ISBN: 978-3-95450-247-9 ISSN: 2673-5490 doi: 10.18429/JACoW-IPAC2024-MOPR75

PARTICLE-IN-CELL MODELING OF LOW-TEMPERATURE PLASMA ION SOURCES FOR ION IMPLANTATION

S. A. Veitzer*, Tech-X Corporation, Boulder, Colorado, USA,
M. P. Dehnel, D-Pace Inc., Nelson, B.C., Canada

Abstract

Numerical modeling of low-temperature plasma (LTP) ion sources provides cost-effective techniques for developing and optimizing beam characteristics for ion implantation and other applications, including plasma processing and etching. Particle-in-cell (PIC) models are a powerful tool for simulating plasma formation and dynamics in LTP sources. Beam formation and transport of the beam through extraction optics can benefit from reduced physical models; for example, one can couple a PIC model for plasma chambers with a different transport model in the extraction region. However, this coupling is *ad hoc*, and it is often not clear that the models are physically consistent with each other.

We present an integrated modeling capability that couples plasma chamber modeling with beam formation using the VSim computational framework. We leverage advanced modeling techniques such as energy-conserving PIC and variable meshing to improve simulation performance. We present results for modeling and optimization of beams for ion implantation. Our results show that our integrated models can improve optimization of beam currents, beam uniformity, and emittance for LTP ion sources.

INTRODUCTION

Modeling ion sources used for industrial applications such as ion implantation and plasma etching is difficult, integrating physics models including electrostatic modeling of plasmas, plasma chemistry and particle collisions, and particle-surface interactions. Externally applied magnetic fields used to confine electrons usually break the model symmetry, and hence 3D models are required. The computational requirements for such 3D models are intensive. Computational models must resolve the relevant physics, such as collision frequencies, which puts an upper limit on the time step size. The spatial resolution of cells must resolve both geometric details of the system, as well as plasma sheaths. In order to avoid computational artifacts such as grid heating, the Debye length must typically also be resolved. The Debye length decreases with decreasing temperature, so for low temperature plasmas (LTPs) resolving the Debye length is often the limiting factor for spatial resolution. Thus in order to model LTP ion sources and beam generation for implantation new techniques are needed to improve the computational efficiency.

Existing codes used to model extraction from ion sources such as Simion [1] and IBSimu [2] do not utilize accurate 3D plasma models to then yield realistic extracted beam characteristics. With such codes it is often very important to have beam phase space and emittance measurements for baseline cases from which useful extrapolations can be made to other configurations. The power of the VSIM code is that the changes to the physical constraints to the system including aperture sizes and shapes, vacuum levels, input gas types, lens voltages etc can be modified and the new plasma can be computed from first principles, and the resultant extracted beams generated in a straightforward manner.

We utilize a number of different numerical techniques to improve the efficiency of our simulations, including energy-conserving PIC methods [?] (which relax the need to strictly resolve Debye length scales), variable grids with higher resolution in the plasma chamber, intra- and inter-node processor domain decomposition for load balancing, and global-model plasma chemistry set reduction. Utilizing reduced ion mass when modeling plasma buildup and beam formation at the meniscus of the plasma chamber, when coupled with separate simulations of beam transport that do not include plasma chemistry can also improve performance. This technique allows us to reuse time-consuming plasma simulations and perform parameter scans for changes to the models outside of the plasma chamber.

Understanding beam properties is the most important important part of the problem for applications. Beam properties are a direct function of the plasma properties and models used to simulate plasma dynamics, so validated models for the plasma are required. In addition, the capability to modify the overall system and measure changes to the beams produced are the key to applying integrated simulation models to industrial ion sources. The shape and extent of the plasma meniscus plays an important role in beam formation in LTP sources, and we compare the meniscus for two different simulations that are the same except for the size of the aperture of the plasma chamber.

We present here advances in modeling LTP ion sources with a focus on understanding how changes to plasma chamber and source properties affect the beam. We simulate plasma formation and beam extraction in a Penning-type source with argon gas as an example of the modeling capability. We focus on how changes to the plasma properties and extraction optics result in changes to beam quality. In addition, we consider how the choice of plasma chemistry sets affects plasma formation, with an eye to modeling ion sources with more complex gas mixtures in the future. We use the plasma simulation framework VSim [6], which employs the Vorpal simulation engine [7] to self-consistently model plasma formation and buildup using accurate plasma chemistry models, as well as beam formation near the aperture of the plasma chamber and beam transport through the puller electrode.

