CYNETICS OF MOLECULAR NITROGEN IONIZATION IN PLASMA OF GAS DISCHARGE ION SOURCE

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A model is suggested wich describes the distruction of N_2 molecules in the gas discharge medium with the pressure of 1 10 Pa. The self-consistent problem is solved using basic different equations system of chemical cynetics. The optimal parameters of discharge are presented which ensure the maximal yield of the N_1^+- component for given energy contribution. The conclusions on mechanism and optimal parameters of gas discharge regime are derived on the basis of comparison of calculated and experimental data achieved on duoplasmatron type injector of RF linear accelerator. The possibilities are discussed of the use of this calculation model for an analysis of physical effects in the region of formation of plasma-type emitter.

1. INTRODUCTION

Nitrogen ion implantation is used widely to increase the surface hardness of metals which results in the large increase in the lifetime of mashines [1]. Deep implanted layers are preferred which make wanted the implantation of N^+ rather than that of N_2^+ ions. Early experimental results show that better wear and corrosion resistances are achieved when implantation is done with only N^+ ions rather than with the mixed N^+, N_2^+ ion beam [2]. A pure beam of N^+ ions is desirable since the mass separation entails the use of a large magnet. Elimination of the mass separation procedure allows a simpler, more efficient and compact ion accelerator as a whole. Application of pure nitrogen beam in technology defines the interest for plasma cynetic parameters of this gas [3,4]. In this paper non - stationary nitrogen plasma is explored. An attempt is made to develop the calculation model of nitrogen plasma in the range of small value of discharge current density. The important purposes of the numerical simulation are the definition of internal plasma parameters (charged particles concentration, exited particles, radicals) when external parameters are given (gas pressure, discharge current and voltage, geometrical factor, sort of the working gas), the calculation of the chemical reactions cynetics in plasma volume and on the electrode surfaces, the search of the discharge parameter (electron temperature, spesific energy contribution and ionization efficiency) leading to the minimal power consumption.

2. EXPERIMENTAL SETUP

The sourse geometry has been already described [5]. The sourse consists of the air cooled electrodes with the duoplasmatron-type configuration. A hollow cathode (2,5 cm diam, 10 cm depth) made of aluminium is positionned on the sourse axis. A magnetic field is produced by permanent magnets, which provide a longitudial magnetic field in the anode region with the magnitude of about 0,2 T at the axis. The open end of the source is enclosed by the two-electrode acceleration system and an einzel lense focusing system. Nitrogen ions are extracted from the source through the 0,5 mm diam aperture. Located downstream from the einzel lense is the magnetic deflection spectrometer to define the ion species in the extracted beam. The Faraday cup is located further downstream. All the measurements are performed with the sourse and extraction operated in dc and pulse mode. The ion energy is estimated near 30 keV.

3. SOLUTION OF NITROGEN PLASMA CYNETICS. THEORETICAL MODEL.

Complicated chemical reaction may be described by the system of stehiometric equations:

$$\sum_{i=1}^{N} \nu'_{ij} M_i \to \sum_{i=1}^{N} \nu''_{ij} M_i \quad , \nu=1,2,\ldots,L \quad , \qquad (1)$$

where L - the number of elementary stages; ν_{ij}', ν_{ij}'' - stehiometrtc coefficients of the i-substance participating in the j-reaction as a initiating reagent and resulting product correspondingly; Mi -the amount of i-substance in the system.

The rate of the process is given by [6]:

$$\frac{dn_i}{dt} = \sum_{j=1}^{M} (\nu''_{ij} - \nu'_{ij})(K_{fj} \prod_{i=1}^{N} n_i^{\nu'_{ij}} - K_{bj} \prod_{i=1}^{N} n_i^{\nu''_{ij}}) \ , \qquad (2)$$

where ni - the density of i-substance; Kfj and Kbj - constants of the direct and inverse reactions correspondingly.

Equation (2) includes value ni for $[N^+]$ ions, where $[N^+]$ - the density of nitrogen atomic ions, obtained in appropriate processes (1,2) so it is necessary to solve the hard basic diferent equations system (BDE) of chemical cynetics.

The following typical process have been analysed:

1. Settling and desactivation of levels $N_2(C^3\Pi_u)$ with constants k1.1 - k1.10;
2. Settling of levels $B^3\Pi g$ with the constants k2.1 - k2.13;
3. Destrustion of levels $B^3\Pi g$ with the constants k3.1 - k3.6,

4. Settling and desactivation of excited levels $N_2(A^3\Sigma_u^+)$ with constants k4.1 - k4.6, k3.1, k3.2, k2.8, k2.6;
5. Formation and destructions of atoms k5.1 - k5.3, k4.3, k4.4;
6. Formation and destruction of ions $N_2^+(B_2\Sigma_{u,v}^+)$ with k6.1 - k6.6;
7. Ionization process k7.1 - k7.8;
8. Ion conversion k8.1 - k8.16.

