Collision Simulation in plasma Sheath Using the Monte Carlo Technic

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In this work we studied the collisions in the sheath and their influence on the energy transferred to the cathode by Monte carlo simulation .The comparison between results obtained by Monte Carlo simulation and those obtained by simulation of Runge Kutta is carried out. We stadied too the influence of the collision on the erosion of the cathode, and we give a technique to calculate the energy of vaporisation

Introduction :

The Monte Carlo method is a statistical approach allowing the resolution of deterministic and probabilistic behavior equations. The use of Monte Carlo technique is not limited to physics, and even less with the modeling of the discharges .The calculation of the number π, with the more lucrative determination of the probabilities of gaining with the plays of hazard, It was the subject of several uses, the evolution of informatic lasting these thirty last years y having fully contributed.

The use of this method in plasma physics allowed the development of particulate models, simulating the behavior of plasma following a microscopic approach, in opposition to models namely <<fluides > > which treat homogeneous plasma like a fluid by characterizing it by averages sizes. The Monte Carlo simulation of a whole of ions or electrons present in a gas in which they make collisions and undergoing a force due to the electric field, makes it possible to follow the temporal evolution of this group of particles in the phase space .This method is based on the generation of random numbers making it possible to recreate a sequence of real events, such as for example the movement of a particle .The Monte Carlo simulation is based on the generation of the random numbers by of the simple algorithms making it possible to create sequences of rational numbers ranging between 0 and 1[8,1,.

plasma Sheath: When a plasma is limited by a border (for example a metalic wall), it is formed around this border a "sheath" where the properties of plasma are different. In general, the sheath is not electrically neutral, there is often a surplus of electrons and ions . The electric potential can vary in an abrupt way through the sheath of plasma. The thickness of the sheath of plasma is typically about the length of Debye[6][7].

In this paper we focus on the modeling and simulation of plasma processes particulary simulation collision in sheath using the technical Monte Carlo simulation.Our aim is the study the effect of collision on energy transferred from thermal plasma to cathode surface through espace sheath and determine the rate of ionization Ki .

In section I we write the governing equations in sheath .In section II we review the concept of technical Monte Carlo simulation and in section III ,we give the results of simulation and comments.

CONTINUUM MODELS : If the neutral-gas pressure is sufficiently high, collisional processes dominate the dynamics of the plasma. To model such a plasma, drift-diffusion equations are widely used. The drift-diffusion equations are "reduced" equations derived from the well-known fluid equations (i.e., mass- and momentum-conservation laws) for ions and electrons under the assumption of high collision frequencies. For example, the momentum-conservation law for electrons may be written as[5,3]

$m_e n_e (\partial_t \underline{\mathbf{v}}_e + \underline{\mathbf{v}}_e \cdot \nabla \underline{\mathbf{v}}_e) = -\nabla \underline{\mathbf{p}}_e - e n_e \underline{\mathbf{E}} - m_e n_e \nu_e \underline{\mathbf{v}}_e$ (1)

$m_i n_i (\partial_t \underline{\mathbf{v}}_i + \underline{\mathbf{v}}_i \cdot \nabla \underline{\mathbf{v}}_i) = -\nabla \underline{\mathbf{p}}_i + e n \underline{\mathbf{E}} - m_i n_i \nu_i \underline{\mathbf{v}}_i$ (2)

where m_e is the electron mass, n_e is the electron density, $\underline{\mathbf{v}}_e$ is the electron "fluid" (drift) velocity, pe is the electron fluid pressure, $\underline{\mathbf{E}}$ is the electric field, and e is the electron collision frequency at which the plasma electrons collide with the neutral gas molecules. Electron-ion collisions are negligible compared with electron-neutral collisions in a high-pressure plasma. If the inertia term (i.e., the left-hand side) of Equation (1) and (2) is negligibly small, we obtain

$\underline{\mathbf{v}}_e = - \nabla \underline{\mathbf{p}}_e / m_e n_e \nu_e - e\underline{\mathbf{E}} / m_e \nu_e .$ (1')

$\underline{\mathbf{v}}_i = - \nabla \underline{\mathbf{p}}_i / m_i n_i \nu_i + e\underline{\mathbf{E}} / m_i \nu_i .$ (2')

