

MATHEMATICAL MODELLING OF KINETICS OF THE COLLISIONAL
AND RADIATIONAL TRANSITIONS IN THE ELECTRIC DISCHARGE
PLASMA

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INTRODUCTION

The use of a Hg-Na vapour mixture under high pressure $p \sim 100-500$ KPa as an active medium for lighting apparatuses poses many problems to scientists. Here mathematical modelling is able to help. The application of mathematical modelling is very effective in the investigation of processes of the collisional and radiational transitions on the microscopical level, such as the kinetics of the collisional and radiational transitions in atoms and ions. These play the main role in low temperature dense plasma.

In a number of papers it is tried to develop a mathematical model adequately describing the processes of the radiational-collisional kinetics in the electric discharge in the Hg-Na dense vapour mixture. It is a fact that the physical conditions in lighting apparatuses using electric discharge under high pressure $p \sim 100$ KPa

This paper has not been published elsewhere.

are not enough investigated (1,3). On the contrary, electric discharges under low pressure $p \sim 100$ Pa are well studied (1,2). Also there are a few works on physics of discharge in the dense medium of mercury and sodium (3,4). At the same time the property of the electric discharges to convert power into radiation is widely used in practice. We must note that the physical conditions in the electric discharges are, as a rule, substantially different for different pressure. Electric discharges under high pressures have a complex spectrum of radiation, at the same time the main part of radiation under low pressure is connected with resonance levels. For instance, in luminescence lamps with pressure $p \sim 100$ Pa about 60% of the electric power of plasma radiate on one resonance level with $\lambda = 2573 \text{ \AA}$ (3). The increase of the density of atoms of mercury under high pressures leads to a substantial self-absorption of radiation of the resonance level and the spectrum of the lamp has high level lines falling in the main in to visual and long-wave ultraviolet regions.

Moreover the use of the Hg-Na-Xe complex mixture and the existence of high currents up to 10 A under high pressures can cause substantially nonequilibrium levels in spite of the equality of temperatures of the electronic and atomic components.

The mathematical model

We designed a system of differential equations describing the kinetics of the collisional and radiational transitions in Hg and Na atoms. We also took into consideration different interaction processes of the atoms: the associative ionization, the Penning reaction, dissociative recombination, the forming of ionic and molecular clusters. On Fig. 1 and 2 we show

schematically all of the essential transitions in Hg and in Na. In the mercury atoms 9 excited states were considered, in sodium - 18.

