Digital Computer Simulation of Three-Dimensional Ion Beam Extraction and Transport Systems

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Abstract

SNOW, a program for the simulation of ion beam extraction from plasmas has been extended into three dimensions. Basic relaxation techniques are employed, alternately solving for voltages (using Poisson's equation expanded in difference form) and computing trajectories through the device. Electrodes are laid out on a large three-dimensional array for the simulation of voltages. The plasma is simulated on a second array (that may be finer than the voltage matrix) by using a background (Boltzmann) electron distribution balanced with the ion space-charge density at the injection plane. The plasma is determined by its electron temperature and the ion drift energy and spatial distribution. The program automatically determines the shape and location of the plasma surface. It is written in generic FORTRAN 77 and can be run on virtually any computer from high end PC's (with DOS extenders) to Cray's with only minor modifications. Execution time can vary from 15 minutes to 8+ hours on the PC. Results can be obtained within a few percent of either theory or experiment.

I. INTRODUCTION

SNOW3D was developed at Varian Ion Implant Systems for the simulation of high current ion beams used in ion beam implanters. These beams are typically extracted from a plasma using a slit, where 2-D and axisymmetric simulations are not adequate. In addition quadrapoles and other lenses, for focusing the beam, and deflection systems, for scanning the beam over the wafer, require 3-D simulations.

The program currently runs on a high end (25 MHz, 80386 or better, with 13 MBytes of memory) IBM PC or clone using DOS extenders. NDP-FORTRAN and NDP-PLOT (from Microway) are used for the compiler and the plotting capability. The program will run small problems (40x40x40 arrays) in as little as 15 minutes, but may require 8 hours or more for large problems (100x100x100 arrays, about the limit for 13 MBytes of memory). Obviously larger memories would permit larger simulations and faster computers would require less time.

The program actually exists in three versions. A full 3-D program permitting uniform magnetic fields along any axis, as well as axisymmetric magnetic fields along the beam axis. A second version with a single plane of symmetry parallel to the beam axis, and allowing a uniform magnetic field normal to the plane. The third version has two planes of symmetry parallel to the beam, with no magnetic fields. The advantage of these other versions is they require less memory (and less time to execute) or permit greater resolution of the simulation.

The method of solution is to alternately solve Poisson's Equation at each point of the array, and to compute representative trajectories (by solving the Lorentz Force Equation) through the device. Space charge is computed from the trajectories and stored on a matrix identical to the voltage array. The plasma region for extraction problems is simulated on a second (and usually finer) matrix so that greater resolution can be obtained in the plasma and most importantly at the plasma surface.

II. THEORY

The voltages are computed by iteratively solving Poisson's Equation;

$$\nabla^2 V = \frac{-\rho}{\epsilon_0} \quad (1)$$

where V is the voltage, ρ the space-charge density, and ε_0 the permittivity of a vacuum (all in SI units). This becomes in cartesian coordinates, in (second order) difference form on a matrix of cubes

$$V_{i,j,k} = \frac{V_{i+1,j,k}+V_{i-1,j,k}+V_{i,j+1,k}+V_{i,j-1,k}+V_{i,j,k+1}+V_{i,j,k-1}}{6} - \rho_{i,j,k} \quad (2)$$

where

$$\rho_{i,j,k} = \frac{(\Delta z)^2 \rho}{6\epsilon_0} \quad (3)$$

where Δz is the matrix increment, and i,j,k are the subscripts for the (x,y,z) three dimensional array.

In the plasma region the space-charge density becomes a function of the voltage due to the presence of the electrons.

$$\rho = \rho_i + \rho_{e0} e^{\left(\frac{eV}{kT_e}\right)} \quad (4)$$

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Where k is the Boltzmann constant, T_e is the electron temperature and ρ_{e0} is the ion space-charge density at the injection plane. Solution of this very non-linear, and somewhat unstable problem, consists of repetitively solving Eq. 2 using the new values computed for the voltage on the left to upgrade the voltage used in the space-charge density term on the right.