Equation (2) states that $\underline{\mathbf{v}}_e$ is determined by the balance among the pressure force, electrostatic force, and drag force. The electron flux $\underline{\mathbf{\Gamma}}_e = n_e \underline{\mathbf{v}}_e$ is then given by

$\underline{\mathbf{\Gamma}}_e = -n_e \mu_e \underline{\mathbf{E}} - \nabla (D_e n_e),$ (3)

where $\mu_e = e/m\nu_e$ is the electron mobility and $D_e = k_B T_e / m_e \nu_e$ is the electron diffusivity. The equation of state $\mathbf{p}_e = n_e k_B T_e$ was also used. The relation $D_e/\mu_e = k_B T_e/e$ is known as the Einstein relation. Similarly, the ion drift velocity $\underline{\mathbf{v}}_i$ and ion flux $\underline{\mathbf{\Gamma}}i = n_i \underline{\mathbf{v}}_i$ can be expressed as

$\underline{\mathbf{\Gamma}}_i = n_i \mu_i \underline{\mathbf{E}} - \nabla (D_i n_i)$ (4)

where μi = Zi e/m_i ν_i is the ion mobility, Z_i e and ν_i are the ion charge and ion-neutral collision

frequencies, and $D_i = k_B T_i / m_i \nu i$ is the ion diffusivity.

If the values of the mobilities and diffusivities are given, we need equations only for the electron and ion densities, n_e and n_i, and the electric field **E** to close the system. This can be achieved by using the mass conservation laws and Poisson's equation:

$$\partial_t n_e + \nabla \bullet \underline{\Gamma}_e = S_e \qquad (5)$$

$$n_i + \nabla \bullet \underline{\Gamma}_i = S_i \qquad (6)$$

$$\Delta\Phi = - e (Z_i n_i - n_e)/\varepsilon_0. \qquad (7)$$

In Equations (5) and (6), S_e and S_i denote the source terms for the electrons and ions, to be discussed below. In Poisson's equation (7), denotes the electrostatic potential, i.e., $E = -\nabla\Phi$. Equations (5)-(7), together with Equations (3) and (4), constitute the drift-diffusion equations for the system. Although we have considered only single-ion species, it is straightforward to extend Equations (5)-(7) to those for the systems of multi-ion species, including negative ions.

Sources and sinks of electrons and ions in the bulk plasma are usually due to ionization, recombination, electron attachment, and charge exchange. In the case of electropositive discharges with single-ion species, we may write :

$$S_e = S_i = k_i n_e n_n - k_r n_i n_e \qquad (8)$$

where k_i and k_r are ionization and recombination rate coefficients. (In general, $S_e \neq S_i$, especially for electronegative plasmas. See for example References [10-12].) As is well known, there is a threshold energy E_{th} for ionization, and the ionization rate coefficient depends on the electron temperature Te. It is often assumed that the electron temperature dependence of the ionization rate coefficient is given by the Arrhenius relation, i.e.,

$$ki = Ai \exp(- Eth/ k_B Te) \qquad (9)$$

where Ai is a constant. For example, for argon, which is commonly used in plasma processing, Ai ≈1 x 10-14 m^3/s.

The particle transport (e ; ion) in a gas under the influence on an electric E can be simulated with the help of a Monte Carlo method from an initially great number of seed electrons. These primary ions are treated one by on from their creation until their disappearance out of the domain of the simulation or by specific collisional processes. Every ion, during its transit in the gas, performs a succession of free flights punctuated by elastic, inelastic, or superlastic collisions with molecules of gas defined by collisions cross sections.

During the successive collisions for every ion, certain, information (velocity, position, etc.) is stored in order to calculate, from appropriate sampling methods, distribution functions and transport coefficients.

The flow chart of Monte Carlo method described here-after is shown in Fig.1. As it can be seen, after definitions of the simulation parameters, the gas, and the initial conditioned, it is necessary to know first the time of free flight.