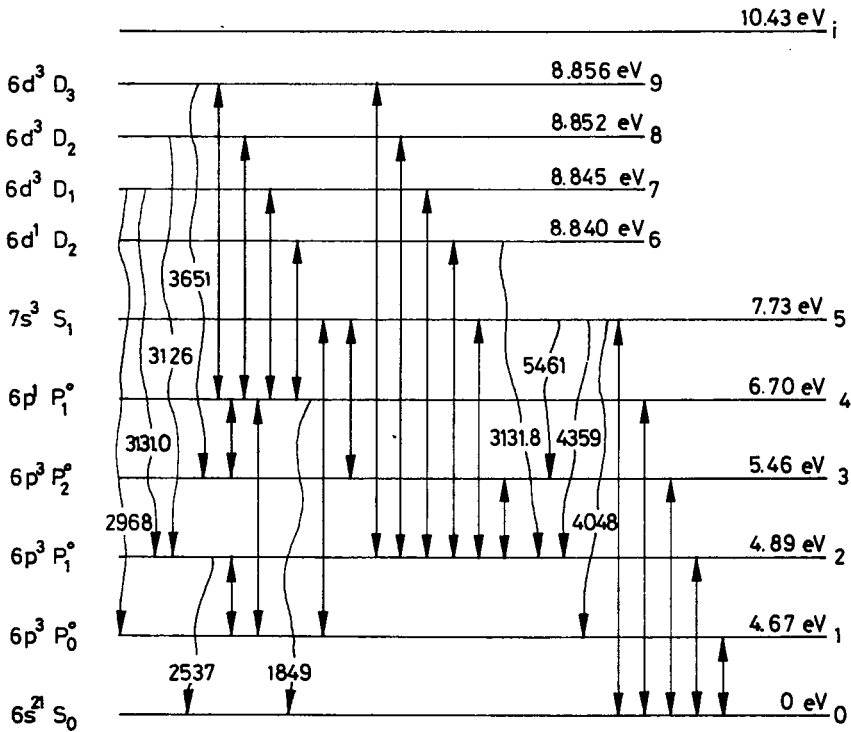


Figure 1
Collisional and radiational transitions in mercury

The system of equations describing these processes has the following form:

$$\frac{dN}{dt} = - \sum_{\beta=1, \dots, 5, i} S_{0\beta} - \sum_{y=1}^3 C_y + \sum_{y=1}^3 (E_y/y) + 4Q + K_{1c}^i M_2^+ N - K_{c1}^i N^+ N^2 + K_{p4} N_4^2 + R_{20} + R_{40}$$

$$\frac{dN_1}{dt} = S_{01} - \sum_{\beta=2,4,5,i} S_{1\beta} - C_1 - E_1 + \sum_{y=2}^3 (E_y/y) + R_{71}$$

$$\begin{aligned} \frac{dN_2}{dt} = & S_{02} + S_{12} - \sum_{\beta=3,5,6,\dots,9,i} S_{2\beta} - C_2 - E_2 + E_3/3 - R_{20} + \\ & + \sum_{y=5}^8 R_{y2} - K_{ass} N_2^2 \cdot 2 \end{aligned}$$

$$\frac{dN_3}{dt} = S_{03} + S_{23} - \sum_{\beta=4,5,i} S_{3\beta} - C_3 - E_3 + R_{53} + R_{93} - 2K_{ass} N_3^2$$

$$\frac{dN_4}{dt} = \sum_{\alpha=0,1,3} S_{\alpha 4} - \sum_{\beta=6,\dots,9,i} S_{4\beta} - R_{40} - 2K_{p4} N_4^2$$

$$\frac{dN_5}{dt} = \sum_{\alpha=0}^3 S_{\alpha 5} - S_{5i} - \sum_{y=1}^3 R_{5y}; \frac{dN_6}{dt} = \sum_{\alpha=2,4} S_{\alpha 6} - S_{66}^i + Q - R_{62}$$

$$\frac{dN_7}{dt} = \sum_{\alpha=2,4} S_{\alpha 7} - S_7^i + Q - \sum_{y=1}^2 R_{7y}; \quad \frac{dN_8}{dt} = \sum_{\alpha=2,4} S_{\alpha 8} - S_8^i + Q - R_{82}$$

$$\frac{dN_9}{dt} = \sum_{\alpha=2,4} S_{\alpha 9} - S_9^i + Q - R_{93}$$

$$\frac{dN^+}{dt} = \sum_{\alpha=0}^5 S_{\alpha i} + \sum_{\alpha=6}^9 S_{\alpha 6}^i - K_{C1}^i N^+ N^2 + K_{IC2}^i M_2^+ N + K_{P4} N_4^2$$

$$\begin{aligned} \frac{dN_e}{dt} &= \sum_{\alpha=0}^5 S_{\alpha i} + \sum_{\alpha=6}^9 S_{\alpha 6}^i + K_{ass} (N_2^2 + N_3^2) + K_{P4} N_4^2 - 4Q + \sum_{\alpha=0}^{18} s_{\alpha i} - q_1 - q_2 + \\ &+ k_{ass} n_1^2 + K_p n N_3 \end{aligned}$$

$$\frac{dM_2}{dt} = \sum_{y=1}^3 C_y; \quad \frac{dM_2^+}{dt} = K_{C1}^i N^+ N^2 - K_{IC2}^i M_2^+ N + K_{ass} (N_2^2 + N_3^2) - 4Q$$