* veitzer@txcorp.com

ISBN: 978-3-95450-247-9 ISSN: 2673-5490 doi: 10.18429/JACoW-IPAC2024-MOPR75

PENNING-TYPE ION SOURCE SIMULATION MODEL

For demonstration purposes, we consider a Penning-type singly-charged ion source. A schematic for the 3D model is shown in Fig. 1. Dimensions are indicated in the figure. For orientation with our analysis below, the beam propagates in the positive Z-direction. The axis parallel to the long direction of the apertures is the Y-direction, and the axis in the short short direction is X. Argon neutral gas at 5 mTorr (number density $n \sim 1.6 \times 10^{20}\ /m^3$) is ionized by electrons emitted from the cathode to form a plasma of singly-ionized argon ions. Electrons in the plasma chamber are confined by a $B_{\text{ext}} = 0.5\ T$ magnetic field that is applied over the entire simulation domain in the vertical (long) transverse direction over the entire simulation domain. Cathodes at the top and bottom of the plasma chamber are at $V_c = -300.0$ Volts, while the anode is grounded. The extraction (puller) electrode is 2.5 mm downstream of the anode, and is at a nominal voltage of $V_e = -15.0$ kV. All electrodes are 1.0 mm thick. The plasma chamber aperture is also one millimeter wide, and is centered on the downstream anode. The puller electrode aperture is 3.0 mm wide and 12.0 mm in height and is offset from the chamber aperture by 2.0 mm to account for the effects of the magnetic field on the beam. The argon ion beam can be seen in the figure.

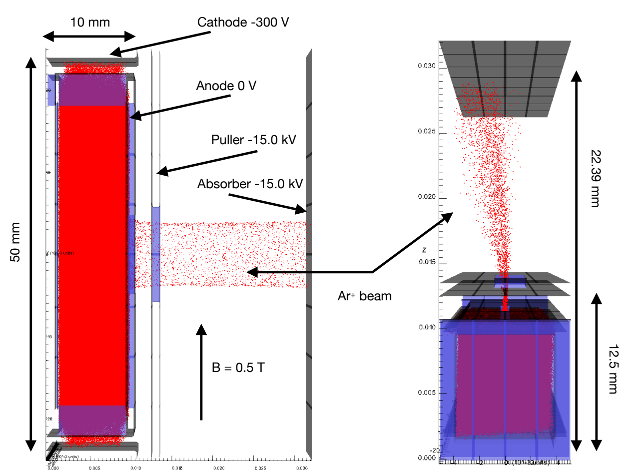

Figure 1: Diagram of the model Penning ion source. Cathodes are at the top and bottom of the plasma chamber. The singly ionized argon beam is deflected by a vertical magnetic field and is measured between 5 and 10 mm downstream from the puller electrode depending on the simulation parameters.

Our simulations start with a cold neutral gas of argon that is ionized by electrons emitted from the cathodes. Electrons are confined to the plasma chamber by a strong magnetic field, and ions are extracted from the chamber by a puller electrode. In our simulations we achieve an electron density of about $N_e \approx 2 \times 10^{17}\ /m^3$ and a temperature of about 1.6 eV.

BEAM EMITTANCE MEASUREMENTS

We measure the transverse beam emittance approximately 10 mm downstream from the puller electrode. The potential on this boundary is set to be the same as that on the puller electrode so that ions are free-streaming in this part of the simulation. Figure 2 shows the transverse emittance for simulations with extraction voltage $V_e = -15.0$ kV. The top plot in the figure is for a chamber aperture height of 10.0 mm. Deflection of the beam by the magnetic field is evident in the phase space plots. The transverse emittance is calculated with respect to the global coordinate system, and so phase space is not projected onto the plane perpendicular to the average beam propagation. Hence the phase space distribution for $X - X'$ is essentially a skewed Gaussian distribution. However, in the direction along the chamber aperture (Y-direction), the phase space is properly transverse but nevertheless the beam distribution is distorted into a S-shape. We surmise this is due to edge effects from the aperture in the plasma chamber. Ions that are created by ionization away from the aperture can only exit the plasma chamber if they have a larger y-component of velocity. This causes the distribution of ions in the long direction to be highly non-uniform, with higher densities at the extremes of the beam, as can be seen in Fig. 2.