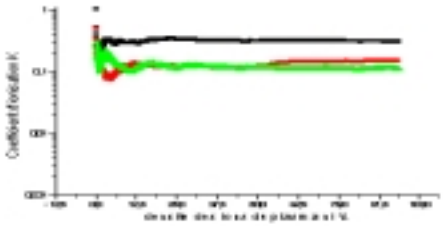

figure 1 : le coefficient d'ionisation pour 3 frequences de collisions 10^{-7} $0.5*10^{-7}$and $0.8*10^{-7}$nous remarquons que la precision de la technique de monte carlo augmente avec le nombre des ions emis du plasma

Time of free flight t_{flight} : The time of free flight is calculated by using the null collision method initially developed by Skullerud [2] for simulation of ion motion in gasses and then used by numerous authors[3] :

$$t_{fliight} = -\frac{ln(r_{flight})}{\upsilon_{tot}}, \qquad (10)$$

where $\mathbf{r_{flight}}$ is a random number uniformly distributed in the [0 ;1] range and $\boldsymbol{\upsilon_{tot}}$ is the total collision frequency including total ion-particle collision frequency $\boldsymbol{\upsilon}$ and a null collision frequency υ_{null} chosen in order to have always υ_{tot} constant :

$$\upsilon_{tot} = \upsilon + \upsilon_{null} = \text{const} \qquad (11)$$

Trajectory between two successive collisions **:**The trajectory between two successive collisions is obtained from the classical mechanic equations. In the from work of this paper, the electric field accelerating ions (with charge +e, mass m, position r, and velocity v) is assumed to be antiparallel to the z axis. Under these conditions, the components v_{x1}, v_{y1}, and v_{z1} in the laboratory frame of velocity $v_1(t_1)$ at time t_1 at the end of the free flight can be written as a function of velocity $v_0(t_0)$ (at initial time t_0 and with components v_{x0}, v_{y0}, and v_{z0} in the laboratory frame). Then, new co-ordinates $r_1(x_1,y_1,z_1)$ of ion at time t_1 can be calculated from co-ordinates $r_0(x_0,y_0,z_0)$ of an ion at time t_0 :

$$x_1 = x_0 + v_{x0}\, \mathbf{t_{fligh}}$$

$$y_1 = y_0 + v_{y0}\, \mathbf{t_{flight}}, \qquad \mathbf{(12)}$$

$$z_1 = z_0 + v_{z0} t_{fliight} + \frac{1}{2}\frac{eE_z}{m} t_{flight}^2$$

with $\mathbf{t_{flight} = t_1 - t_0}$

So, starting from the ion parameters t_0, v_0, r_0 at the beginning of the free flight, the new ion parameters

t_1, v_1, r_1 at the end of the free flight are obtained, respectively, from relation (1) and classical mechanic equations. Then just after collision occurring at time t1, ion parameters become t'_1, v'_1, r'_1. However, it is necessary to calculate only ion velocity v'_1 because the ion-particle interaction is assumed to be instantaneous ($t'_1 = t_1$) and local ($r'_1 = r_1$). In order to calculate the velocity v'_1, it is necessary to know the collision type.

Type of collision : The collision type necessities knowledge of the likelihood's ($p_{col,el}$, $p_{trasf,ch}$,p_{ion}, or $p_{col,null}$) of the occurrence of every collision kind (elastic, transfert of the charge, ionisation , or null) .

Simulation :

The cross section used for for frontal collision(transfert of the charge) is given by the relation proposed by Phelps 9:

$$\sigma_b = 1/2\left\{A\varepsilon_i^{-0.1}\left(1+B/\varepsilon_i\right)^{0.6} - \left[\frac{C}{\varepsilon_i^{0.5}\left(1+\varepsilon_i\right)} + \frac{D\varepsilon_i}{\left(1+\varepsilon_i/3\right)^2}\right]\right\}$$

where A= 1.15 10^{-18} , B=0.015, C= 2 10^{-19} , D= 3 10^{-19} , ε_I the energy (eV) of the ion.

For the elastic collision we are used the relation:

$$\sigma_i = \left[\frac{C}{\varepsilon_i^{0.5}\left(1+\varepsilon_i\right)} + \frac{D\varepsilon_i}{\left(1+\varepsilon_i/3\right)^2}\right]$$

where C= 2 10^{-19} , D= 3 10^{-19}.

For the ionization we are useed the interpolation of the cross section given by Phelps:

$$\sigma = A + B\varepsilon_i + C\varepsilon_i^2$$

where A = -209.99044 10^{-23} , B = 4,8335225 10^{-23}, C = -0.0020614624 10^{-23}.