$$\frac{dn}{dt} = - \sum_{\beta=1}^{18} s_{0\beta} - s_{0i} - \sum_{y=6,8}^{18} p_y + q_1 + 2q_2 + \sum_{y=1,4,7,10,13,15} r_{y0} -$$

$$- K_p n N_3 - (K_{1c} n^2 - K_{c1} n_2^M) n$$

$$\frac{dn_1}{dt} = s_{01} - \sum_{\beta=2,3,i} s_{1\beta} - 2k_{ass} n_1^2 - r_{10} +$$

$$+ \sum_{y=2,3,5,6,8,9,11,12,14,16} r_{y1}$$

$$\frac{dn_2}{dt} = \sum_{\alpha=0,1} s_{\alpha 2} - \sum_{\beta=4,i} s_{2\beta} - r_{21}; \quad \frac{dn_3}{dt} = \sum_{\alpha=0,1} s_{\alpha 3} - \sum_{\beta=4,i} s_{3\beta} +$$

$$+ \sum_{y=6,9,12,16} r_{y3}^f - r_{31}$$

$$\frac{dn_4}{dt} = \sum_{\alpha=0,2,3} s_{\alpha 4} - \sum_{\beta=5,6,i} s_{4\beta} - r_{40} + q_2;$$

$$\frac{dn_5}{dt} = \sum_{\alpha=0,4} s_{\alpha 5} - \sum_{\beta=7,i} s_{5\beta} - r_{51}$$

$$\frac{dn_6}{dt} = \sum_{\alpha=0,4} s_{\alpha 6} - \sum_{\beta=7,i} s_{6\beta} - r_{61} - r_{63}^f + q_1 + p_6;$$

$$\frac{dn_7}{dt} = \sum_{\alpha=0,5,6} s_{\alpha 7} - \sum_{\beta=8,9,i} s_{7\beta} - r_{70}$$

$$\frac{dn_8}{dt} = \sum_{\alpha=0,7} s_{\alpha 8} - \sum_{\beta=10,i} s_{8\beta} + p_8 - r_{81}; \quad \frac{dn_9}{dt} = \sum_{\alpha=0,7} s_{\alpha 9} - \sum_{\beta=10,i} s_{9\beta} +$$

$$+ p_9 - r_{91} - r_{93}^f$$

$$\frac{dn_{10}}{dt} = \sum_{\alpha=0,8,9} s_{\alpha,10} - \sum_{\beta=11,12,i} s_{10,\beta} + p_{10} - r_{10,0};$$

$$\frac{dn_{11}}{dt} = \sum_{\alpha=0,10} S_{\alpha,11} - \sum_{\beta=13,i} S_{11,\beta} + p_{11} - r_{11,1}$$

$$\frac{dn_{12}}{dt} = \sum_{\alpha=0,10} S_{\alpha,12} - \sum_{\beta=13,i} S_{12,\beta} + p_{12} - r_{12,3}^f;$$

$$\frac{dn_{13}}{dt} = \sum_{\alpha=0,11,12} S_{\alpha,13} - \sum_{\beta=14,16,i} S_{13,\beta} + p_{13} - r_{13,0}$$

$$\frac{dn_{14}}{dt} = \sum_{\alpha=0,13} S_{\alpha,14} - \sum_{\beta=15,i} S_{14,\beta} + p_{14} - r_{14,1};$$

$$\frac{dn_{15}}{dt} = \sum_{\alpha=0,14} S_{\alpha,15} - \sum_{\beta=16,17,i} S_{15,\beta} + p_{15} - r_{15,0}$$

$$\frac{dn_{16}}{dt} = \sum_{\alpha=0,13,15} S_{\alpha,16} - S_{16,i} + p_{16} - r_{16,1} - r_{16,3}^f;$$

