SIMULATION-DRIVEN OPTIMIZATION OF HEAVY-ION PRODUCTION IN ECR SOURCES*

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Abstract

Next-generation heavy-ion beam accelerators require a wide variety of high charge state ion beams (from protons to uranium) with up to an order of magnitude higher intensity than that demonstrated with conventional Electron Cyclotron Resonance (ECR) ion sources. Optimization of the ion beam production for each element is therefore required. Efficient loading of the material into the ECR plasma is one of the key elements for optimizing the ion beam production. High-fidelity simulations provide a means to understanding the deposition of uncaptured metal atoms along the walls. This information would help to optimize the loading process into the ECR plasma. We are currently extending the plasma simulation framework VORPAL with models to investigate effective loading of heavy metals into ECR ion source via alternate mechanisms, including vapor loading, ion sputtering and laser ablation. First results of the ion production for different loading scenarios are presented.

INTRODUCTION

The development of a high performance electron cyclotron resonance ion source (ECRIS) has been identified as one of the key requirements for a successful development of the next-generation rare isotope beam facilities such as RIA, the FAIR project at GSI and the radioactive ion beam factory in RIKEN. These next generation heavy ion beam accelerators require a great variety of high charge state ion beams (from protons to uranium) with up to an order of magnitude higher intensity than demonstrated with conventional Electron Cyclotron Resonance (ECR) ion sources. A particular focus is set on the reliable production of high-intensity metal ion beams, especially uranium. In the US, the fully superconducting 28 GHz ECRIS VENUS (**V**erstaile **E**CR ion source for **NU**clear **S**cience, [1]) at LBNL has been selected as a prototype source for such a next-generation heavy ion accelerator. Since it started operation with 28 GHz microwave heating in 2004, many world record ion beam intensities have been produced. For example 2.8 emA of O^{6+}, 200 eμA of U^{33+}or U^{34+}, and in respect to high charge state ions, 1 eμA of Ar^{18+}, 133 eμA of Ar^{16+}, 28 eμA of Xe^{35+} and 4.9 eμA of U^{47+} have been produced. However, reliable and efficient long-term production of intense uranium beams is still the subject of intense R&D, including a longer term program at LBNL.

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In addition to uranium, some of isotopes such as ^{48}Ca, ^{96}Zr, ^{112}Sn, ^{64}Ni etc., that required for the production of radioactive isotopes are quite expensive and rare and it is therefore critical to efficiently load them into the ECR plasma. While capturing efficiencies for gases into ECR sources like VENUS can be higher than 80% and the efficiency for producing one charge state can reach 20% [2] the capture efficiency for metals, especially for high-temperature materials is very small, typically lower than a few %, since the metal atoms stick to the cold plasma chamber walls and are lost from the plasma.

High-fidelity simulations provide the best approach for understanding where along the interior walls the un-captured metal atoms are deposited and, hence, to optimize loading of the metal into the ECR plasma.

Here we report on initial results of a novel fully-kinetic simulation code, based on the VORPAL simulation framework, to investigate effective loading of heavy metals into ECRIS via alternate mechanisms: vapor loading, ion sputtering and laser ablation.

THE VORPAL PLASMA SIMULATION FRAMEWORK

The VORPAL plasma simulation framework [3,4] is a joint project between the University of Colorado and Tech-X Corporation. While originally designed as a tool for simulating the interaction of intense laser beams with plasmas, the versatility of the code has allowed modeling in a variety of different areas over time.

In order to model ECR ion source plasmas, VORPAL had to be extended to include kinetic ionization, in order to simulate the generation of higher charge states. In addition, mechanisms to allow the simulation of devices on meter scale length over timescales of milliseconds had to be developed for the VORPAL simulation framework. In the following, some of these enhancements are described.

Kinetic Ionization Model

The kinetic ionization model in VORPAL is based on the so-called Monte Carlo Collisions (MCC) algorithm, which determines at each time-step the probability that a collection of particles undergoes a certain process. In our case, this process is the ionization or recombination of a particle. Based on a random variable, the process is then either performed or not. Originally, this algorithm was developed for collisions among particles, but ionization is a straight forward extension of this process.

A major challenge in modeling ionization and recombination processes via MCC is the ionization cross

sections model, especially for high-Z elements. VORPAL currently has access to three different ionization cross-section models: The empirical Lotz formula [5], the Shull&VanSteenberg [6] refinement, mainly based on newer measurements and including both ionization and recombination, and the binary encounter dipole model of electron-impact ionization [7], a generalization of the classic Lotz model, which provides ionization cross-sections for arbitrary elements. These models have been incorporated into the physics library TxPhysics, which is available independently of VORPAL[8].

