DEVELOPMENT AND ANALYSIS OF SOFTWARE FOR THE NUMERICAL SIMULATION OF FIELD EMISSION ELECTRON SOURCES

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Abstract

The open-source DAISI C++ package (Design of Accelerators, optImizations and SImulations) is extended with the ability to simulate the operation of electron sources in the field emission mode, with the user-defined initial distribution of emitted electrons velocities, as a model parameter, and with the automated calculation of current-voltage characteristics. Particles injection scheme is suggested. Computational experiments are performed for silicon carbide field emission electron source nanostructure with bimodal energy spectrum, revealed from experimental study, and comparative analysis with Maxwell distribution is presented.

INTRODUCTION AND MOTIVATION

It is extremely important for effective functioning of the field emission electron sources to prevent beam particles from getting to the the periphery of the beam. So it is an actual problem to improve approaches of simulation of the field emission electron sources, because the initial velocity distribution has a significant influence on the emission picture, but the simplest models are utilizing zero initial velocity spread or Maxwell distribution, that doesn’t always match experimental data [1–3].

SOFTWARE DEVELOPMENT

In DAISI the particle-in-cell (PIC) method is split into two modules [3], one of which consists of solvers and the other is a software abstraction of the physical model. Calculation of current density with the Fowler-Nordheim model is being realized in software abstraction of physical device. The exact modified parts are shown in the fragment of the UML class diagram (Fig. 1).

Figure 1: Fragment of the UML class diagram of DAISI implementation of PIC calculations and particle injection scheme. Red colored blocks show modified part of C++ code, which allow to simulate the operation of electron sources in the field electron emission mode, with the choice of the initial distribution of electron velocities.

where \( \varphi \) — azimuth coordinate:

\[
\frac{\partial^2 U(r, z)}{\partial r^2} + \frac{\partial^2 U(r, z)}{\partial z^2} + \frac{1}{r} \frac{\partial U(r, z)}{\partial r} = -\frac{\rho(r, z)}{\varepsilon_0}, \quad (r, z) \in G, \quad (1)
\]

\[
E_r(r, z) = -\frac{\partial U(r, z)}{\partial r}, \quad E_z(r, z) = -\frac{\partial U(r, z)}{\partial z},
\]

\[
\int_G U = g(r, z), \quad (r, z) \in \partial G_1,
\]

where \( \rho(r, z) \) — space charge density, \( \varepsilon_0 \) — electric constant, \( g(r, z) \) — function that describes boundary potential, \( \hat{n} \) — normal vector to the boundary \( \partial G_2 \) (axis of symmetry and side boundary of electron source cell). The motion of particles is described with reduced momentum \( p_r, p_z \) by following equations in Lagrangian cylindrical coordinates \( (r, z) \) (for model macroparticles, the relativistic form of the equations of motion is used, taking into account the realization of the particle-in-cell method [3]):

\[
\begin{align*}
\frac{d r}{d \tau} &= p_r \gamma, \\
\frac{d p_r}{d \tau} &= \frac{e E_z}{m_0 c^2} + \frac{p_r^2}{r^2}, \\
\frac{d z}{d \tau} &= p_z \gamma, \\
\frac{d p_z}{d \tau} &= \frac{e E_z}{m_0 c^2}, \\
\frac{d \varphi}{d \tau} &= 0,
\end{align*}
\]

\[
(r(0), z(0)) \in \partial G_1, \quad (p_r(0), p_\varphi(0), p_z(0)) = \vec{p}_0. \quad (4)
\]

where initial positions of particles are given on part of boundary \( \partial G_1 \) including emission area; \( \gamma = \sqrt{1 + p_r^2 + p_z^2 + (p_\varphi/r)^2} \), \( \tau = ct \), \( c \) — speed of light, \( m_0/q \) — ratio of rest mass to electron charge (model particles have the same ratio). Initial momentums

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related with initial velocities $v_0$ that are given by Maxwell distribution or user-defined distribution (as described in next section), $\hat{p}_0 = v_0\gamma/c$.

Current density is determined according to the Fowler-Nordheim field emission model [1]:

$$j(E) = \frac{A(\beta \gamma E(s))^{2}}{t^{2}(y)\Phi} \exp \left( -\frac{B\gamma^{3/2}}{\beta \gamma E(s)}\nu(y) \right), \quad (5)$$

where $j(E)$ — current density ($A$/m$^2$ for $E$ measured in V/m), $\Phi$ — work function of material (eV), $\beta_f$ — local field enhancement factor [4, 5], $E(s)$ — magnitude of the field strength vector in point $s$, $A$ and $B$ — Fowler–Nordheim constants, $\nu(y)$ — Nordheim parameter, $\gamma(y), t(y)$ — approximations of elliptic Nordheim functions found by Forbes and Deane that give a more accurate approximation in comparison with the classic Schmidt approach [6].

**METHODS OF SIMULATION**

Injection of particles is suggested by the following scheme:

1. Emission surface is represented as a partition of an interval in 2D space $\sigma_N$ with the number of subparts equals $N$, which value depends on the grid.

2. Current density from the whole subpart is considered to be equal to current density calculated at the center point of the subpart.

3. Emission surface is represented as a partition of an interval in 2D space $\sigma_K$ with the number of subparts equals $K < N$ and it is a model parameter.

4. Macroparticle is injected from the center of every subpart of the $\sigma_K$ and current calculation is based on the current sum from all subparts of $\sigma_N$ that are covered with considered $\sigma_K$ subpart.

