A Methodology of Field-Emission Modeling with Space-Charge Effects

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ABSTRACT

In this paper, we present a methodology for modeling and simulating 3D field-emission devices (FED) with space-charge effect. This approach applies an accelerated boundary-element-method (BEM) electrostatics solver and an adaptive explicit integrator. The charges emitted from the tip are evaluated as the function of the surface electric field distribution on the tip by the Fowler-Nordheim equation. The displacement and velocity of emitted particles in each time step is calculated by the Runge-Kutta integration method. The results by this methodology are verified with the results by a commercial electromagnetic package MAGIC. The simulation results show that the approach in this study is efficient and accurate in solving electrostatic problems with space charge effect.

Keywords: field emission, microtip, space charge, boundary element method.

1 INTRODUCTION

For electrostatic simulations, there are two major types of solvers in the industry: the finite-element/difference method (FEM/FDM) solvers and the boundary-element method (BEM) solvers. The approach of the finite-element/difference method receives wide acceptance due to its availability. Therefore, most of the modeling works in field-emission device (FED) studies use finite element method. The most significant challenge in FED modeling is the very different dimensional scales surrounding the tip region compared to the regions around and above the gate. 3-D FEM/FDM approaches [1] typically need several hundred thousand elements and tremendous computational resources (memory and CPU time) to simulate a simple emitter model; 2-D FEM/FDM approaches, while requiring less resource, lack the ability to simulate emitter arrays because of the assumption of azimuthal symmetry. BEM approaches, intrinsically, have a reduction in dimension, and thus are ideal for FED 3D-electrostatics calculations. Previous approach has proved that 3D BEM solvers significantly improve the computational efficiency for 3D geometries [2][3].

In this paper, we focus on the modeling of charged-particle behaviors of micro-emitters. We present a methodology for modeling and simulating 3D field-emission devices with space-charge effect, which was assumed negligible in previous works. This approach applies a BEM electrostatics solver FastLap to calculate the electric field distribution in the simulation domain [4]. The space charge effect is modeled by a method similar to the particle-in-cell (PIC) method [5]. The results are compared with those from MAGIC [6], which utilizes the PIC method to analyze the charged particles behaviors, such as trajectories, potential, electric fields, current density, and so on. We also demonstrate that the boundary element method is efficient and accurate in solving electrostatic problems.

2 SIMULATION METHODS

The BEM solver FastLap is used to calculate the surface electric field on the panels of BEM model. This procedure is very similar to that presented in [2]. After the initial step of electrostatic calculation, the emission current density distribution from the various panels on the tip is determined from the Fowler-Nordheim equation [7]

$$J = A \cdot \frac{F^2}{\phi \cdot t^2(y)} \exp\left(-B \cdot \frac{\phi^{\frac{2}{3}}}{F} v(y) \right) \qquad (1)$$

where J is in A/cm^2, A=1.54×10^{-6}, B=6.87×10^7, $t^2(y)$=1.1, $v(y)$=0.95-y^2 and y=3.79×10^{-4} · $F^{1/2}$ / ϕ, ϕ is work function and usually in the range 3.4 to 11.6.

According to the information of current density, the total charge of the electrons emitted out of each panel in each time step is computed according to the panel area and time step. The electrons emitted out of each panel in each time step will be grouped as a "charged macro particle" (space charges) in this methodology.

Using the Newton's laws and Runge-Kutta integration method, the new position of each emitted charged macro-particle is calculated by equation (2). Here we assume that the initial velocity of electron emitted from a panel is its thermal velocity. The initial direction of the thermal velocity is the normal direction of the panel from which the electrons are emitted.

$$m\ddot{x}_i = -qE_i \qquad i = 1,2,3 \qquad (2)$$

The emitted charge macro-particles are treated as new BEM cubes for the BEM electrostatic calculation in the next time step. Before the second cycle start, the mesh of the panels of the new cubes are added into the original mesh of the BEM model. The six panels of each cube are assigned as Neumann-type boundaries with a total surface charge which is the same as the charge of the emitted electrons. Similar to the first cycle, the electric field on the tip panels and on the locations of those emitted macro-particles are calculated by the FastLap. Then the new emission charges from the tip can be calculated by the Fowler-Nordheim equation while the charges of "old" emitted macro-particles are the same as in the previous cycle. Again, the Runge-Kutta method is used to compute the new positions and velocities for the macro-particles emitted from the tip and for those emitted in previous cycle based on the newly calculated electric field distribution. Note that the amount of emitting charges is not the same as those emitted in last cycle since the BEM mesh has been changed after each time step. The new emitted electrons are again treated as BEM cubes and added to the original BEM mesh. The simulation repeats the same cycle until reaching steady state. In addition, the emitted macro-particles reaching the boundary of the calculation domain are omitted. Figure 1 shows the procedure of the simulation proposed in this work.