The binary encounter model currently includes parameterized ionization cross sections for Hydrogen, Helium, Lithium, Oxygen and Uranium. The parameters include the ionization potential as well as the number of outer shell electrons for each charge state. For a more accurate estimate one would have to sum over atomic orbitals and have knowledge of the binding energy, the mean kinetic energy, and the number of electrons of each orbital. Refined cross sections also use the orbital dipole moment as a parameter.

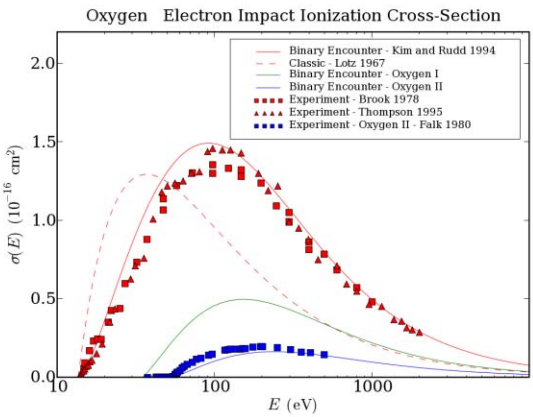

Figure 1: Comparison of different theoretical and experimental ionization cross-sections for the lower ionization states of Oxygen.

Figure 1 shows a comparison of the different cross-section models, as well as experimental data, for the lower ionization states of Oxygen.

Figure 2 shows the temporal evolution of the different charge states of oxygen for a plasma initially consisting of neutral Oxygen, O^+ and e^- and the Shull&VanSteenberg model for the ion cross-section was used.

Higher Order Particle Shapes

A challenge in kinetically modeling ECRIS is the large discrepancy of time- and length scales encountered in these devices. One of the key requirements to model plasmas with first order particle-in-cell methods is that the Deybe length has to be resolved by the spatial grid in order to prevent artificial heating of the plasma. However, for plasmas encountered in ECRIS, the Debye length often is on the order of a few micron, whereas the device scale length is on the order to tens of cm. This results in prohibitively large computational grids. However, if the Debye length is not resolved by the grid, an unphysical instability known as 'grid heating' develops resulting in an increase of the mean thermal velocity of the plasma.

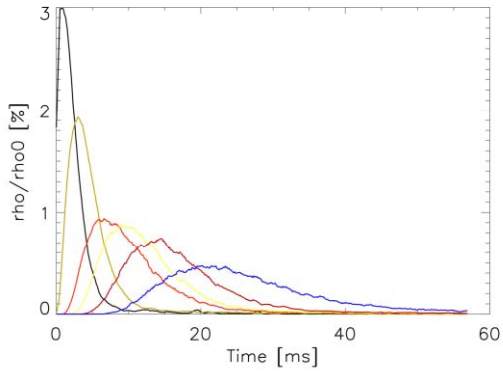

Figure 2: Temporal evolution of the different ionization states of oxygen in a plasma initially loaded with Oxygen, O^+ and e^-. O^{2+} (black), O^{3+} (brown) , O^{4+} (orange), O^{5+} (yellow), O^{6+} (purple) and O^{7+} (blue). O^{8+} was not included in this model.

One approach to prevent the numerical heating of electrons within a manageable grid size is to eliminate the effect of the self-consistent electric field onto the electrons. This approach can be justified in an ECRIS, since the electrons are highly magnetized and their dynamics is mainly determined by the motion along the magnetic field consisting of a sextupole field and a magnetic bottle.

Another way of avoiding numerical heating is to use higher order particle shapes, which essentially extends the particle over multiple grid cells, making the particle less susceptible to numerical noise and prevents numerical heating., even if the Debye length is not resolved.

Therefore, we implemented higher-order particle shapes in VORPAL and investigated their performance. Figure 3 shows the evolution of the plasma temperature for different particle shapes in a 2D electrostatic simulation, starting with a highly unresolved Debye length of $\lambda_D/dx=0.01$.

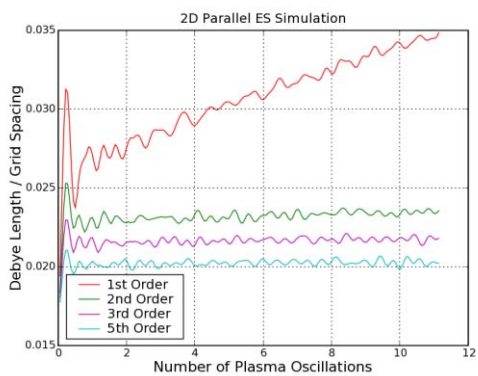

Figure 3: Evolution of the electron Debye length relative to the grid size for different particle shapes. Higher order particle shapes avoid the numerical heating observed in 1st Order particles.

