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NUMERICAL MODEL OF AFTERGLOW PLASMA IN GAS MIXTURES[1]

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Processes of diffusion, electron-ion recombination, ionmolecular reactions and Penning ionization are taken into account in our model of the afterglow plasma in inert gas mixtures. Time and spatial dependences of the particle densities are calculated by the numerical solution of the system of partial differential equations. The model is applied to He-Ne mixtures.

МЕТОД ЧИСЛЕННОГО РАСЧЕТА ПОСЛЕСВЕЧЕНИЯ ПЛАЗМЫ В СМЕСИ ГАЗОВ

В работе приводится модель для послесвечения плазмы в смесях инертных газов, в которой учтены процессы диффузии, электронно-ионная рекомбинация, ионно-молекулярные реакции и ионизация Пеннинга. На основе численного решения дифференциальных уравнений в частных производных вычислена временная и пространственная зависимости плотностей частиц. Модель применена к смеси газов гелия и неона.

I. PROCESSES IN AFTERGLOW PLASMA

In the afterglow plasma of the periodical pulsed d.c. glow discharge the kinetics of charged and metastable particles is determined by their mutual collisions. We consider the following processes: — *ambipolar diffusion of electrons and ions*; — *diffusion of the metastable atoms of the main gas*; — *electron-ion recombination with photon emission*

$$\begin{tikzcd}[row sep=tiny] & X^* + h\nu \\ X^+ + e \arrow[ur] \arrow[dr] & \\ & X + h\nu \end{tikzcd} \qquad (1)$$

X^+ is the atomic ion, X^* is the excited atom

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— *electron-ion recombination in three body collision processes*

$$X^{+}+e+Y \rightarrow X^{*}+Y \tag{2}$$

Y is the electron or neutral atom

— *dissociative recombination*

$$XY^{+}+e \rightarrow X^{*}+Y \tag{3}$$

— *ion-molecular reactions*

$$X^{+}+Y+Z \rightarrow XY^{+}+Z \tag{4}$$

$$X^{+}+Y+Z \rightarrow Y^{+}+X+Z \tag{5}$$

$$XY^{+}+Z \rightarrow XZ^{+}+Y \tag{6}$$

Y, Z are neutral particles

— *Penning ionization*

$$X^{m}+Y \rightarrow Y^{+}+e+X \tag{7}$$

X^{m} is the metastable atom of the main gas. In a more precise discussion further processes such as associative ionization can be taken into account.

II. MODEL EQUATIONS AND METHOD OF THEIR SOLUTION

The system of the partial differential equations which describe plasma decay can be generally written in the form

$$\frac{\partial n^{(\eta)}}{\partial t}=D^{(\eta)}\Delta n^{(\eta)}-\sum_{\xi} A^{(\eta,\xi)}n^{(\xi)}, \tag{8}$$

where $n^{(\eta)}$ is the column vector, the components of which are densities of particles, $D^{(\eta)}$ is the line vector with diffusion coefficients as components, Δ is the Laplacian operator, t is time. The elements of the matrix $A^{(\eta,\xi)}$ are the coefficients in corresponding continuity equations for particles under consideration. In the cylindrical geometry the densities are dependent only on the r a t coordinates as it is the case of the positive column of the d.c. glow discharge. We have approximated the system (8) by the system of the difference equations

$$\frac{n_{j,k+1}^{(\eta)}-n_{j,k}^{(\eta)}}{\Delta t}=D^{(\eta)}\left(\frac{n_{j+1,k}^{(\eta)}-2n_{j,k}^{(\eta)}+n_{j-1,k}^{(\eta)}}{(\Delta r)^{2}}+\right. \tag{9}$$

$$+\frac{n_{j+1,k}^{(\eta)}-n_{j-1,k}^{(\eta)}}{2j(\Delta r)^{2}}-\sum_{\xi} A_{j,k}^{(\eta,\xi)}n_{j,k}^{(\xi)},$$

where j, k indicate the number of the nets points in the directions r and t, respectively. By using this scheme we have calculated values $n_{j,k+1}$ from $n_{j+1,k}$, $n_{j,k}$ and $n_{j-1,k}$, i.e. the system (9) leads to the explicit difference scheme. The numerical solution converges on the exact solution if the following stability criterion is fulfilled [1]

$$\Delta t \leq \min_{j,k,\eta} \frac{2(\Delta r)^{2}}{8D^{(\eta)}+A_{j,k}^{(\eta,\xi)}(\Delta r)^{2}}. \tag{10}$$

We have solved numerically Eqs. (8) with the initial distributions $n^{(\eta)}(r,0)=J_0(2.405r/R)n_0^{(\eta)}$ and the boundary conditions $n^{(\eta)}(R,t)=0$ and $\partial n^{(\eta)}/\partial r|_0=0$ $(t \geq 0)$, R is the diameter of the discharge tube.

