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Secondary electrons photoemission in PF breakdown

In Plasma Focus (PF) devices electrical breakdown, the first avalanche ionization phase leads the system to the formation of a plasma seed by the cathode-insulator junction: this results only in a pre-breakdown mechanism. In order to simulate the evolution of the system towards the final plasma sheath configuration, a further mechanism of free charges production is needed, leading to a greater ionization degree of the filling gas. Such a mechanism was found to be supplied by secondary electrons photoemission from cathode: during the plasma seed formation, electrons colliding with gas neutral molecules produce an excited molecules spatial distribution. The de-excitation process of this population leads to a photons production rate delayed in time, which is responsible of the secondary emission of electrons from cathode.
A description of the photoemission mechanism is briefly presented, together with a detailed study of the excited molecules distribution and of a spatial map for cathode sight factor.

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Abstract

In Plasma Focus (PF) devices electrical breakdown, the first avalanche ionization phase leads the system to the formation of a plasma seed by the cathode-insulator junction: this results only in a pre-breakdown mechanism. In order to simulate the evolution of the system towards the final plasma sheath configuration, a further mechanism of free charges production is needed, leading to a greater ionization degree of the filling gas. Such a mechanism was found to be supplied by secondary electrons photoemission from cathode: during the plasma seed formation, electrons colliding with gas neutral molecules produce an excited molecules spatial distribution. The de-excitation process of this population leads to a photons production rate delayed in time, which is responsible of the secondary emission of electrons from cathode.
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Contents

1 Introduction

The aim at simulating the PF discharge initial stage, the electrical breakdown of the gas filling the device chamber, is devoted to a better understanding of the phase-space description of the plasma sheath used as initial condition for well-known snowplow codes, used both to design and optimize PF devices.

The standard mechanism of bulk ionization via electron impact on gas neutral molecules was found [1] to produce only an initial low-density plasma seed: the fast electrons indeed reach very quickly ($10 \div 12$ ns) energies of several tens of eV, at which the collision cross sections (and the ionization one in particular) decrease making the runaway effects – by absorption on both the anode and the dielectric sleeve – predominant. A Secondary Electrons Emission (SEE) mechanism is therefore necessary to take the process toward the complete plasma sheath formation.

The classical SEE by ion impact is negligible at the first stages of a discharge development, due to both the low mobility of the heavy ions with respect to the electrons one, and the short times proper of highly overvoltaged breakdown phenomena. Preliminary estimations indeed show that the mean time needed for an ion, created in the region of highest electric field, to impinge on the cathode is greater than tens of nanoseconds: referring to the numerical values of the case of study [1, 2], if collisions are neglected and a rise rate of 10^{11} Vs^{-1} is assumed for an uniform planar gap of $d = 1$ cm, the time-to-impact of an initially stationary ion can be evaluated as $t = \sqrt[3]{6md/(qE_{0,t})}$ $\sim 10^{-7}$ s. First simulations [1] confirmed the result showing only spurious secondary emissions due to ion impacts, which lead to a non-continuity between the sheath and the cathode preventing the electrode short-circuiting.

Since experimental data predict characteristic closure times of the order of tens of nanoseconds, an alternative mean of electrons emission from the cathode had to be investigated. It can be therefore noticed that every inelastic collision of electrons with neutral gas molecules is followed by the emission of a photon which impacts either the electrodes or the dielectric walls. Such photon may be responsible of the emission of a secondary electron by means of the so called photoelectric effect [3, 4, 5], providing a possible alternative SEE mechanism. The hypothesis of internal excited states decay as source of secondary electrons, as proposed by Blagoev [6], has been recently confirmed [7].

2 The physical model

The de-excitation of a molecule previously excited by electron inelastic impact to a specific excited level l is a stochastic phenomenon characterized by the isotropic emission of a photon with energy $\mathcal{E}_{\mathrm{ph}}$, and vacuum radiative decay time τ, which depend only on the molecule species and the involved excitation type of the latter.

The emitted photon will travel roughly unperturbed in the background gas, due to the low pressure of the medium and to the low attenuation parameter μ (its characteristic energy being of about 10 eV), until it reaches a boundary or an external surface, being absorbed. The emission of free electrons from the boundary surfaces is therefore a function of the excited nuclei population. Since the characteristic times of the electrical discharge of interest are very short (few tens to one hundred ns), the time evolution of the excited state densities can be neglected.