The Lorentz force equation can be solved in either cartesian coordinates (for uniform or no magnetic fields) or in axisymmetric-cylindrical coordinates (the beam does not have to be symmetric) for axisymmetric magnetic fields;

$$F = -e(E+v\times B) \tag{5}$$

where e is the electronic charge, and B the applied magnetic field. The solution (again in second order difference form) for cartesian coordinates, and zero magnetic field, becomes

$$\begin{aligned} x_{i+1} &= 2x_i - x_{i-1} - \eta(dt)^2 E_x \\ y_{i+1} &= 2y_i - y_{i-1} - \eta(dt)^2 E_y \\ z_{i+1} &= 2z_i - z_{i-1} - \eta(dt)^2 E_z \end{aligned} \tag{6}$$

where η is the charge to mass ratio, and E the electric field. These equations become more complex and consume a great deal of space [1] as the magnetic fields are added and will not be discussed here. The electric fields (as well as other derivatives) are expressed in second order differences similar to Eq. 7.

$$E_x = -\frac{\partial V}{\partial x} = -\frac{V_{i+1,j,k}-V_{i,j,k}}{2\Delta x} - \frac{V_{i+1,j,k}-2V_{i,j,k}+V_{i-1,j,k}}{(\Delta x)^2}h_x \tag{7}$$

where h_x is the normalized distance (to Δz) between x_i and the i column. This calculation is made at all four corners of the square at the nearest x (i) plane through which the particle is passing.

III. THE PROGRAM

The three versions of the program make it quite flexible. All versions can simulate multiple injected beams of varying mass, energy, and distribution. The programs can calculate electron and positive or negative ion trajectories in the same simulation, aiding the calculations for negative ion sources or neutralizing positive ion beams.

The program has a limited (but multiple) extracted electron beam capability, requiring flat, thermionic cathodes. Beam (and potential) data from any simulation can be saved at any plane for reinjection into later simulations. In addition to the beams injected in the plasma, multiple beams of electrons and ions can be injected (or reinjected) from almost any boundary. The program can save and restore data for restarts of the same (or slightly modified) data.

The configuration is described by entering integer matrices describing the electrode shapes at each cross (x-y) plane of the simulation. This can be quite complex for tapered electrodes requiring many planes to be defined, but may be very simple for a series of quadrapoles as only one cross section need be defined. No partial matrix squares are employed, the program relies on the fineness of the mesh to provide adequate resolution. The fine matrix covering the plasma region is similarly defined.

Plots of the trajectories and equipotentials can be obtained in two or three dimensions. Current density distributions and emittances can also be plotted.

IV. RESULTS

Accuracy of results are proportional to the fineness of the mesh employed, the density of trajectories, and the care employed in setting up the problem. An example of a theoretical "Pierce" diode is shown in Figures 1 and 2. The quotes are employed because the Pierce [2] theory does not cover this configuration. It was found necessary to form a blend from the 2-D beam theory, along the slit, to the axisymmetric theory at the end of the slit. Figure 1 shows the x-z and y-z plane plots of the beam trajectories and equipotentials through the center of the beam, and Fig. 2 shows the three-dimensional

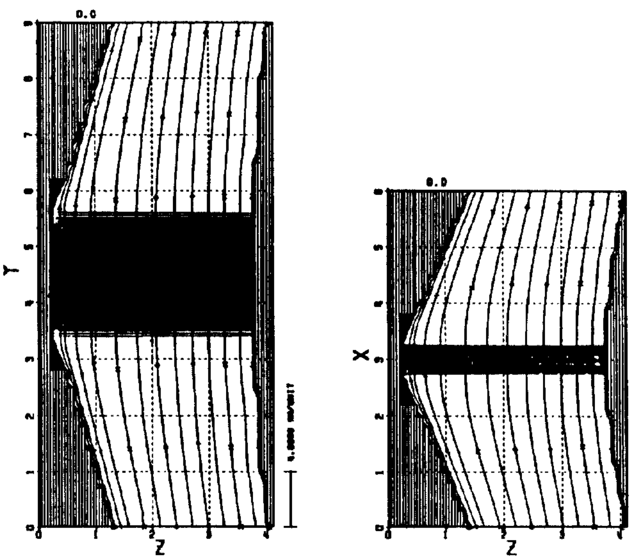

Figure 1. Trajectories and Equipotentials for a theoretical "Pierce" diode, about four percent of the trajectories are plotted.