III. RESULTS — MIXTURES He AND Ne

Ions of He^{+}, Ne^{+}, He_2^{+}, Ne_2^{+} and $HeNe^{+}$ are present in the afterglow plasma in He and Ne mixtures. In addition to the recombination and diffusion processes we have considered six ion-molecular reactions according to [2, 3]. We have calculated space and time dependences of the ion densities at helium (main gas) pressure $p_{He}=3040$ Pa and 666.6 Pa and various relative concentrations of the neon atoms s. The discharge tube diameter was 2.2 cm. Metastable He atoms have not been taken into account.

Time dependences of the ion densities at the point $r=0$ are shown in Fig. 1 for two different sets of initial conditions. It can be seen that these dependences differ a little. Fast processes (conversions of atomic to molecular ions) which are described by the following equations

$$Ne^{+}+2\,Ne \rightarrow Ne_2^{+}+Ne \tag{11}$$

$$Ne^{+}+Ne+He \rightarrow Ne_2^{+}+He \tag{12}$$

$$Ne^{+}+2\,He \rightarrow He_2^{+}+Ne \tag{13}$$

created new initial conditions for slow processes, which are efficient in the late afterglow. In this part of the afterglow period Ne_2^{+} ions are dominant. With increasing Ne percentage, the relative concentration of Ne_2^{+} ions increases due to processes (11, 12) and the process

$$HeNe^{+}+Ne \rightarrow Ne_2^{+}+He, \tag{14}$$

which is also present.

The calculated spatial profiles of the densities of the molecular Ne_2^{+} and complex $HeNe^{+}$ ions are changing in the afterglow period. In Fig. 2 the time dependences of the ratio of the normalized ion flux at $r=R$ to central ion density are given for various ions. This ratio changes during the afterglow mostly for Ne_2^{+} ions, which is caused by the great efficiency of the nonlinear recombination of these ions. The

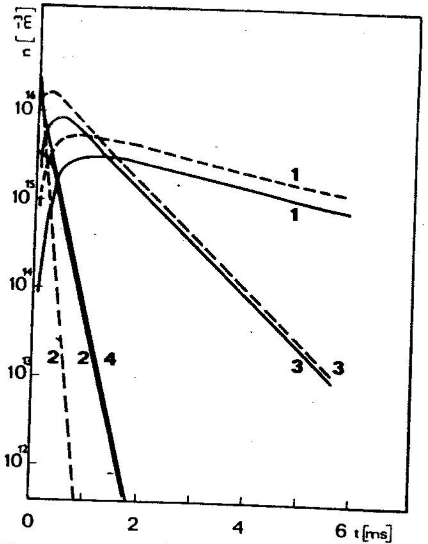


Fig. 1. Time dependences of the ion densities for two sets of initial conditions: dashed lines $n^{(2)}(0) = 1.5 \times 10^{16}\,\mathrm{m}^{-3}$; full lines $n^{(2)}(0) = 7.35 \times 10^{11}\,\mathrm{m}^{-3}$, $n^{(4)}(0) = 1.5 \times 10^{16}\,\mathrm{m}^{-3}$ (1 Ne_2^+, 2 Ne^+, 3 $HeNe^+$, 4 He_2^+, $p_{He} = 3040$ Pa, $s = 4.9 \times 10^{-5}$).

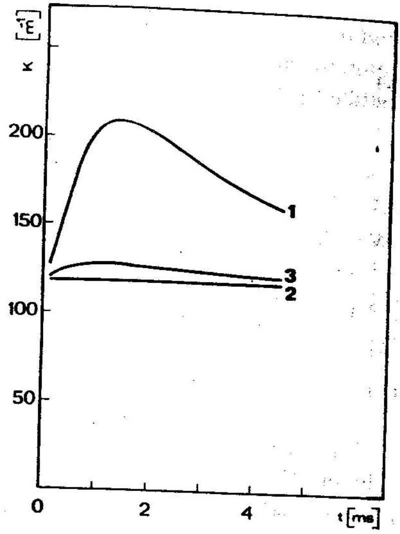


Fig. 2. Time dependences of the ratio K for various ions ($p_{He} = 3040$ Pa, $s = 1.9 \times 10^{-4}$, 1 Ne_2^+, 2 Ne^+, 3 $HeNe^+$).

obtained results are important for mass-spectrometry of the afterglow plasma. The assumption that K is constant is used often, but according to our experience it is not valid in all cases.