Comments and Conclusion : The figure(1) represent the results of variation of energy of ion versus the distance between through the sheath obtained by Runge Kutta simulation whileThe figure2 represent the same of variation of energy of ion versus the distance between through the sheath obtained by Monte Carlo simulation.The results of energy variation for two technic (Monte Carlo simulation and Runge Kutta simulation)are in good agreement.

We have also calculated using our simulation the rate ionisation in sheath K_i.The slope of curve(figure 3) is proportional to value of K_i.We have found for K_i at order of the 10^{-16}.This value is in agreement with the theoritical result[5,3].

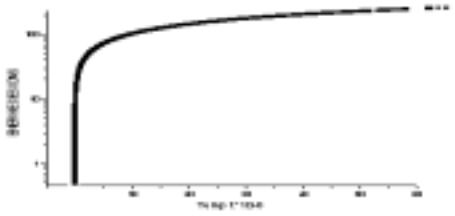

Figure 2 : variation de l'energie des ions dans la Gaine avec le temps.

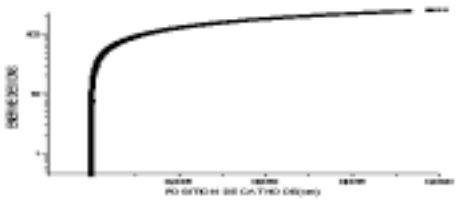

Figure 3 : variation de l'energie des ions dans la Gaine avec la position du gaine.

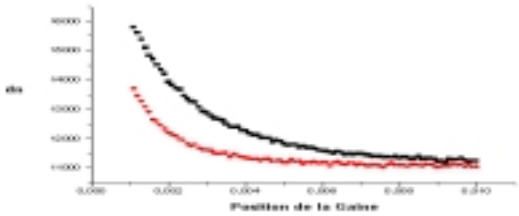

Figure 4 : variation de la densité des ions dans la Gaine avec la distance au cathode.

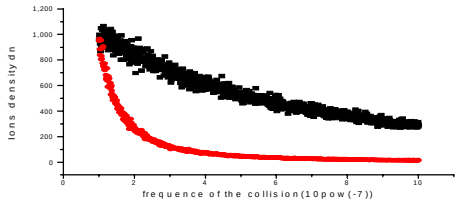

Figure 5 : variation de la densité des ions dans la Gaine avec la frequnce des collisions.

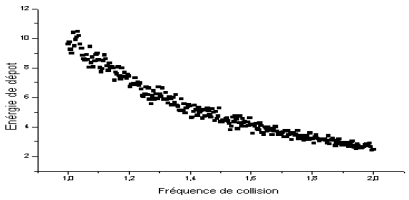

Figure 6 : variation de l'energie de dépôt sur la cathode avec la frequence de collision.

References

[1] Monte carlo models of electron and ion transport in non-equilibrium plasmas Savino Longo Elsvier 200-213 2000

[2] Self-consistent monte Carlo simulation of the Dc positive column in Argon Vasilii hakhovski, Katssunobu Nishihara and Takeshi Arakawa Rev. Sci. Instrum. 50 ,210 1999

[3] A model of the cathode of atmospheric pressure arcs M.S. Benilov and A.Marotta Qebec 2000

[4] Calculated gas temperature profiles glow disharges I.Revel, L.C.Pitch ford,and J.P.Bœuf

Journal of applied physics , Vol 88 N° 5 (2000).
[5] Modeling and simulation methods for plasma processing S.Hamaguchi IBM Journal of Research &Development Vol .43 N0 1-2 Plasma processing 1999
[6] Theory of sheath in a collisional multi-componenet plasma M.K.Mahanta and K.S Goswami Pramana Journal of Physics Vol 56 N04 April 2001 pp 579-584
[7] Modeling of plasma sheath D.Saifaoui Plasma technology and applications Fac Sc-Ain Chock July 2001
[8] Monte carlo Simulation of electron swarms at low reduced electric fields M.Yousf,A Hennad and A.Alkaa Physical Review E Vol 49 N0 4 April 1994
[9]A. V Phelps, "the application of scattering cross sections to ion flux models in discharge sheath", J. Appl, Phys. 76(2), 747-753 (1994)

MONTE CARLO METHOD :
Flow chart for Monte Carlo :