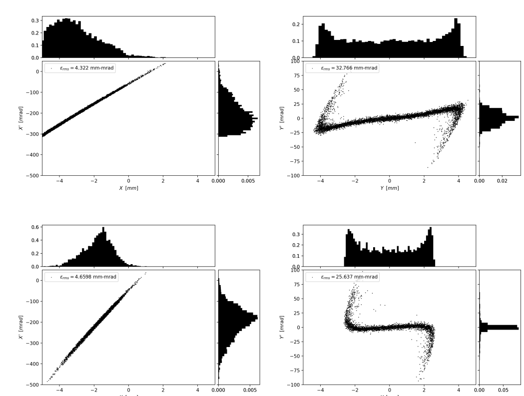

Figure 2: Transverse beam emittance in simulations with chamber aperture height 10.0 mm (top) and 7.5 mm (bottom).

Compare this with simulations where the plasma chamber aperture is 7.5 mm in height instead of 10.0 mm, as shown in Fig. 2(bottom). Here there is less of a skew in the transverse phase space in X and the Y-velocity does not have a pronounced tilt. While the beam size in the long transverse direction is smaller (hence smaller emittance in this direction), the S-shape is still observed. In addition, there is lower beam current in this case compared to the previous case.

As one would expect, an aperture that is 25% smaller in the Y-direction results in a lower emittance in that direction. In our simulations, the $Y - Y'$ emittance is about 21.75% lower for the smaller aperture, but the total beam current is lower by approximately 70%. We calculate that the beam

ISBN: 978-3-95450-247-9 ISSN: 2673-5490 doi: 10.18429/JACoW-IPAC2024-MOPR75

brightness of the small aperture case is approximately 38% of the brightness of the beam in the larger aperture case.

MODELING THE PLASMA MENISCUS

The shape of the plasma meniscus plays an important role in both beam formation and quality [8], and so accurate modeling of the electric potential in the plasma chamber is needed in order to accurately predict beam quantities. VSim is able to self-consistently compute both plasma buildup and beam formation in the plasma chamber, as well as beam transport through the extraction optics. This is an improvement over models that are calibrated to experimental measurements and only follow the beam after it has left the plasma chamber.

In VSim, we can either import geometries from CAD files or construct geometries using primitive shapes. Geometries are assigned material properties, and we model both dielectrics and conductors. Uniquely for VSim, our geometric models are 2^{nd}-order accurate for cut cells, meaning that the calculation of electric potential in computational cells that are *cut* by geometry are treated as conformal boundaries instead of stair-stepped [9]. This provides more accurate approximations of the potential near surfaces, which is especially important for particle/surface processes, such as sheath formation and secondary electron emission.

Figure 3 shows a comparison of the unperturbed electric potential in simulations with different plasma chamber aperture sizes. The plasma meniscus can be seen in Fig. 3. Because of the large range of scales for the potential, note the scale in the figure. Differences in the shape and extent of the meniscus in the two simulations are significant enough to translate to differences in the beam formation.

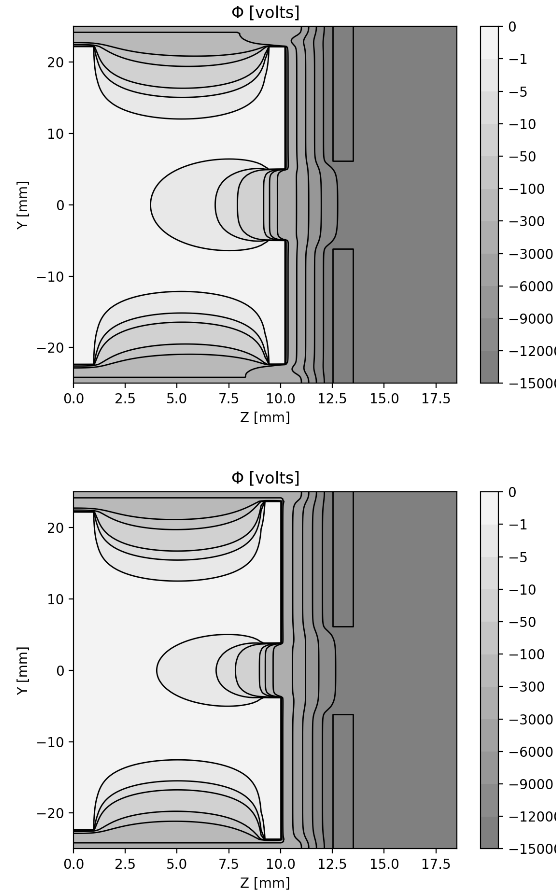

Figure 3: Comparison of electric potential for two different simulations. Note the differences in the shape and extent of the meniscus. Top figure is with an aperture of 10.0 mm and bottom figure is for of 7.5 mm.

