STUDY OF COLLISION PROCESSES IN POSITIVE COLUMN OF GLOW DISCHARGE BY MEANS OF COMPUTER EXPERIMENT[1)]

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The computer experiment for the simulation of processes in weakly ionized plasma was proposed. The results obtained give us information about the influence of individual elementary processes on plasma characteristics and allow to build a very simple model of inert gas plasma. As a criterion for qualitative correctness of the model its ability to maintain the Maxwellian energy distribution of electrons was chosen. The simulation based on experimental data for Ar plasma showed that the minimum set of scattering mechanisms is: elastic collisions, one-level excitation, ionization and intensive electron-electron interactions.

I. INTRODUCTION

The method of computer experiment can be applied to various problems in plasma physics, together with more usual experimental and theoretical approaches. In our previous papers (e.g. [1], [2]) we studied the probe charateristics of the positive column of dc glow discharge both in the inert gases and in their mixtures with hydrocarbons for plasmachemistry. For realistic computer experiments in this field it is necessary to have a model of undisturbed Ar and Ne plasma. As the simulations are typically very time consuming, the model must be simple enough but not oversimplified. The purpose of this contribution is, therefore, to find the minimal number of interactions in plasma which is sufficient for its qualitative characterization. As a criterion the ability to maintain the Maxwellian distribution was chosen. The first results were published in [3].

1) Contribution presented at the 8th Symposium on Elementary Processes and Chemical Reactions in Low Temperature Plasma. STARÁ LESNÁ, May 28 - June 1, 1990

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II. MODEL

The simulation procedure used in our computer experiment is the combination of molecular dynamics and the Monte Carlo method, i.e. while the electron trajectories in the external electric field are derived from the Newton equation of motion, the scattering processes are treated on the basis of the theory of probability. In the model the large group of electrons is processed simultaneously, which justifies the probabilistic approach.

The simulation of the inert gas plasma is based on these simplifying assumptions:

- The total number of electrons in our model is constant (the increase of their number being compensated by the ambipolar diffusion).
- The external electric field is constant (the working region of our model is placed into the positive column of a dc glow discharge).
- The scattering of electrons is isotropic (it concerns their angular distribution).

There exist several tens of more or less important interactions even in the plasma of atomic gases like Ar and Ne. After some preliminary evaluations we included into our model only four kinds of interactions for electrons in plasma :

1. elastic collisions
2. inelastic collisions - excitation
3. inelastic collisions - ionization
4. electron-electron collisions.

The cross-sections and parameters of these interactions were given by experiments or calculated from experimental data (e.g. [5]–[8]).

The elastic collision of an electron is represented in the model from the energetic point of view by an energy loss equal to $2(m/M)$, m and M being the masses of electrons and gas atoms, respectively. The direction of an elastically scattered electron is chosen according to our assumption randomly, i.e. the components of its velocity are generated by the relations [9]:

$$\begin{aligned} v_x &= v\cos\vartheta \\ v_y &= v\sin\vartheta\cos\phi \\ v_z &= v\sin\vartheta\sin\phi \\ \cos\vartheta &= 2\gamma - 1 \\ \phi &= 2\pi\gamma, \end{aligned} \qquad (1)$$

where γ is a random number unoformly distributed between 0 and 1. The cross-section for elastic collisions were taken from [7].

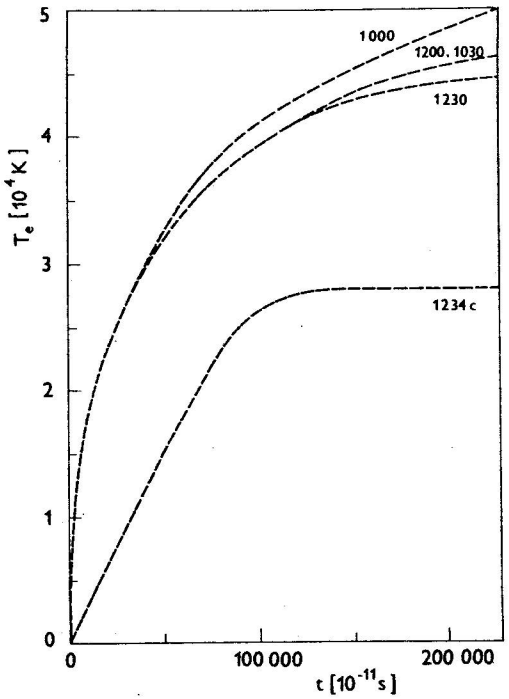

Fig. 1a. The time dependence of mean energies of electron distributions for various combinations of scattering mechanism.