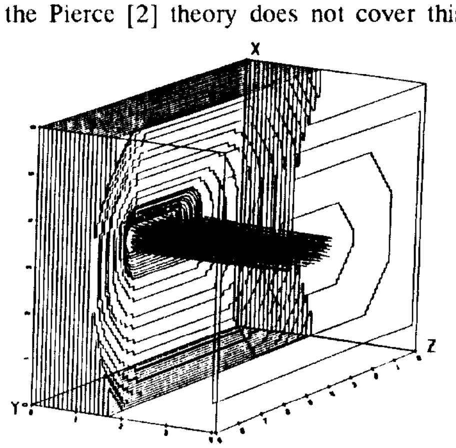

Figure 2. 3-D view of electrodes and trajectories for theoretical "Pierce" diode.

plot of the same simulation. Typically four to ten percent of the trajectories are plotted in both plots. The dark regions on the electrodes around the plasma in Fig. 1 demark the fine matrix. The x-z plane equipotentials on this fine (plasma) mesh, for the center of the slit, are seen in Fig. 3. With an electron temperature of 1.1 V and an ion drift energy of 3 Ev there is no sharp dividing line between the plasma and the beam. This transition region, which is caused by the Boltzmann electron distribution, seems to be what permits the greater current density. The current density was set 3 percent above the theoretical value determined from Child's Law for space-charge limited emission.

The current density distribution at the anode is seen in Fig. 4. One measure of the errors in the beam is shown in Fig. 5 where the x and y emittance plots are shown. The beam has a small overall divergence in x and a small convergence in y, both of less than 10 mrad. The beam is quite symmetrical and has a net deflection angle of less than 0.1 mrad in either plane. It is difficult to determine quantitatively an overall percentage error in the simulation but agreement with theory appears quite good.

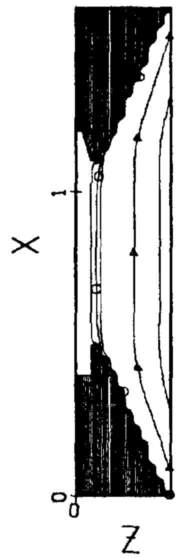

Figure 3. Equipotentials on plasma mesh.

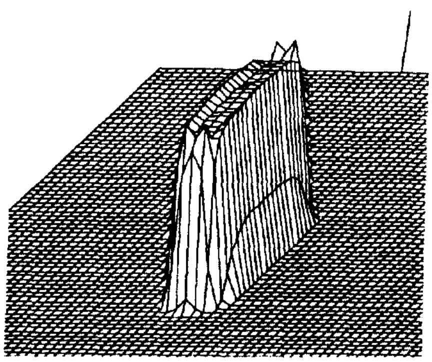

Figure 4. Current density distribution at anode for "Pierce" diode.

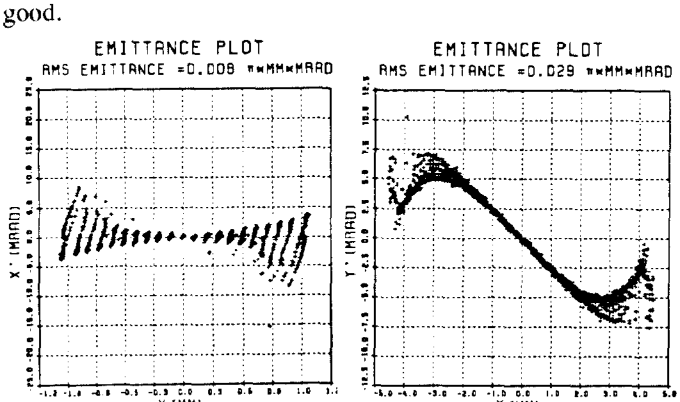

Figure 5. X and Y emittance plots for theoretical diode.