Equations describing the main processes mentioned above are given below.

Electrons:

$N_2(x,v) + e \rightarrow N_2^+ + 2e$

$N + e \rightarrow N^+ + 2e$

$N_2^+ + e \rightarrow N_2^+ + e$

$N_2^+ + e$ -wall $\rightarrow N_2$

$N^+ + e$ -wall $\rightarrow N$

$N_2^+ + e$ -wall $\rightarrow N_2 + N$

N_2^+ ions:

$N_2^+(x,v_1)+N_2(x,v_2) \rightarrow N^+ + N + N_2(x,v_3)$

$(E_{v1} + E_{v2} - E_{v3} = 8{,}73\ eV)$

N^+ ions: (3)

$N_2^+(x) + e \rightarrow N^+ + N + e$

$N + e \rightarrow N^+ + 2e$

$N + N_2^+(x,v) \rightarrow N^+ + N_2(x,v)$

$N + N_4^+ \rightarrow N^+ + 2N_2$

$N^+ + 2N_2 \rightarrow N_3^+ + N_2$

$N_2^+ + N + N_2 \rightarrow N_3^+ + N_2$

$N_2^+(x,v_1) + N_2(x,v_2) \rightarrow N_3^+ + N$

where x - the basic electron state of particle;
V - the number of oscillation levels;
E - the energy of internal excitation.

Excitation cross-sections of electron levels and ionization cross-section used in calculation are shown on figure 1 [3].

The BOE system (2) was written using the parameters n_e, $[N_2^+]$, $[N^+]$, $[N_3^+]$, $[N_4^+]$, $[N]$, $[N(^2P)]$, $[N(^4S)]$, $[N_2(X_v)]$, $[N_2X_\Sigma]$, $[N_2(A)]$, $[N_2(B^3\Pi)]$, $[N_2(C^3\Pi)]$.

There is some difficulty with the analysis of process $N^+ + e$-wall $\rightarrow N$ with the constant $k8.13=(0.6-3.7)*10^4\ S^{-1}$ for definition of $[N^+]$ concentration. Velosity constants of electron impact reactions are extrapolated and specified by [2,7,8].

The self - consistent problem is solved in the following way:

1. Calculatin of particle concentrations:

$$\frac{\partial n_i}{\partial t} = f_i(n_1, n_2, \dots, n_N, t), \quad (4)$$

with the inital conditions $n_i(t_0) = n_{i0}$, $i=1,2,\dots,N$, is reached by means of the subroutine S2STIF for determination of hard BOE systems.

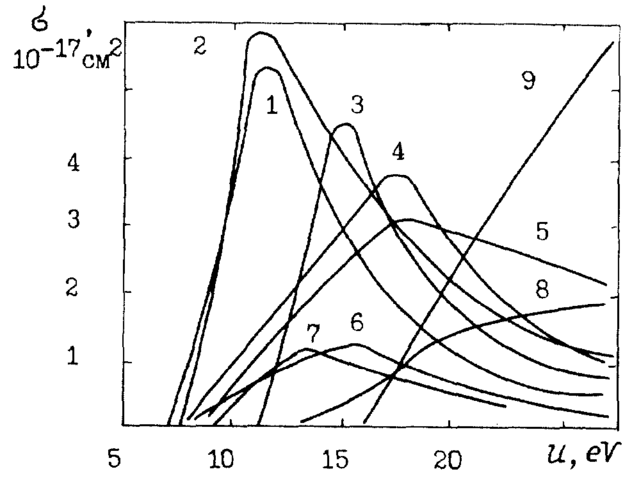

Figure 1 Exciting cross-section of nitrogen electron levels [3]: 1- $A^3\Sigma_u^+$; 2- $B^3\Pi g$; 3- $C^3\Pi u$; 4- $W^3\Delta u$; 5- $a^1\Pi g$; 6- $B'^3\Sigma^-u$; 7- $W^1\Delta u$; 8- $B'\Pi u$; 9- ionization.