The source of excited states is known from the MCC module which gives the time- and space-dependent inelastic collision rate $\nu_{k,\mathrm{exc}}(\vec{r}, t)$ for each species k:

$$\Delta N_k^+ = (N_k(\vec{r}, t + \Delta t) - N_k(\vec{r}, t))^+ = \nu_{k,\mathrm{exc}}(\vec{r}, t)\Delta t\,.$$

The number of photons emitted at each time step Δt depends on the number of excited molecule $N_k(\vec{r},t)$ and on their characteristic life-time τ_k by the relation

$$\Delta N_k^- = (N_k(\vec{r},t) - N_k(\vec{r},t+\Delta t))^- = -\int_0^{\Delta t} -\frac{N_k}{\tau_k}\exp\left(-\frac{t'}{\tau_k}\right)\,\mathrm{d}t' =$$
$$= -N_k(\vec{r},t)\left(\exp\left(-\frac{\Delta t}{\tau_k}\right)-1\right) \simeq N_k(\vec{r},t)\frac{\Delta t}{\tau_k}\,,$$

where the main approximation is the assumption of a sufficiently small Δt to consider a constant number of excited molecules during Δt and to allow the substitution of the exponential form with its first order series expansion. The net effect in Δt is then

$$\Delta N_k = \Delta N_k^+ - \Delta N_k^-\,,$$

which is summed to $N_k(\vec{r},t)$ to obtain the number of excited states $N_k(\vec{r},t+\Delta t)$ at the next time step.

Beyond the surface the photon loses energy by subsequent interactions with the electrons of the medium. If a single electron receives an energy which overtakes the material work function, the electron is removed from its place within the lattice and travels free in the medium. Unless the electron collides with other electrons or nuclei, losing energy and being captured again, and if its velocity is directed outside the surface it can be emitted towards the reaction chamber as a free charge. This results in an overall emission probability for every surface. To produce an electron through photo-electric effect, therefore, a photon must have at first an energy greater than the work function ϕ of the material on which it collides; the energy depends only on the molecular energy level l involved in the de-excitation as $\mathcal{E}_{\mathrm{ph}} = \mathcal{E}_l - \mathcal{E}_g$, the suffix g denoting the ground state of the molecule, and is fully deterministic. Secondly, assuming an isotropic source of radiation, a "sight-factor" $\Omega(\vec{r},\vec{r}_0)$ will give the portion of photons emitted from $\vec{r}$ and impinging the boundary in $\vec{r}_0$. Lastly, the secondary emission coefficient γ_ν gives the probability of emission of an electron per each photon impacting on the surface. Thus, the number of electrons emitted per de-excitation photon is

$$N_{\mathrm{e}}(\vec{r}_0) = \Omega(\vec{r},\vec{r}_0)\gamma_\nu(\vec{r}_0)\sum_k \Delta N_k^-(\vec{r})\,,$$

where a nearest integer has to be calculated in order to obtain an integer number of electrons.

The generic outcoming electron is isotropically sampled in direction as done for secondary emission by electron or ion impact. Under the hypothesis of a cool emitting surface, the electron energy distribution function is approximately triangular-shaped with $\mathcal{E}_{\mathrm{F}}(T=0)$ as sharp maximum cutoff energy. Once sampled a random number R, the energy is simply given by

$$\int_{r_1}^{r_i} f(r)\,\mathrm{d}r = R\int_{r_1}^{r_2} f(r)\,\mathrm{d}r\,,$$

as $\mathcal{E} = \sqrt{R}\mathcal{E}_{\mathrm{F}}$.

In many cases, the calculation of a precise sight factor is a hard task and a MC ray-tracing procedure is often the only practicable solution. Alternatively, an approximate 0D model

can be used, assuming a generic averaged sight factor for all the excited molecules depending on the expected region of maximum concentration.

3 A rough 0D model

A zero-dimensional model has been developed to take into account an average global effect and to sample, via MC techniques, a source of electrons from the back-wall of the cathode: since the excitation energy threshold is reached at first in the region of highest electric field (the cathode edge on the insulator sleeve) [1], the excited gas atoms or molecules can be thought localized on the insulator sleeve, following the maximum deposited charge on it (mainly given by the more mobile electrons impacting on its surface). This allows to easily calculate a global approximated sight-factor of the cathode wall from such a pointwise isotropic source: as shown in Figure 1, less than one quarter of the photons emitted in 4π are directed towards the wall, depending on the radial and axial position ($r_\nu = r_{\text{int}}, z_\nu$) of the emitting source. Referring to the notations of Figure 1, one can estimate