The extraction system in Fig. 6 takes advantage of the half symmetry version of the program. Here a 129 Ma, 24 kV negative ion beam is being extracted along with the associated electrons from the plasma. There is a uniform 0.24 Tesla magnetic field along the y axis. The electrons are injected in the transition region from the plasma to the beam, injected in the plasma the electrons will just travel in circles (there are no collisions in the program). Most of the electrons cycloid back into the extraction plate but some are deflected sideways and do not have enough z directed energy to return to the plate.

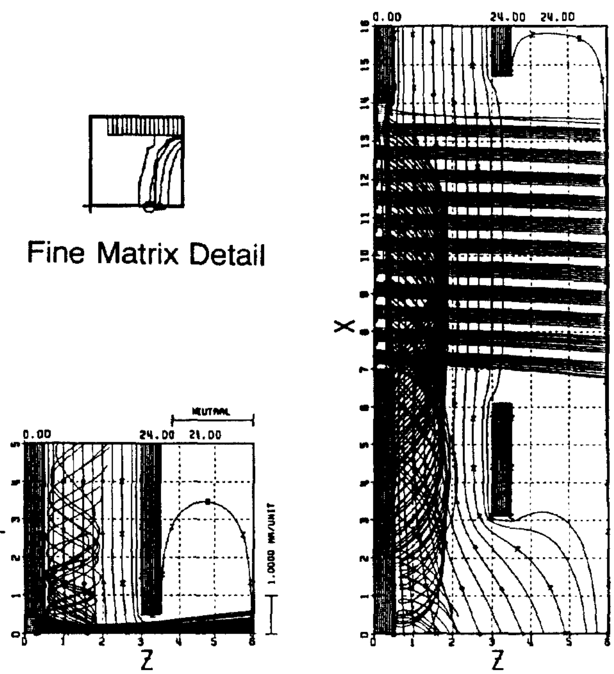

Figure 6. Half symmetry plot of negative ion beam extraction system with accompanying electrons and fine matrix detail of beam fillet.

Figure 7 is a 3-D plot of the same data looking down the z axis, with the escaping electrons going off at an angle to the side of the slit. The cause of the transverse energy of the electrons at the edge of the slit is the plasma fillet along the edge. This can be seen in the inset in Fig. 6 where the x-z equipotentials, at the center of the slit (remember the symmetry in y) on the plasma matrix are shown. The experimental device [3] produces two electron beams travelling off in similar directions.

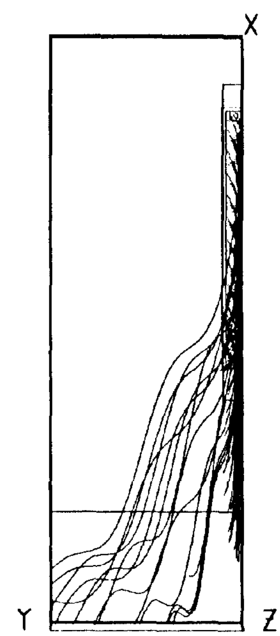

Figure 7. Three dimensional plot looking down z-axis showing electrons escaping.

V. REFERENCES

[1] J. E. Boers, "Computer Simulation of Space-Charge Flows," University of Michigan, Ann Arbor, Mich., Ph.D. dissertation, 1968.

[2] J.R. Pierce, *Theory and Design of Electron Beams*, New York: D. Van Nostrand Co., Inc., 1950.

[3] Joe Sherman, LANL, private communication.