ACCURATE AND EFFICIENT MODELING OF PLASMA CHEMISTRY

We model argon gas in our examples here, and restrict our simulations to only include singly-ionized argon ions. This is appropriate for Penning sources in many cases, however for other real-world applications more complex plasma chemistry models are required. We use quantemolDB [10] to obtain reaction cross sections for electron interactions with charged and neutral species of interest. QuantemolDB has a plugin to export cross sections into VSim format so the inclusion of accurate plasma chemistry into our ion source models is seamless. In general for singly-ionized, single-species plasmas, it is important to include not just ionization from the the ground state neutral atoms, but also excitiation/de-excitation and ionization from excited states as well. This can have a significant affect on the total ionization rates; typically increasing the ionization since low-energy electrons can ionize excited states more easily than from the ground state. To improve performance, we reduce the number of possible reactions using quantemol's Boltzmann global (0-D) model.

More complex plasma chemistries are important for ion implantation and etching devices. These include using both multi-species gasses and modeling higher ionization states. The plasma chemistry models built into VSim allow us to self-consistently simulate ion sources with more complex dynamics.

CONCLUSION AND FUTURE WORK

In this paper we presented simulation results of a Penning-type ion source that integrates complex, accurate plasma formation modeling with beam extraction and measurement. In future work we will compute the bend plane phase space transverse to the beam radius of curvature, and will focus on expanding our modeling to more complex plasma chemistry sets and higher ion charge states relevant to ion implantation and etching sources We also intend to model similar ion source types, including Bernas sources, which are often used for implantation.

ACKNOWLEDGMENTS

The authors would like to thank Dr. Nicolas Savard for his invaluable assistance in determining the model parameters.

ISBN: 978-3-95450-247-9 ISSN: 2673-5490 doi: 10.18429/JACoW-IPAC2024-MOPR75

REFERENCES

[1] Simion Website, `https://simion.com`

[2] IBSimu Website, `https://ibsimu.sourceforge.net`

[3] A.T. Powis and I.D. Kaganovich, "Accuracy of the Explicit Energy-Conserving Particle-in-Cell Method for Under-resolved Simulations of Capacitively Coupled Plasma Discharges", *Phys. Plasmas*, vol. 31, no. 2, pp. 023901, Feb. 2024. `doi:10.1063/5.0174168`

[4] D. Main *et al.*, "Comparing Momentum-conserving and Energy-conserving Electrostatic Particle-In-Cell Schemes in VSim", *Journal of Physics: Conference Series*, vol. 2743, no. 1, p. 012021, 2024. `doi:10.1109/ICOPS45740.2023.10481505`

[5] S. Veitzer and D. Main, "Advances in Particle-In-Cell Modeling of Low-Temperature Plasma Ion Sources", *J. Phys. Conf. Ser.*, vol. 2743, p. 012021, May 2024. `doi:10.1088/1742-6596/2743/1/012021`

[6] VSim Website, `https://txcorp.com/vsim`

[7] C. Nieter and J.R. Cary, "VORPAL: A versatile plasma simulation code", *J. Comput. Phys.*, vol. 196, no. 2, pp. 448-473, 2004. `doi:10.1016/j.jcp.2003.11.004`

[8] D. Faircloth *et al.*, "The Child Langmuir Illusion", presented at the ICIS 2023, 2023.

[9] S. Dey and R. Mittra, "A locally conformal finite-difference time-domain (FDTD) algorithm for modeling three-dimensional perfectly conducting objects", *IEEE Mic. and Guided Wave Lett.*, vol. 7, no. 9, 1997. `doi:10.1109/75.622536`

[10] QuantemolDB Website, `https://www.quantemoldb.com`.