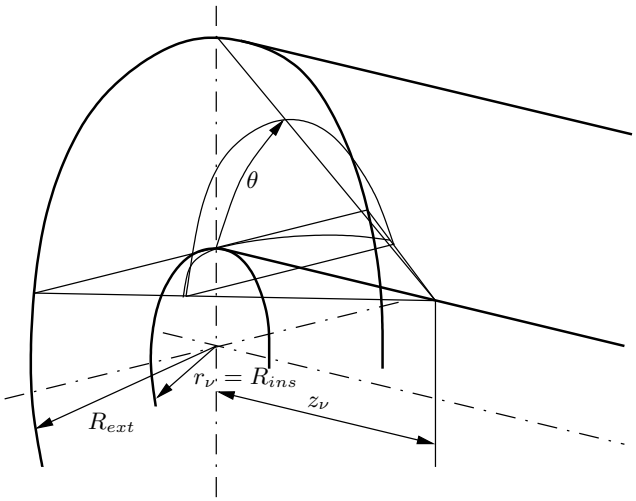

Figure 1: Sketch of the closed end of the electrodes and of the fictitious pointwise isotropic photon source used to estimate a global 0D sight factor.

$$\Omega = \int_0^{\pi} \mathrm{d}\varphi \int_0^{\vartheta_{\max}} \sin\vartheta \,\mathrm{d}\vartheta = \pi \cos\left(\arctan\left(\frac{r_{\text{ext}} - r_{\text{int}}}{z_\nu}\right)\right) = \pi \frac{z_\nu}{\sqrt{z_\nu^2 + (r_{\text{ext}} - r_{\text{int}})^2}},$$

assuming $r_{\text{ext}} \simeq r_{\text{ext}} - r_{\text{int}}$. Seeking for a refinement step, one should consider the distance of the source point from the generic element of the cathode wall in order to define a source of secondary electrons to sample as a function of the radial coordinate on the cathode back-wall.

The contribution on the insulator sleeve is neglected due to the high work function of dielectric materials; the effect of photons directed towards the cathode cylindrical electrode

is assumed negligible due to the unfavorable sight factor, even lowered if the cathode is made of rods.

4 The "exact" model

An extension to a 3D case should start from a local count of the excited states and decay fractions. The evaluation of a cell by cell sight factor would allow to calculate the cumulate of impinging photons on each radial position of the cathode back-wall and to define a more precise source distribution function. The same could be done for all the boundary surfaces of the simulation domain.

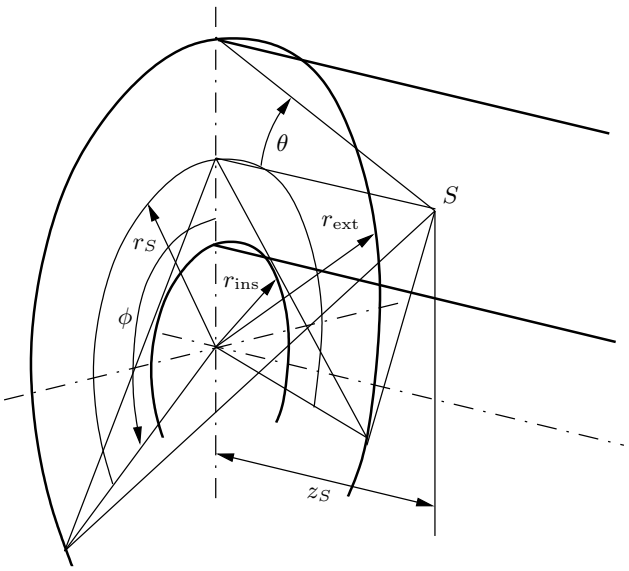

Figure 2: Sketch of the closed end of the electrodes and of a generic real pointwise isotropic photon source used to estimate a global 3D sight factor.

Referring to the scheme of Figure 2, let therefore S be a fixed point of coordinate (r_S, z_S) in a 3D cylindrical geometry (the poloidal coordinate is not important by now). Let P be a generic point of interest of coordinate (r, ϕ) and null z–coord. P is intended to move on an arc of radius r for increasing ϕ from 0 (which correspond to the axial plane containing the source S) to a maximum value denoted by ϕ_{lim}, corresponding to the intersection of the tangent from S to to the innermost circumference of radius r_{int}.

4.1 2D formulation

The axial-symmetric assumption lets us consider the source S as an uniform annular distribution of radiation source of total intensity I_S at the same fixed positions (r_S, z_S). The

intensity of the emitted flux will decrease proportionally to the inverse square of the distance d between S and the target of interest P, given by

$$d = \sqrt{z_S^2 + r_S^2 + r^2 - 2r_S r\cos\phi}$$

where the *cosine theorem* has been used to define the distance $\overline{PS}$ on the plane $(r,\, \phi)$.

Since a 1D radial dependence of the radiation intensity on the target is wanted, the radial coordinate of P can be considered as fixed. Hence only its angular coordinate ϕ will vary. Exploiting the axial symmetry of the problem for a fixed point source S, the angle ϕ will vary in the range $[0,\, \phi_{\mathrm{lim}}]$ with ϕ_{lim} given by the tangent condition above mentioned. The angle $\gamma = \widehat{\mathrm{SOP}}_{\mathrm{max}}$ can be seen as the sum of $\alpha = \widehat{\mathrm{SOT}} = \arccos(\mathrm{r_S}/\mathrm{r_{int}})$ and $\beta = \widehat{\mathrm{TOP}}_{\mathrm{max}} = \arccos(\mathrm{r}/\mathrm{r_{int}})$.