$$\frac{dn_{17}}{dt} = \sum_{\alpha=0,15} S_{\alpha,17} - S_{17,i} + p_{17}$$

$$\frac{dn_{18}}{dt} = -S_{18,i} + p_{18}; \quad \frac{dn^+}{dt} = \sum_{\alpha=0} S_{\alpha,i} - (K_{1c}^+ n^+ n - K_{c1}^- n_2^+) n + K_p n N_3$$

$$\frac{dn_2^+}{dt} = (K_{1c}^+ n^+ n - K_{c1}^- n_2^+) n + k_{ass} n_1^2 - q_1; \quad \frac{dn_3^+}{dt} = (K_{2c}^+ n_2^+ n - K_{c2}^- n_3^+) n - q_2$$

$$\frac{dn_2^M}{dt} = (K_{1c} n^2 - K_{c1} n_2^M) n$$

We used the following notations and expressions:
 $N_i \cdot n_j$ ($i=0, \dots, 9$; $j=0, \dots, 18$) are the concentrations of the mercury and sodium atoms in the basic and excited states; N_e denotes the concentration of electrons,

$$S_{\alpha\beta} = (K_{\alpha\beta} N_{\alpha} - K_{\beta\alpha} N_{\beta}) N_e, \quad S_{\alpha i} = (K_{\alpha i} N - K_{i\alpha} N^+ N_e) N_e,$$

$S_{\alpha\beta}^i = (K_{\alpha\beta}^i N_{\alpha} - K_{\alpha\beta}^k N_e^+ N_e) N_e$, $C_y = (K_{yc} N_y N - K_{cy} M_2) N$, $R_{\alpha\beta} = A_{\alpha\beta} N_{\alpha}$,
 $E_y = K_{yex} N_y M_2$, $Q = \alpha M_2^+ N_e / 4$ for mercury, and $s_{\alpha\beta} =$
 $= (k_{\alpha\beta} n_{\alpha} - k_{\beta\alpha} n_{\beta}) N_e$, $s_{\alpha i} = (k_{\alpha i} n_{\alpha} - k_{i\alpha} n_e^+) N_e$, $r_{\alpha\beta} = a_{\alpha\beta} n_{\alpha}$,
 $p_y = k_{yx} (N_1 + N_2) n$, $q_j = \alpha_j n_{j+1}^+ N_e$ ($j=1,2$) for sodium. Here
 $K_{\alpha\beta}$, $k_{\alpha\beta}$ denote the number of transitions by electron
 impact from state α to state β per unit volume and time;
 $A_{\alpha\beta}$, $a_{\alpha\beta}$ - radiational coefficients; N_e^+ , n_e^+ , M_2^+ , n_2^+ , n_3^+
 atomic and molecular ions; K_{yc} , k_{yc} , k_{yc}^+ , K_{ass} , k_{ass}
 coefficients of conversion and associative ionizations;
 K_{py} , k_p coefficients of Penning, K_{yex} coefficient of
 extinguishing. The coefficients $K_{\alpha\beta}$, $K_{\alpha i}$, $A_{\alpha\beta}$, K_{yass} ,
 $k_{\alpha\beta}$, $k_{\alpha i}$, $a_{\alpha\beta}$, k_{lass} , k_{yx} were calculated from experi-
 mental data of cross sections whereas K_{yc} , K_{1c}^i , K_{yex} ,
 K_{3p} , α , h_{1c} , k_{yc}^+ , k_{lass} , k_p , α_1 , α_2 are data found in
 the literature.

Results of modelling

At the first stage the kinetics of the transitions
 of the mercury atoms was analysed in detail. For that
 aim the first fourteen equations were numerically
 solved with fixed temperature $T_e = T_g = 0.8$ eV. The
 results are shown in Fig. 3, 4. We call your attention
 to the nonmonotonic character of exit to the stationary
 state of the $N_{6-9}(t)$ curves, moreover, these stationary
 states are substantially different from the Boltzmann
 distribution. Our analysis shows that both facts are due
 to the ignoration of the high excited states, the so-
 called quasicontinuum (5). The introduction of the
 quasicontinuum, according to (5), into the above system
 of equations made it possible to obtain the correct
 limiting transmission to the distribution of Saha-
 Boltzmann in the Hg dense plasma, Fig. 3. From the