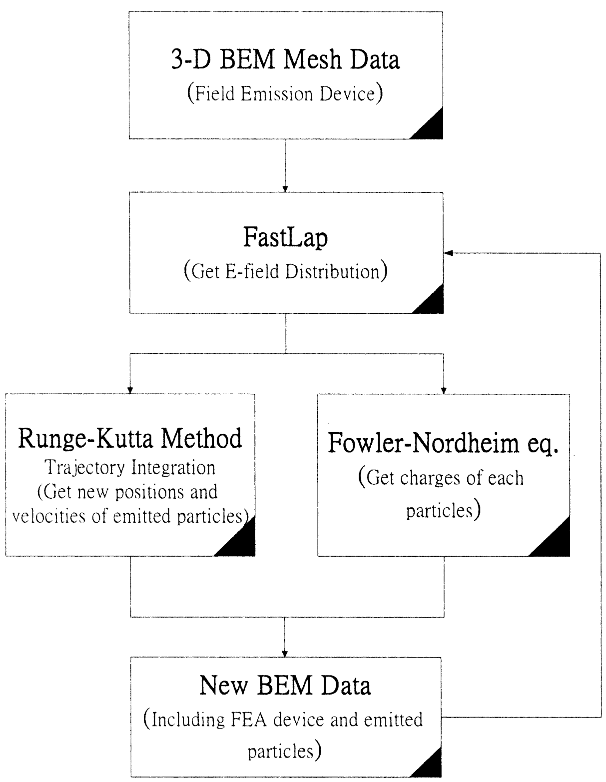

Figure 1: Simulation procedure using FastLap to solve BEM problems of this work.

3 MODELING

The boundary element model of a field emission device is shown in Figure 2. The solid lines in the figure indicate the surfaces of the Dirichlet-type boundaries which sustain constant electric potential, and the dotted lines indicate the Neumann-type boundaries which sustain constant values of the normal derivatives of potentials. In order to simulate the tip array, the Neumann-type boundaries with zero constant value are used to represent symmetric conditions. In this condition, the electric field perpendicular to the surface is equal to zero. In other words, there are no electric field components that are normal to the side-walls of the simulated domain. Figure 3 shows the 3-D BEM surface mesh of the field emission device where we used in this work. The tip radius of curvature is 100 nm, and the gate radius is 0.5 μm.

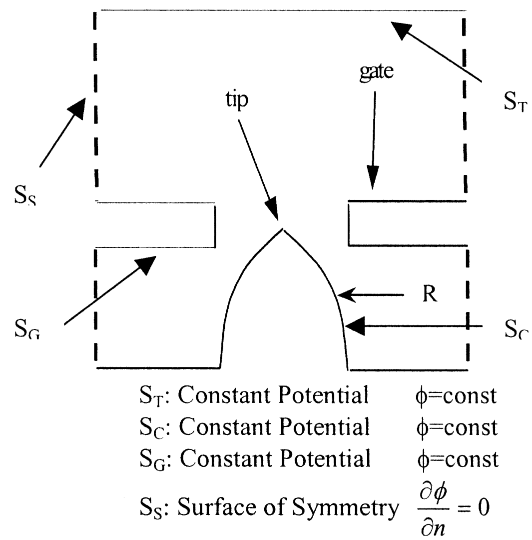

***Figure 2:** Boundary conditions of the model for the field emission device.*

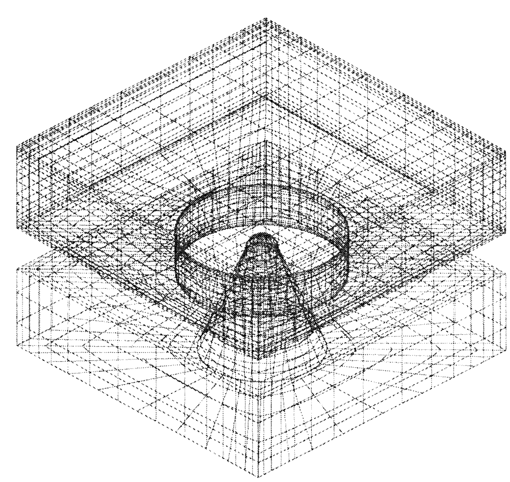

***Figure 3:** 3-D boundary element mesh plot of the simulated emitter.*

The schematic of emitted charge (space charge) outside the emission tip after the first and the second time step is shown in Figure 4.

