

Modelling of chemical reactions in plasma

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Abstract. The paper is devoted to theoretical investigation of interaction of pulsed high current electron beam with gas substance. As a result of the interaction the formation of chemical active plasma can be observed. One of the key parameter for theoretical analyze of the process is the electron distribution function. Within the framework of the Boltzmann approach we obtained the dynamical equation for electron distribution function depending on the electron energy, coordinate and time.

1. Introduction

The influence of concentrated of energy fluxes on the gas substance attracts the interest of many theoretical groups [1-9]. As a source of the energy fluxes it is often used the discharge and lasers. The action time of the energy fluxes is small ($\approx 10^{-3} - 10^{-6}$ sec) compared with typical time of physical and chemical processes in created plasma ($10^{-7} - 10^{-12}$ sec). In these cases the stationary equations for describing the electron distribution function (EDF) is applicable [1, 2, 4, 6, 8].

Another method of action on gas is the using of pulsed high current electron beams [10]. The pulsed duration of such accelerators is nearly $10^{-6} - 10^{-10}$ sec and the power flow of $10^6 - 10^9$ W/cm². Under the action of the beams on a chemical active gas the nonequilibrium plasma is formed. Note that the physical and chemical processes occur simultaneously with spreading of beam. In this case the stationary describing is not applicable. Moreover, the concentration of chemical active particles changes significantly for small time interval. In addition if one use the power flow of $10^6 - 10^9$ W/cm² the priority and rates of physical and chemical processes are changed.

In present paper we obtained the dynamical equation for time evolution of EDF based on the Boltzmann equation. The equation allows investigating the electron beam spreading in the gas substance.

2. Boltzmann equation

The time evolution of electron distribution function $f = f(\vec{r}, \vec{v}, t)$ in the space of the coordinates \vec{r} and the velocities \vec{v} is described by means of Boltzmann equation

$$\frac{\partial f}{\partial t} + \vec{v} \nabla_r f + \frac{\vec{F}}{m} \nabla_v f = \left(\frac{\delta f}{\delta t} \right), \quad (1)$$



where e , m are the elementary charge and mass of electron respectively, \vec{F} is the electromagnetic force created by beam electrons, $(\delta f / \delta t)$ is the collision integral. Under the assumption of weak anisotropy it can be used a Legendre polynomial expansion P_n for EDF [1]

$$f = \sum_{n=0}^{\infty} f_n P_n \left(\frac{\vec{v}}{v} \right). \quad (2)$$

Inserting in Boltzmann equation (1) the expansion (2) to first order the second term is written as

$$\vec{v} \nabla_r f = \vec{v} \left(\frac{\vec{r}}{r} \frac{\partial f_0}{\partial r} + \frac{\vec{v}}{v} \frac{\vec{r}}{r} \frac{\partial \vec{f}_1}{\partial r} \right), \quad (3)$$

and the second term is

$$\frac{\vec{F}}{m} \nabla_v f = \frac{\vec{F}}{m} \left[\frac{\vec{v}}{v} \frac{\partial f_0}{\partial v} + \frac{1}{3v^2} \frac{\partial}{\partial v} (v^2 \vec{f}_1) \right], \quad (4)$$

where f_0 , f_1 are the isotropic and anisotropic parts of EDF respectively. Thereby, after EDF expansion the (1) can be represented as the two equations for zero and first order of velocity

$$\begin{cases} \frac{\partial f_0}{\partial t} + \frac{v}{3} \frac{\vec{r}}{r} \frac{\partial \vec{f}_1}{\partial r} + \frac{\vec{F}}{3mv^2} \frac{\partial}{\partial v} (v^2 \vec{f}_1) = \left(\frac{\delta f_0}{\delta t} \right) \\ v^{-1} \frac{\partial \vec{f}_1}{\partial t} + \frac{\vec{r}}{r} \frac{\partial f_0}{\partial r} + \frac{\vec{F}}{mv} \frac{\partial f_0}{\partial v} = v^{-1} \left(\frac{\delta \vec{f}_1}{\delta t} \right) \end{cases}. \quad (5 \text{ a, b})$$

3. Dynamical equation

The left part of (5b) after substitution (2) is written as

$$\left(\frac{\delta \vec{f}_1}{\delta t} \right) = -v \vec{f}_1 \cdot \sum_k N_k(t) \left[Q_{el}^k(v) + \sum_j Q_{inel}^{jk}(v) \right], \quad (6)$$

where $N_k(t)$ is the time function of molecular concentration of various sorts k , Q_{el}^k is the cross section of elastic interaction between electrons and k -molecules, Q_{inel}^{jk} is the cross section of j -type inelastic interaction. For obtaining (6) we supposed that the decreasing velocity of f_1 is proportional to the collision frequency between electrons and molecules. Substituting the (6) in (5 b) it is gets

$$v^{-1} \frac{\partial \vec{f}_1}{\partial t} + \frac{\vec{r}}{r} \frac{\partial f_0}{\partial r} + \frac{\vec{F}}{mv} \frac{\partial f_0}{\partial v} = -\vec{f}_1 H(v, t), \quad (7)$$

$$H(v, t) = \sum_k N_k(t) \left[Q_{el}^k(v) + \sum_j Q_{inel}^{jk}(v) \right], \quad (8)$$