During the excitation collision an electron loses one part of its energy corresponding to the excitation energy of a gas atom (11.55 eV for Ar - one level only, the stepwise processes are not taken into account). The direction of the electron after this interaction is generated again according to the relation (1) with velocity v corresponding to the resultant electron energy.

At the ionization collision an electron loses an energy corresponding to the ionization potential of gas (15.76 eV for Ar). The process of generation of a new electron after this collision is simulated (according to our assumption about the constant number of electrons in the model) in such a way that the remaining energy of the scattered electron will be shared randomly with another electron from our test group of electrons. The isotropic angular scattering was again generated by the relations (1) and the corss-sections for inelastic collisions were taken from [7] and [8].

The electron-electron collision is described according to [4] and [5] by the

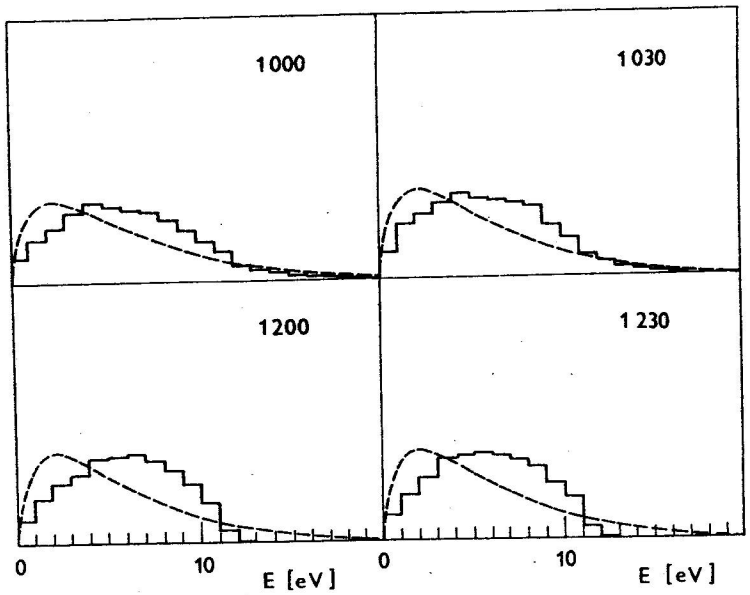

Fig. 1b. The energy distributions of electrons at the time t=250000 time steps and the Maxwellian distributions with the same electron temperature (dotted lines).

quadratic dependence of the cross-section on the reciprocal value of energy E, K/E^2, K being parameter of the model. This collision was treated with the help of the Monte Carlo method, too, i.e. an electron after the electron-electron collision shares its energy randomly with another electron from the test group and its direction is randomly generated by the relation (1).

III. COMPUTER EXPERIMENT

The group of electrons (typically 10^3 to 10^4 - the minimum number from the point of view of statistical noise) was randomly generated in the 2D or 3D working area with cyclic boundary conditions. The initial velocities of electrons were generated according to the Maxwellian distribution with a given temperature (typically 300 K). The trajectories of electrons in the external electric field were calculated by means of the *constant time step method* with the elementary time step 1×10^{-11}s. As stated above, the interactions of electrons were treated by the Monte Carlo method (e.g. [9]) with some new techniques for a better convergence [4], [10]. For an easier evaluation of individual scattering events the *null collision*

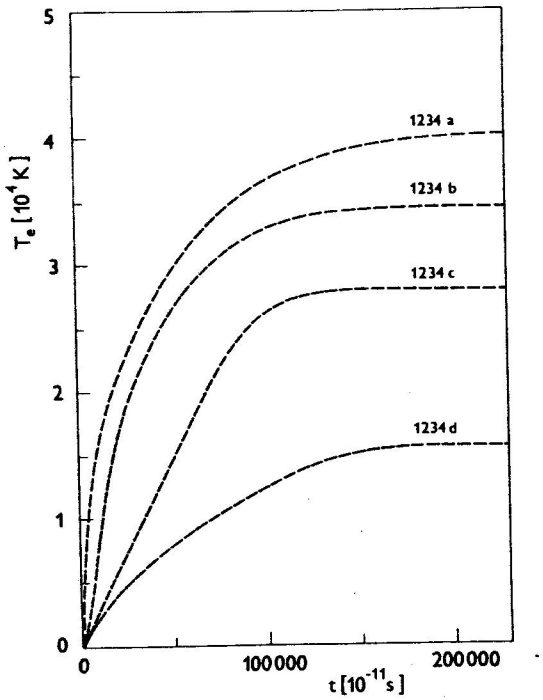

Fig. 2a. The time dependence of electron temperatures for the combination of collisions {1234} and four values of intensity of electron-electron interaction a–d.

method with the total cross-section 30×10^{-16} cm^2 was applied. All the electrons in the test group were processed simultaneously.