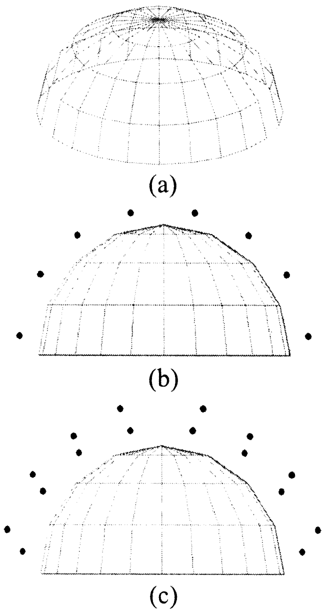

Figure 4: *(a): The BEM mesh of the emission tip. (b) and (c): The schematic of emitted charge (space charge) outside the emission tip after the first and the second time step*

4 RESULTS AND DISCUSSION

With the model described previously, we calculate the electric field distribution first without any space charge effect. The electric field is about 8.42×10^{8} V/m at the top of the tip and 5.7×10^{8} V/m at the bottom of the tip. The emitted charged macro-particles are then formed based on the surface electric field and their trajectories are calculated in each time step. A typical distribution of the emitted macro-particles calculated by the methodology is shown in Figure 5 (not to scale) after 15 time steps. Here a time step is 5×10^{-15} second.

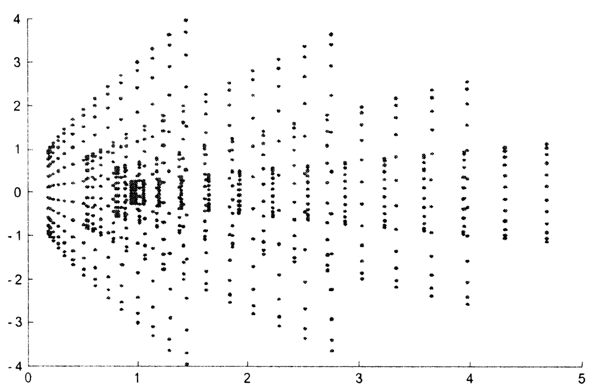

Figure 5: *The electrons distribution calculated by our work.*

According to the plots, a few macro-particles will hit the ceiling (the top surface in Figure 2) at 1×10^{-13} second (after 20 time steps), and will be neglected in successive steps to make the simulation running correctly. The current density is about 1.8×10^{9} Amps/m^2 at the top of the tip and 4×10^{7} Amps/m^2 at the bottom of the tip.

We also compared our results with those calculated by the MAGIC. Figure 5 shows a 2-D MAGIC finite-difference (FDM) model of a field emission tip assuming cylindrically symmetric. The gray areas are ideal conductors and the simulation domain is meshed by the finite difference method. The boundary conditions are the same as those in our work. The electron distribution calculated by the MAGIC is shown in Figure 6.

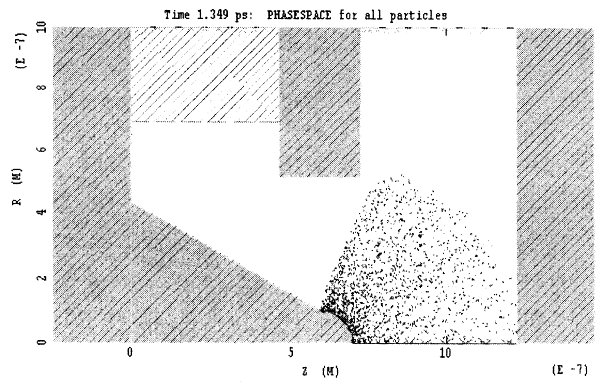

Figure 6: *The electrons distribution calculated by the MAGIC at t=1.349 ps*

Compare the results of our work with the MAGIC example, we find that the phase space of these two are very similar. Besides, the MGAIC results show that the electrons emit from the tip at 1.235×10^{-12} seconds and hit the ceiling at 1.349×10^{-12} seconds. It costs 1.14×10^{-13} seconds for the front electrons to reach the ceiling, which is very close to the results (10^{-13} sec) calculated by our methodology. Figure 7 shows the surface electric field distribution on the tip.