The solution of the differential equation (8) is

$$\vec{f}_1 = \left[\mathbf{v} \frac{\vec{r}}{r} \frac{\partial f_0}{\partial r} + \frac{\vec{F}}{m} \frac{\partial f_0}{\partial \mathbf{v}} \right] (H\mathbf{v})^{-1} + \exp(-H\mathbf{v}t). \quad (9)$$

The second term can be neglected because the $H\mathbf{v}$ has the order of magnitude is nearly 10^{-12} sec that ever for pulsed regime (10^{-7} sec) is very small time. Then the (9) is rewritten

$$\vec{f}_1 = \left[\mathbf{v} \frac{\vec{r}}{r} \frac{\partial f_0}{\partial r} + \frac{\vec{F}}{m} \frac{\partial f_0}{\partial \mathbf{v}} \right] (H\mathbf{v})^{-1}. \quad (10)$$

Substituting the (10) in the (5 a) we get

$$\frac{\partial f_0}{\partial t} + \frac{1}{3H} \frac{\vec{r}}{r} \frac{\partial}{\partial r} \left[\mathbf{v} \frac{\vec{r}}{r} \frac{\partial f_0}{\partial r} + \frac{\vec{F}}{m} \frac{\partial f_0}{\partial \mathbf{v}} \right] + \frac{\vec{F}}{3m\mathbf{v}^2} \frac{\partial}{\partial \mathbf{v}} \left[\mathbf{v} \left(\mathbf{v} \frac{\vec{r}}{r} \frac{\partial f_0}{\partial r} + \frac{\vec{F}}{m} \frac{\partial f_0}{\partial \mathbf{v}} \right) \right] = \left(\frac{\delta f_0}{\delta t} \right). \quad (11)$$

For convenient let us transform from velocity space to energy space $u = m\mathbf{v}^2 / 2e$, where $\partial / \partial \mathbf{v} = m\mathbf{v}e^{-1} \partial / \partial u$ [2]. Then dynamical equation (11) can be rewritten as

$$\frac{\partial f_0}{\partial t} + \frac{1}{3H} \sqrt{\frac{2u}{m}} \frac{\vec{r}}{r} \frac{\partial}{\partial r} \left[\sqrt{e} \frac{\vec{r}}{r} \frac{\partial f_0}{\partial r} + \frac{\vec{F}}{\sqrt{e}} \frac{\partial f_0}{\partial u} \right] + \frac{\vec{F}}{3e} \sqrt{\frac{2}{mu}} \frac{\partial}{\partial u} \left[\frac{u}{H} \left(\sqrt{e} \frac{\vec{r}}{r} \frac{\partial f_0}{\partial r} + \frac{\vec{F}}{\sqrt{e}} \frac{\partial f_0}{\partial u} \right) \right] = \left(\frac{\delta f_0}{\delta t} \right). \quad (12)$$

The right path of the equation (12) contains the inelastic and the hyper elastic terms

$$\left(\frac{\delta f_0}{\delta t} \right) = \left(\frac{\delta f_0}{\delta t} \right)_{inel} + \left(\frac{\delta f_0}{\delta t} \right)_{hyperl}. \quad (13)$$

In work [2] the relation for the inelastic term was derived. We have generalized this relation for the time dependent case and have obtained the relation for hyper elastic term

$$\left(\frac{\delta f_0}{\delta t} \right)_{inel} = \sqrt{\frac{2e}{mu}} \sum_j \sum_k \left[(u + u_{jk}) f_0(u + u_{jk}) N_k(t) Q_{inel}^{jk}(u + u_{jk}) - u f_0(u) N_k(t) Q_{inel}^{jk}(u) \right], \quad (14)$$

$$\left(\frac{\delta f_0}{\delta t} \right)_{hyperl} = \sqrt{\frac{2e}{mu}} \sum_j \sum_k \left[(u + u_{jk}) f_0(u + u_{jk}) N_{jk}(t) Q_{inel}^{(-j)k}(u + u_{jk}) - u f_0(u) N_{jk}(t) Q_{inel}^{(-j)k}(u) \right]. \quad (15)$$

where u_{jk} is the energy of j -type excitation state of k -molecule, $N_{jk}(t)$ is the time function of molecular concentration of various sorts k at the j -type excitation state. The cross section of the hyper elastic collisions is related with the Q_{inel}^{jk} by means of the ratio

$$Q_{inel}^{(-j)k} = \frac{u + u_{jk}}{u} Q_{inel}^{jk}(u + u_{jk}). \quad (16)$$

4. Correspondence principle

The relations (12)-(15) are described the time evolution of electron distribution function. The main features are the possibilities to imply the equation (12) for the gas substance and the time dependence of the concentration of molecules at the various stages: ground and excited. If in (12) we eliminate the mixed derivatives, the coordinate and time dependences in (14) and (15) we obtain the “classical” formulae derived by W.L. Nighan [2].

5. Conclusion

The dynamical equation for describing of spreading process of pulsed high current electron beam in a gas substance is obtained. The relation was derived by using Boltzmann equation. The time dependence of chemical active particle concentration is a main feature of the dynamical equation. It is argued that the obtaining relation in limit case transform to the equation previously received in other works.

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