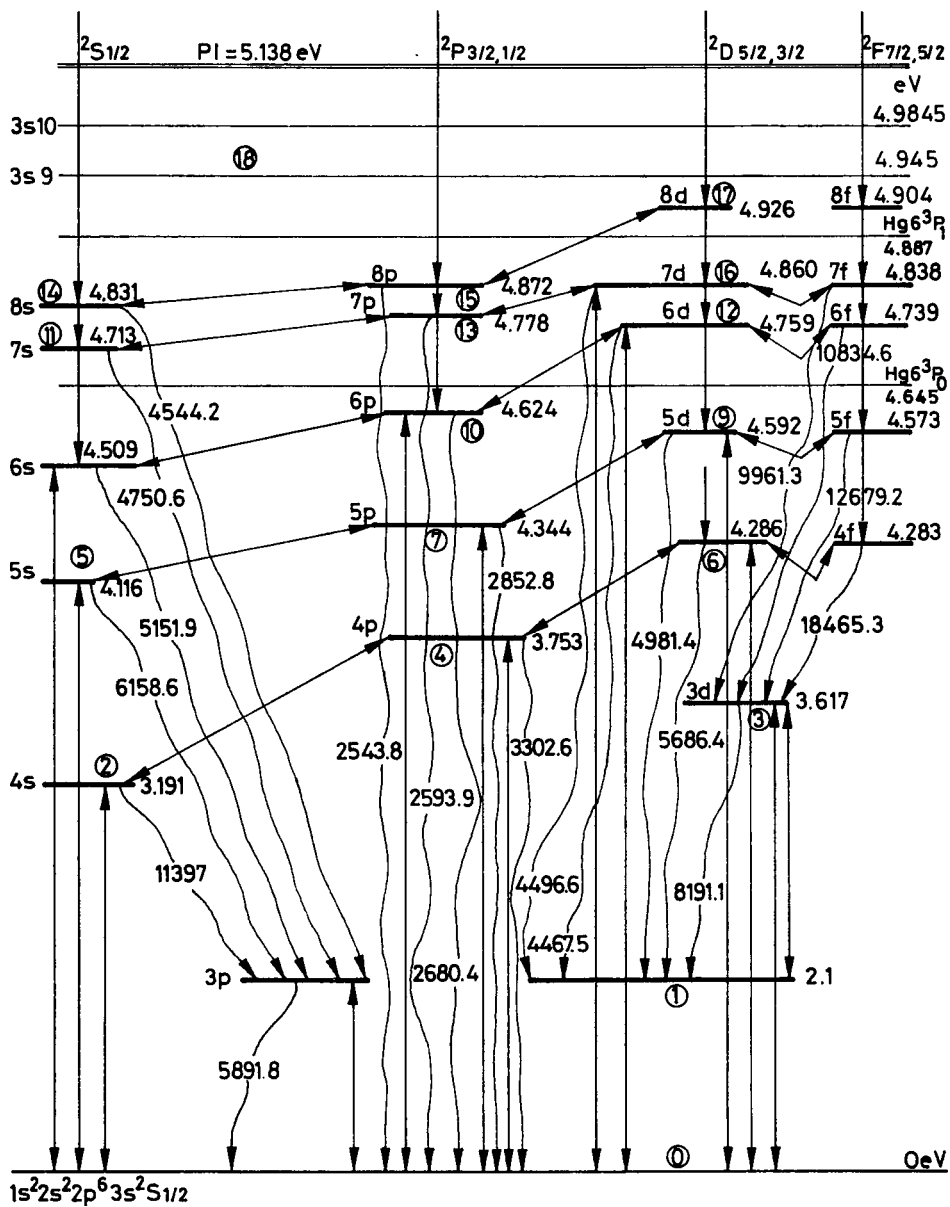


Fig. 2. Collisional and radiational transitions in sodium

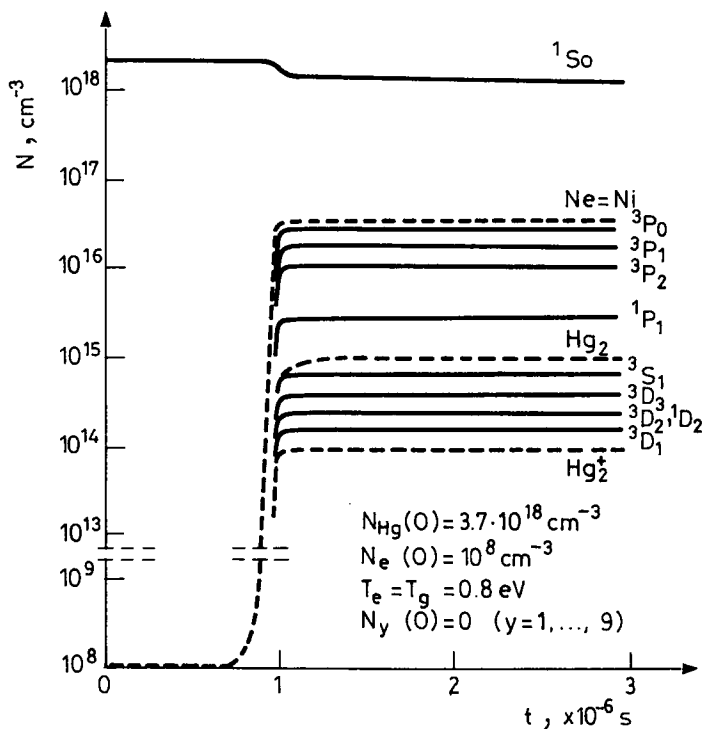


Figure 3. The concentration of the excited states in Hg

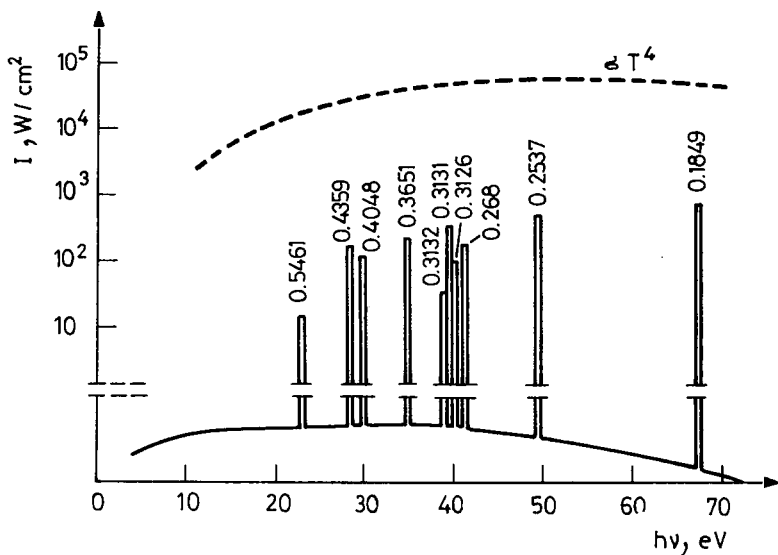


Figure 4. Intensities of radiation in Hg

derived concentration values of the excited states the intensities of radiation of the corresponding transmissions were calculated Fig. 4. The numerical analysis of the spectrum of radiation was carried out according to the methods (6). Doppler and Lorentz mechanisms of broadening were taken into account. We didn't taken into account the self-absorption of radiation and the presence of the lines with wave length of 2573 and 1874 Å in the spectrum.

The dashed line in Fig. 4. shows the theoretical limit of the radiation intensity which is equal to σT^4 . The brief analysis of the results shows that the designed mathematical model qualitatively correctly describes the main processes in the gas discharge. Similar calculations were made also for sodiums vapour.

The case of low pressure was investigated by I. Joó (personal communication).

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