The program was prepared in the FORTRAN 77 language and processed by the microcomputer.

IV. RESULTS

The simulation was performed for the Ar and the Ne plasma. The results presented in this contribution are based on the experimental data derived for the Ar plasma (pressure 1 Torr, electric field 3 V/cm - except for Fir. 4, gas temperature 300 K).

We prepared several sets of model data with various combinations of electron scattering mechanisms (1–4) and in the case of electron-electron interactions with their various intensities described by the parameter K. The range of K parameters

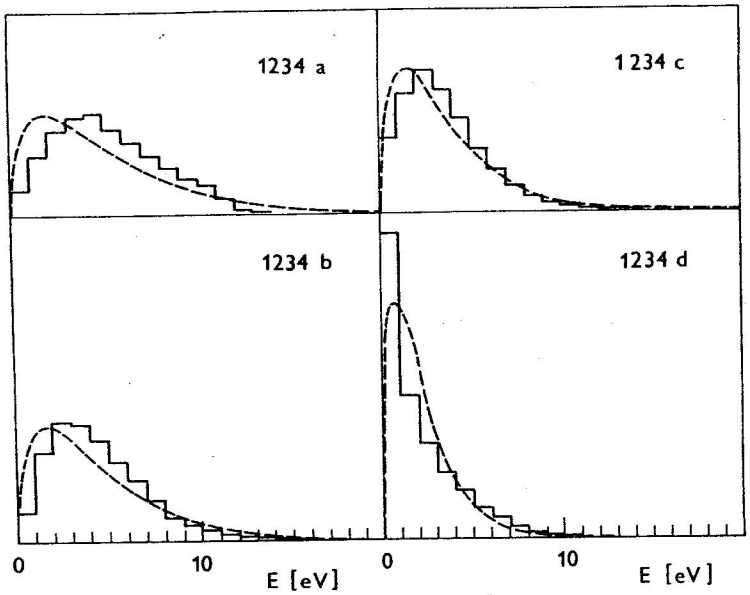

Fig. 2b. The steady-state energy distributions and the corresponding Maxwellian distributions.

extended from 1×10^{-17} cm^{2}eV^2 to 1×10^{-14} cm^{2}eV^2. In the following figures the used combinations of scattering processes are described by their numbers (e.g. {1230}, {1000}, {1234*b*}), where 0 denotes the missing kind of interactions and the letter a – d the intensity of electron-electron interacion:

$$\begin{aligned} a: q_{e-e} &= 1 \times 10^{-17}/E^2 \text{cm}^2\text{eV}^2 \\ b: &\quad 1 \times 10^{-16}/E^2 \\ c: &\quad 1 \times 10^{-15}/E^2 \\ d: &\quad 1 \times 10^{-14}/E^2 \end{aligned}$$

Fig. 1a brings the time dependencies of the mean energies of electrons (expressed by the equivalent electron temperature T_e) for various scattering events. In Fig. 1b the energy distributions of these electrons evaluated at the time equal to 250000 time steps are shown together with the corresponding Maxwellian distributions calculated for the same temperature. It can be seen that except for the single elastic interactions {1000}, the energy distributions do not maintain the high energy parts, which are presented in the Maxwellian distribution. The case of elastic interactions {1000} is not applicable, either as the electron temperature