Additional partition of an interval $\sigma_K$ is required because constructed grid according to Runge rule leads to too high value of $N$. DAIISI computational algorithms perform particle injection at fixed points during the simulation. If particles will be injected from each subpart from $\sigma_N$ then it will lead to very low performance and injected particles will carry a very small amount of charge, significantly lesser than elementary. To reduce the influence of $N$ new smaller partition $\sigma_K$ is introduced and it is used as an aggregator of current density from subparts of $\sigma_N$ at one fixed point required for DAIISI.

This scheme allows one to take into account the nontrivial specifics of the emission surface. And macroparticles that carry the most charge are matching surface regions with the highest current density. Also, it is should be noted that emission surface length is a model parameter. Let us introduce the probability density function (PDF) of the bimodal random variable based on the field electron emission energy distribution spectra (Fig. 2). Considering spectrum as a function of energy $x$ it can be described as a piecewise linear function $g(x)$ that equals to spectrum value within obtained energy interval $[E_{\text{spec},\text{min}}, E_{\text{spec},\text{max}}]$ and zero otherwise, where $E_{\text{spec},\text{min}}, E_{\text{spec},\text{max}}$ — minimal and maximum spectrum values. PDF can be obtained $f(x)$ after the normalization of the $g(x)$:

$$f(x) = k_{\text{norm}}g(x), \quad (6)$$

where $k_{\text{norm}}$ is normalization factor. The cumulative distribution function now can be easily obtained integrating (6) on $(-\infty, x]$.

To simulate this random variable, the inverse function method based on uniform random numbers [8] is used, but because the spectrum is set for limited energy values $[E_{\text{spec},\text{min}}, E_{\text{spec},\text{max}}]$, the following problem is to model the truncated distribution [8]. To simulate a truncated random variable on the segment $[a,b]$, it is necessary to obtain the values of the random numbers on the segment $F(a), F(b)$:

$$x = F^{-1}(R(F(E_{\text{spec},\text{min}}), F(E_{\text{spec},\text{max}}))). \quad (7)$$

The following equation can be solved with respect to $x$:

$$\gamma = F(x) = \sum_{i=1}^{N_{\text{spec}}} f(y)dy, \quad (8)$$

where $\gamma \sim R(F(E_{\text{spec},\text{min}}), F(E_{\text{spec},\text{max}}))$. Considering $E_{\text{spec},\text{min}} = x_{1} < x_{2} < \ldots < x_{N_{\text{spec}}} = E_{\text{spec},\text{max}}$ where $N_{\text{spec}}$ — number of value of the spectrum numerical representation, and because the integration nodes are fixed, and not equidistant, for the numerical approximation of the integral the trapezoid rule can be used:

$$\int_{E_{\text{spec},\text{min}}}^{E_{\text{spec},\text{min}}} f(y)dy = \frac{1}{2} \sum_{j=2}^{i} (f(x_{j-1}) + f(x_{j})) \cdot (x_{j} - x_{j-1}). \quad (9)$$

Combining Eqs. (9) and (8) with respect to $i$ is obtained, from which the velocity of the particle can be expressed in explicit form using the particle’s kinetic energy equation.

**ANALYSIS OF THE RESULTS**

The cell of a field emission array electron source with a blade structure of vertical type emitters [1] in a triode configuration is considered to illustrate capabilities of the software.

The surface of the emitter is modeled as an ideal conductor without a dielectric coating associated with the presence of adsorbates, the edge of the blade is approximated by the toroid surface with an elliptical section with semi-axes of the ellipse 120 and 50 nm.
Computations are performed for two emission surfaces length 144 nm (Fig. 3) and 30 nm to eliminate influence of this model parameter. Both results (Fig. 4) are obtained with fixed $\sigma_N$ and with $\sigma_K$ for $K = 600, 1000$ to show that with additional $\sigma_K$ partition of an interval there is no qualitative difference in simulation results.

Figure 3: Silicon carbide nanostructures under the study [9–11]: a) SEM-image of field emission cell with razor-blade emitter; b) SEM-image of cylindrical blade structure [10]; c) geometric configuration of the electron source cell with two emission surface lengths — 144 nm (red and green combined) and 30 nm (red).

Influence of $\sigma_K$ doesn’t cause significant changes on simulation results for different $K$. Also, Maxwell distribution leads to the injection of particles that are faster and carry a lesser charge (Fig. 5).

Figure 4: Pairwise comparison for both emission surface lengths: a) anode current from the gateway potential with bimodal and Maxwell initial velocity distribution; b) cathode current from the gateway potential with bimodal and Maxwell initial velocity distribution.

CONCLUSION

DAISI PIC code related to the calculation of the current density is extended with a field emission simulation, and injection of charged particles is extended with a such model parameter, as initial velocity distribution. Particle injection scheme was suggested and simulation results are obtained for the considered silicon carbide nanostructure as field emission electron source within the foregoing model assumptions. Simulated emission current collected on anode with bimodal initial velocity distribution approximately two times lesser than with Maxwell distribution with its parameter equals the expected value of the energy spectra.

ACKNOWLEDGEMENTS

Scientific research were performed at the Research park of St. Petersburg State University “Centre for Nanofabrication of Photoactive Materials (Nanophotonics)”, “Interdisciplinary Center for Nanotechnology” and “Computing Center”.

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