Due to the reversibility of the axial symmetry of the problem, a section $(r,\, z)$ of the domain will feel the contributes of the axial symmetric annular source; then the fraction f of the radiation emitted by the source impinging in the point P' on an infinitesimal area $\delta A = r\delta r\delta\phi$ about position r is given by

$$f = \frac{1}{4\pi}\int_{-\gamma}^{\gamma} \frac{r^2\delta r}{\left(z_S^2 + r_S^2 + r^2 - 2r_S r\cos\phi\right)^{3/2}}\,\mathrm{d}\phi = c\int_0^{\gamma} \frac{\mathrm{d}\phi}{a - b\cos\phi}\,,$$

with $c = r^2\delta r/\left(2\pi\right)$, $a = z_S^2 + r_S^2 + r^2$ and $b = 2rr_S$.

4.2 3D formulation

The extension of the 2D formulation to the 3D case is immediate: each point of the annular receiver must be considered by itself, and therefore the integration on ϕ doesn't subsist anymore. The differential $\mathrm{d}\phi$ becomes the infinesimal $\delta\phi$ and the resulting intensity of radiation simply reduces to the

$$f = \frac{1}{4\pi}\frac{r^2\delta r\delta\phi}{\left(z_S^2 + r_S^2 + r^2 - 2r_S r\cos\phi\right)^{3/2}}\,. \tag{1}$$

4.3 Coding features within *es-c*PIF

The coding transposition of such a multidimensional approach of the photoelectric effect articulates over two important modifications, following the spatial discretization of both the domain (where sources are considered) and the boundaries (where photons impinge):

1. the need of a spatial mapping variable for the local intensity of the photons emitting source due to molecules de-excitation;

2. a sight factors matrix for the assignment to the boundary elements of the proper fraction of received photons from every spatial source location.

The first point is easily codeable since the local nature of the excitation collision already implemented in the ***es-c*PIF** code within the Monte Carlo Collisional (MCC) module. Every electron-molecule excitation impact should be registered on the proper position in an array to count the local production of a possible photon emitter. After each simulation timestep the array should be glanced through to randomly extract the number of emitted photons at each cell for source distribution definition.

The second point, which should appear the most time consuming, requires instead only a single computation at the beginning of the simulation to retrieve the sight factor matrix. It is to be noticed that the only differences between the 2- and 3D cases lie in the dimension of the sight matrix and in its coefficients definition: if n_r, n_z and n_ϕ are the number of cells for every dimension in the domain discretization, for the first case it results in a $n_r \times (n_r n_z)$ matrix, which elements are defined by the equation4.1, while in the latter case it results in a $(n_r n_\phi) \times (n_r n_z n_\phi)$ matrix. Such a matrix, kept in memory and recalled at each timestep, will give the photons colliding each boundary cell by means of a simple multiplication with the source array of point 1.

A Hydrogen excitation levels and de-excitation times

The multitude of excitation cross sections for molecular Hydrogen results in a wide series of excitation levels involved in electron-molecule collisions. Each excitation level is charachterized therefore by an exact excitation (and de-excitation as a consequence) energy and an exact decay mean time. Table 1 summarizes the energies and decay times for common applications excitation phenomena: it can be noticed that, among all the processes usually considered in the MCC module (the ones charachterized by an electron collision cross section higher than an effective threshold of 1.E-3 $Å^2$ [8]), only few ones are considered for photoemission in the simulation of the PF breakdown since the de-excitation times must be comparable with the proper times of the studied phenomenon and the energies compatible with the electrodes work function to effectively lead to photoemission from the latter.

Excitation	Energy [eV]	Decay mean time [ns]
$H_2(X^1\Sigma_g^+) \rightarrow H_2^*(B^1\Sigma_u^+)$	11.37	0.8
$H_2(X^1\Sigma_g^+) \rightarrow H_2^*(C^1\Pi_u)$	12.41	0.6
$H_2(X^1\Sigma_g^+) \rightarrow H_2^*(a^3\Sigma_g^+)$	11.90	11.1
$H_2(X^1\Sigma_g^+) \rightarrow H_2^*(c^3\Pi_u)$	11.89	106
$H_2(X^1\Sigma_g^+) \rightarrow H_2^*(d^3\Pi_u)$	13.98	68.0

Table 1: Molecular Hydrogen inhelastic collisions of interest for PF breakdown and related excitation energies and decay mean time.

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