2. Calculation of the ratio E/N, where E - the electric field in discharge; N - neutral particle density, using current equation and dependence of drift velocity Wd(E/N):

$$J = eS\left(W_{de} n_e + \sum_i W_{di} n_i\right)$$
$$W_d = W_{do}\left(\frac{E/N}{(E/N)_0}\right)^{\alpha} \quad (5)$$

Thus form eq. (4), one obtains

$$\frac{E}{N} = \left(\frac{E}{N}\right)_0 \frac{J\,(W_{do})}{eS\left(W_{de}n_e + \sum_i W_{di} n_i\right)^{\frac{1}{\alpha}}}, \quad (6)$$

where S - the cross-section of discharge tube. This calculation is realized by the subroutine DIFFUN. The E/N value is chosen in accordance whith the real conditions in anode region of duoplasmatron ion source, when anode potential fall is given by the relation [9] :

$$U = \frac{KT_{e1}}{2e} \lg\left(\frac{2M}{\pi m}\right), \quad (7)$$

where T_{e1} - the electron temputure in the cathode plasmxa; M - ion mass; m - electron mass.

3. Calculation of coefficients depending on eletric field (E/N) with the use the energy distribution of electrons $k_{ij} = k_{ij}(E/N)$, $Di=Di(E/N)$, which may be realized by subruotine COEF for determination of plasma cynetics coefficients.

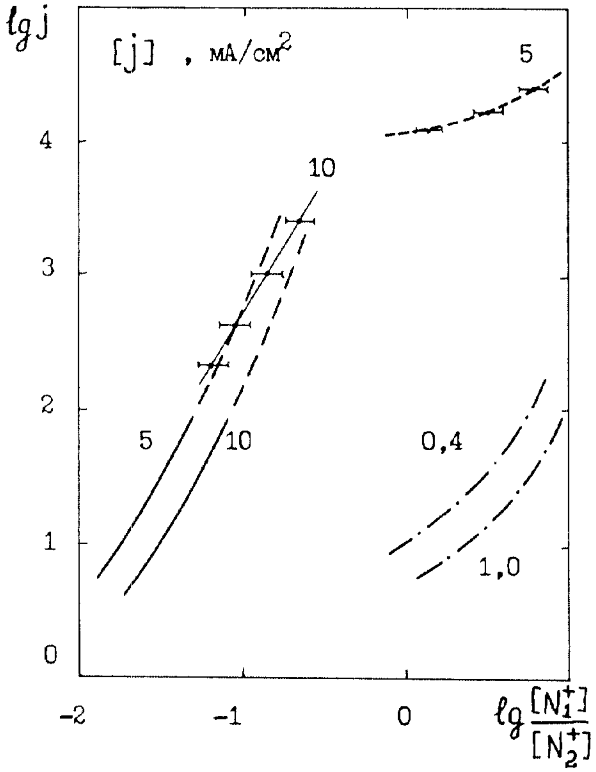

Figure 2 Calculated and experimental value of $\log[N_1^+]/[N_2^+]$ in dependence on discharge current density logJ: ——— - theoretical results (small currents); ——— - experiment (dc mode of operation); ------ - experiment (pulse mode of operation) —·—·— - experimental data [10]; — — - extrapolation of theoretical data (high discharge currents); parameter of curves - the gas pressure in discharge chamber, Pa.

4. THEORETICAL AND EXPERIMENTAL RESULTS.

We present some mechanism of nitrogen ions generation which may be used for description of $[N_1^+]/[N_2^+]$ experimental dependences on initial neutrals density and discharge current density. Errors are stipulated by mistakes in particle density as well as coeficients of processes rate. Theoretical and experimental data for small discharge currents are shown on fig. 2. Theoretical investigation of feasible mechanisms of nitrogen destruction has shown that high efficiency is reached in non-equilibrium conditions (Te>>To),where To - neutral gas temputure), when dissociation is stimulated by oscillation excitation of N_2 electron levels. Furthermore, the creation of N_1^+ ions by electron impact, their recharging and destruction by diffusion or diffusion with the three-particle conversion may not explain the experimental data. It is necessary to take into account the ambipolar diffusion across magnetic field.

Experimental dependences of $\log[N_1^+]/[N_2^+]$ for high discharge currents in the range of working gas pressure 5-10 Pa are shown on the same fig.2. Experimental data inside considered error range for inverstigated space of parameters accounting extrapolation procedure are in good agreement with the theoretical results.It seems that significant distinction of theoretical and experimental data [10] (see fig.1.), may be explained by the specific discharge conditions of multicusp anode system posessing of high efficiency of electron energy transfer into plasma by means repeated oscillations. Oscillation of plasma electrons leads to high non-equilibrium state of discharge conditions (Te>>To).

Theoretical analysis of plasma cynetics in the range of high discharge currents shows that additional efforts should be taken to get more correct cynetics coefficients of considered reactions.

5. CONCLUSION.

Theoretical model and experimental data obtained on duoplasmatron ion sourse for small discharge current are discussed. Considered calculation algorithm may be sucsessfully applied to an analysis of physical effects in the region of formation of plasma-type emitter. In addition this calculation model might be useful for cousidering more complicated plasma-creating media, for example, halogens.

6.REFERENCES

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