COMPARISON OF DIFFERENT LOADING LOCATIONS

With the new models in place, VORPAL can now be used to investigate and optimize vapor loading variables of an ECRIS such as the initial angle of the injected neutral gas.

These simulations were run on a 20 x 20 x 100 cell grid, spanning a 0.2 m x 0.2 m x 1 m domain. Electrons were only affected by the magnetic field. The imposed magnetic field, consisting of a magnetic bottle and a sextupole field, was loaded with electrons by expanding a cubic electron population of density 10^{18} m^{-3} in the center of the bottle. The magnetic bottle is modeled as

$$B_z = B_0(z) + \frac{r^2}{4}\partial_z^2 B_0(z)$$

$$B_r = -\frac{r}{2}\partial_z B_0(z) - \frac{r^3}{16}\partial_z^3 B_0(z)$$

where $B_z(r,z)$ and $B_r(r,z)$ are the axial and radial fields, respectively, expanded from the axial magnetic field $B_0(z)=B_z(r=0,z)$.

The neutral Oxygen source is located close to the magnetic bottle neck and the Oxygen either streams into the domain radially or axially to the magnetic bottle. In order to accelerate these initial simulations, all ionization cross-sections were scaled by a factor of 10^3.

Figure 4 shows the spatial ion density distribution 10 μs after the simulation was launched. In case of radial loading, the O^{3+} and O^{4+} ions are captured by magnetic field and leave the device. Basically no O^{3+} and O^{4+} ions can be found in the center of the magnetic bottle.

In case of axial loading, a larger number of neutrals can penetrate into the low-magnetic field region close to the center of the magnetic bottle. This leads to a large population of O^{3+} and O^{4+} in the center of the source, where they eventually can be extracted. All modeled charge states can be observed in the center of the magnetic bottle.

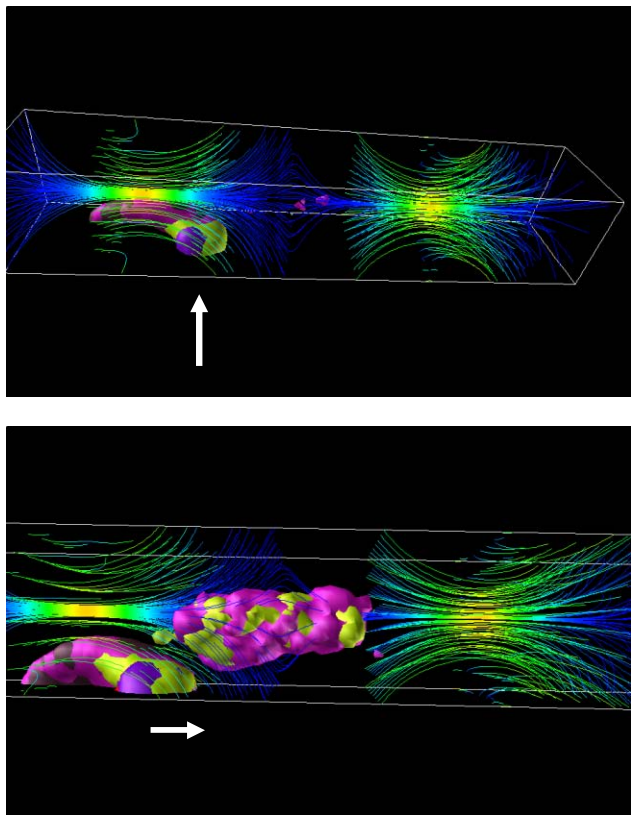

Figure 4: Comparison of different loading scenarios for oxygen: Radial loading (top) vs. axial loading (bottom). The arrow indicates the location and direction of the neutral Oxygen source. The iso-surfaces for O^{3+} (purple) and O^{4+} (yellow) are shown at the same levels in both figures. In addition, the field lines of the magnetic bottle are shown.

SUMMARY

The plasma modeling framework VORPAL has been extended with models to help simulate the plasma in ECRIS. This includes a kinetic ionization model with different parameterizations for the ionization cross-sections, as well as higher order particle shapes which help to prevent numerical heating for coarse grid resolutions. Initial simulations of ECR plasma configurations show that a significantly different ion population can result depending on the initial injection angle of the vapor.

The results agree with experimental practice, where the neutral gas is injected in axial direction, rather than radial to the magnetic bottle. This is a first indication that the modeling tool can be used in order to guide experiments.

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