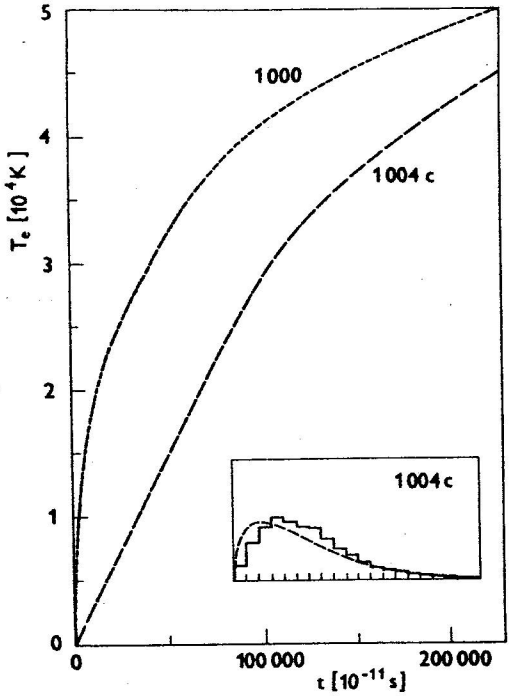

Fig. 3. The time dependence of electron temperatures for the combination of collisions {1004} and its (not stable) energy distribution for t=250000 time steps.

T_e can never stabilize.

From the physical considerations it is clear that the realistic scattering mechanisms must be created by the combination of elastic and electron-electron interactions. Good results can be obtained with the combination of all four processes - Fig. 2, while the influence of a smaller number of interactions is not sufficient, either for the derivation of the steady-state energy distributions (e.g. combinations {1204}, {1034}) or for the stabilization of rising electron temperature (combination {1004} - Fig. 3). From Fig. 2b it can be seen that the best correspondence with the Maxwellian distribution is achieved for the combination {1234} with a rather large intensity of electron-electron interactions - with parameter K between 10^{-15} and 10^{-14}cm^{2}eV^2].

Fig. 4 shows the influence of the electric field on the best combination of interactions {1234}. The corresponding steady- state energy distributions will remain Maxwellian for all tested values of field F.

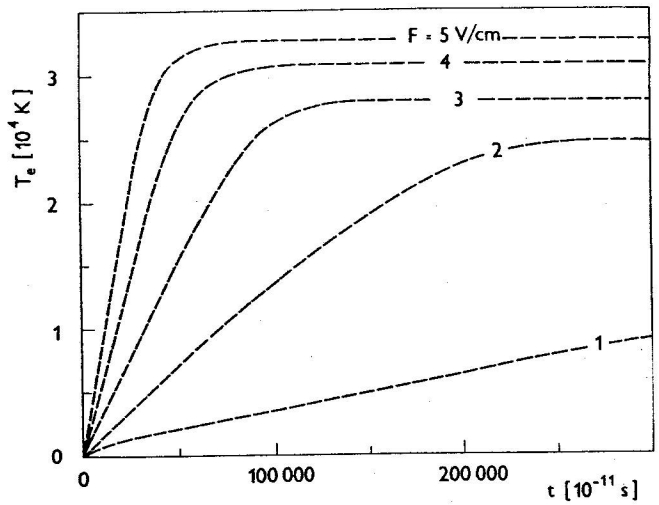

Fig. 4. The time dependence of electron temperatures for the combination of collisions {1234c} for various values of electric fields F.

All the energy distributions were generated from the starting electron temperature T_e=300 K. When the initial temperature is higher, the time necessary for its stabilization will decrease [3] and the modelling will be more efficient.

V. CONCLUSIONS

From our computer experiment it follows that for purposes of a realistic modelling of probe characteristics, when a simple model of inert gas plasma must be used as an electron source, the simulation is very time consuming even in its simple form. It is necessary, therefore, to generate electrons with the right combination of interactions and with the right initial electron temperature. The best minimal combination of scattering processes in argon plasma is the elastic interaction, excitation, ionization and intensive electron-electron interaction.

A further modification of our model (inclusion of drift velocities, non-Maxwellian distributions, etc.) is in progress.

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Received October 18th 1990
Accepted for Publication February 1st, 1991

ИССЛЕДОВАНИЕ ПРОЦЕССОВ СОУДАРЕНИЙ В ПОЛОЖИТЕЛНОМ СТОЛЬБЦЕ ТЛЕЮЩЕГО РАЗРЯДА В КОМПЮТЕРНОМ ЭКСПЕРИМЕНТЕ

В работе приводится компютерный эксперимент симулирования процессов в слабо ионизированной плазме. Полученные результаты дают сведения о влиянии отдельных элементарных процессов на характеристике плазмы, что позволяет построить простую модель плазмы инертного газа. Критерии качественной менравности модели является максвелловское распределение энергии электронов. Симулирование, основанное на эксперименталных данных плазмы аргона показывает, что упругое рассеяние, одноуровневое возбуждение, ионизация и сильное электронное взаимодействие оказывается минимальным набором механизмов рассеяния.