at $pd<pd$* or before the occurrence of a self-sustained discharge in the system with an anode ion source is in the range of values from 1 to about 5.55. Note, these values relate to the cathode surface. Indeed, a real workpiece is disposed on some distance from the back surface of the cathode and it is needed to introduce some correction to these values in order to know the flow of fast neutral atoms on the surface of the distant workpiece. Taking into account the interception of the neutrals by the cathode, *i.e.* transparency coefficient of the cathode $\eta<1$ (*e.g.*$\eta=0.5$), one may obtain at the back cathode surface $e\Gamma_{n.c}/j_{i.a} \times \eta = e\Gamma_{n.b.c}/ji.a = 0.5...2.75$. The absolute values of $\Gamma_{n.c}$ and $\Gamma_{n.b.c}$ are bigger with increasing U at the same d, hence, the work at higher U may be preferable.

Thus, the physical-kinetic model of the fast neutral atoms flow source on the base of AGD channel rays has been created. The model allows estimating the parameters of the generated fast atom flow. The limits of applicability of the created model and the range of the operating parameters of the source are established. The model will be used for implementation of beam technology for dielectric optical nanostructured metamaterials [4, 5].

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