In Fig. 3 the time dependences of the reciprocal average electron density are shown for various s. From the slope of these curves the effective recombination coefficient α_{eff} can be determined. This slope increases with increasing s. The value of the coefficient α_{eff} determined from the linear portion of the calculated curve for $s = 1.3 \times 10^{-3}$ is nearly equal to the value for the Ne_2^+ ions.

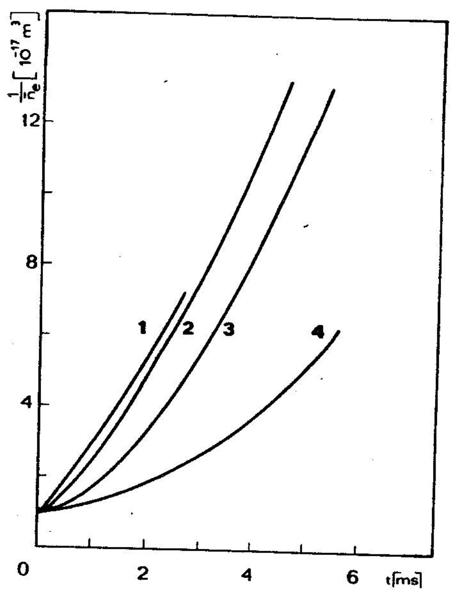
The results of the calculations for the He pressure 666.6 Pa and a small s ($s = 1.6 \times 10^{-5}$) show that He_2^+, $HeNe^+$ and Ne^+ ions are dominant and the role of Ne_2^+ ions is not important. It is in agreement with experimental data [3]. If s increases, the efficiency of the processes (12—14) and also of the following processes

$$He_2^+ + Ne \rightarrow Ne^+ + 2\,He \tag{15}$$

$$Ne^+ + 2\,He \rightarrow HeNe^+ + He \tag{16}$$

increases. Therefore He_2^+ ions disappear more rapidly for a larger value of s. Simultaneously the role of the Ne_2^+ ions is more significant. Spatial distributions of all ions change very slowly.

Fig. 3. Dependences of the reciprocal electron density $1/n_e$ versus time t for various values of the relative concentration s (1 $s = 1.3 \times 10^{-2}$, 2 $s = 1.9 \times 10^{-4}$, 3 $s = 4.9 \times 10^{-5}$, 4 $s = 10^{-5}$, $p_{He} = 3040$ Pa, $n^{(2)}(0) = s \times n^{(4)}(0)$, $n^{(4)}(0) = 1.5 \times 10^{16}\,\mathrm{m}^{-3}$).



IV. CONCLUSION

We have obtained new information about time and spatial dependences of the ion densities from calculations based on the model of the afterglow plasma. This model gives a possibility for the evaluation of experimental results, for the

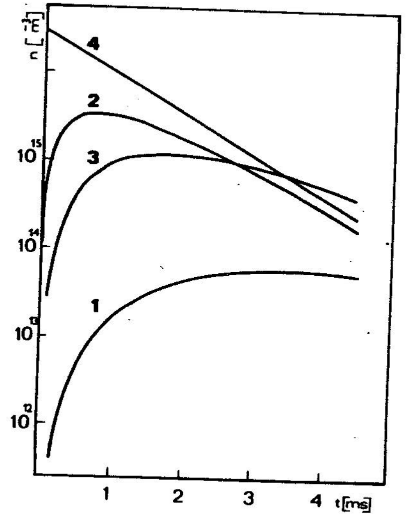


Fig. 4. Time dependences of the ion densities at $r = 0$ ($p_{He} = 666.6$ Pa, $s = 1.6 \times 10^{-5}$, $n^{(2)}(0) = 4.8 \times 10^{11}\,\mathrm{m}^{-3}$, $n^{(4)}(0) = 3 \times 10^{16}\,\mathrm{m}^{-3}$, 1 Ne_2^+, 2 Ne^+, 3 $HeNe^+$, 4 He_2^+).

optimization of experimental conditions and it can also be used for the investigation of kinetics of the excited atoms in the afterglow plasma.

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