If the charge effects are concerned, the electric field distribution will be changed. Assume that the electric field without concerning charge effects is E1 while the electric field concerning charge effects is E2, then the discrepancy is defined as

$$discrepancy = \frac{|E1 - E2|}{E1}$$

Figure 8 shows that the discrepancy of the tip surface electric field between the results of this work and the MAGIC is less than 0.3%.

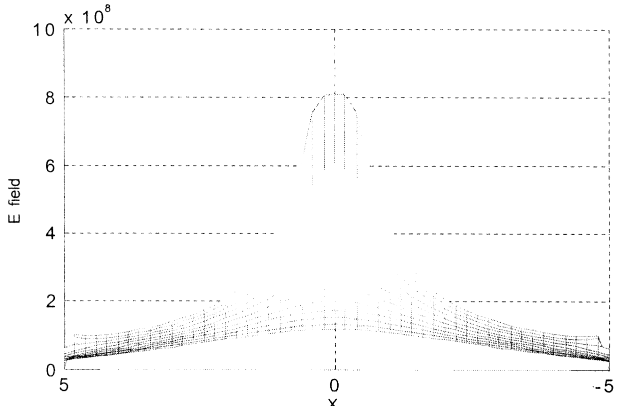

Figure 7: The electric field distribution on the emission tip (ceiling:85 volts, gate:80 volts).

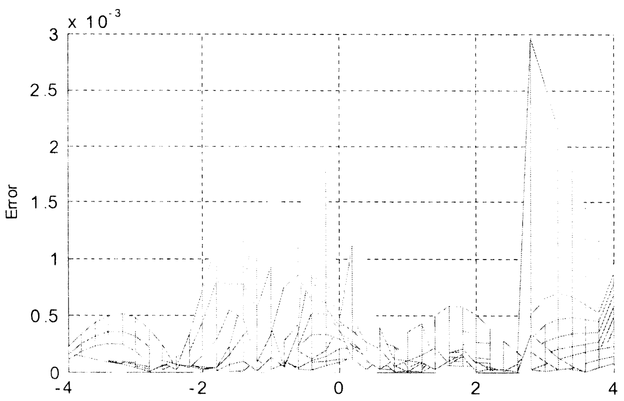

Figure 8: *The discrepancy of tip surface electric field between the results of this work and the MAGIC (ceiling:85 volts, gate:80 volts).*

We also calculate the maximum electric fields vs. different gate voltages (with fixed voltage difference (5 volts) between the gate and the anode), as shown in Figure 9. This figure indicates that the electric field will change linearly with the variation of the ceiling (gate) volts.

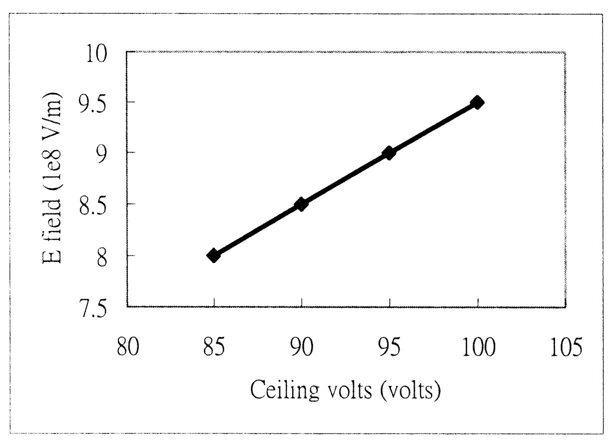

Figure 9: *The maximum electric field obtained in different boundary conditions*

5 CONCLUSION

In this paper, electrostatic simulations of field emission devices are performed by the boundary element method solver FastLap. The electric field distribution is calculated by Fowler-Nordheim equation to determine the charges emitted form the tip. The electrons emitted out of each panel in each time step will be grouped as a "charged macro-particle" (space charges). The moving distances of the macro-particles in each time step are calculated by Runge-Kutta method. The results are compared with those from MAGIC with good agreement, and demonstrate that the boundary element method is efficient and accurate in solving electrostatic problems. We also show that this methodology not only provides excellent accurate results, but also reduces the effort of creating 3-D solid models of field emission tips.

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