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Los Angeles

DC Plasma Interactions with Structured Surfaces

A dissertation submitted in partial satisfaction
of the requirements for the degree
Doctor of Philosophy in Aerospace Engineering

by

Cesar Eduardo Huerta

2019

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2019

ABSTRACT OF THE DISSERTATION

DC Plasma Interactions with Structured Surfaces

by

Cesar Eduardo Huerta

Doctor of Philosophy in Aerospace Engineering

University of California, Los Angeles, 2019

Professor Richard E. Wirz, Chair

Plasma-material interactions (PMI), such as sputtering, electron emission, and deposition, play an important role in the evolution of surface geometry and its effects on the plasma and sheath properties for a wide range of plasma devices and applications. In the work presented herein, the effects of sputtering, deposition, and secondary electron emission are modeled in order to better understand these physical phenomena and the effect of surface structure on PMI.

The sputtering model developed in this work accurately captures surface architecture effects via a computationally-efficient view factor model. The model reveals that increasing the surface pitch angle beyond about 45° can lead to significant decreases in the normalized net sputter yield for all simulated ion incident energies (i.e. 75, 100, 200, and 400 eV) for both smooth and roughened surfaces. At higher incident energies, smooth triangular surfaces exhibit a nonmonotonic trend in the normalized net sputter yield with surface pitch angle with a maximum yield above unity over a range of intermediate angles. The resulting increased erosion rate occurs because increased sputter yield due to the local ion incidence angle outweighs increased deposition due to the sputterant angular distribution. For nano-rod surfaces, the model captures the coalescence of sputterants at the protuberance sites and accurately illustrates the structure's expansion due to deposition from surrounding sputtering surfaces, thus demonstrating the capability to aid in developing favorable surface

applications for plasma applications.

Similarly, a particle pushing model is used to investigate secondary electron emission for varying effects of complex surfaces by using simple geometric constructs. Geometries used in the model include: vertical fibers for velvet-like surfaces, tapered pillars for carpet-like surfaces, and a cage-like configuration of interlaced horizontal and vertical fibers for nano-structured fuzz. The model shows that unlike other structured surfaces previously studied, tungsten fuzz exhibits secondary electron emission yield that is independent of primary electron incidence angle, due to the prevalence of horizontally-oriented fibers in the fuzz geometry.

The PMI physics simulated in these models are implemented into a DC discharge plasma model, DC-ION. Along with these additions, the code is improved and modified to simulate a canonical plasma column incident on a variable anode surface. Simulation results are compared with experimental data obtained for an aluminum slab surface, as well as two aluminum foams with different porosities. Simulation results show good agreement with the experimental data and agree with analytical expectations of the impact that architected surfaces have on the plasma. These results show that these featured surfaces are the promising candidates for improving a wide range of plasma devices, including electric propulsion, laboratory plasma sources, and high-temperature fusion devices.

The dissertation of Cesar Eduardo Huerta is approved.

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University of California, Los Angeles

2019

*I am eternally grateful to my mother and father,
your sacrifice lit my way.*

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PUBLICATIONS

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Huerta C E, Patino M I, Wirz R E, “Secondary electron emission from textured surfaces”, *Journal of Physics D: Applied Physics* **51** (14), 2018

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Li G Z, Huerta C E, Wirz R E, “Computational Modeling of an Axial Ring Cusp Hybrid Discharge for the MiXI Thruster”, *54th AIAA Propulsion and Energy Forum*, 2018

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CHAPTER 1

Introduction

The interactions of bounded plasmas with surface materials through sputtering, redeposition, and electron-induced secondary electron emission (SEE) significantly impacts the performance of plasma devices. These plasma-material interaction (PMI) effects are important for a wide variety of applications, such as plasma processing [1, 2], electric propulsion [3, 4, 5, 6, 7, 8, 9, 10, 11], and fusion [12, 13, 14, 15, 16, 17].

Ions, accelerated by the sheath, bombard plasma-facing surfaces and lead to sputtering of neutrals which can contaminate the plasma. These neutrals can also be ionized by primary electrons and redeposit onto surfaces, leading to increased downtime for fusion reactors [18]. Sputtering of surfaces results in erosion, which for many devices, can limit the lifetime of certain components (tokamak divertors, ion thruster grids, etc.). SEE leads to a reduction in the sheath potential and plasma bulk electron temperature, as well as increased wall heat losses [19]. In combination, these SEE effects could lead to a decrease in the rate of ionization in the plasma bulk.

Surface texturing suppresses the effects of PMI by capturing and trapping particles emitted from the surface, thereby reducing the net sputtering and SEE yields (the ratio of emitted to incident particle fluxes) [20, 21, 22, 23, 24]. In 1962, Rosenberg and Wehner observed the effects of surface features on net sputter yield by exposing a threaded surface to argon ions and noting a decrease in measured sputter yield due to sputterant deposition [25]. More recently, tungsten fuzz has generated interest due to its natural occurrence under tokamak disturbance-like conditions [26, 27, 28, 29, 30], which could allow for the sustained reduction

of SEE. A similar reduction in the yield has also been estimated for ion-induced electron emission (IIEE) from tungsten fuzz [31].

The work presented herein focuses on computationally efficient modeling of sputtering and SEE. These models are used to gain insight into the effects of surface texturing on PMI and are integrated into a self-consistent plasma-surface model to help understand the dynamic interactions between the surface, the sheath, and the plasma (see figure 1.1).

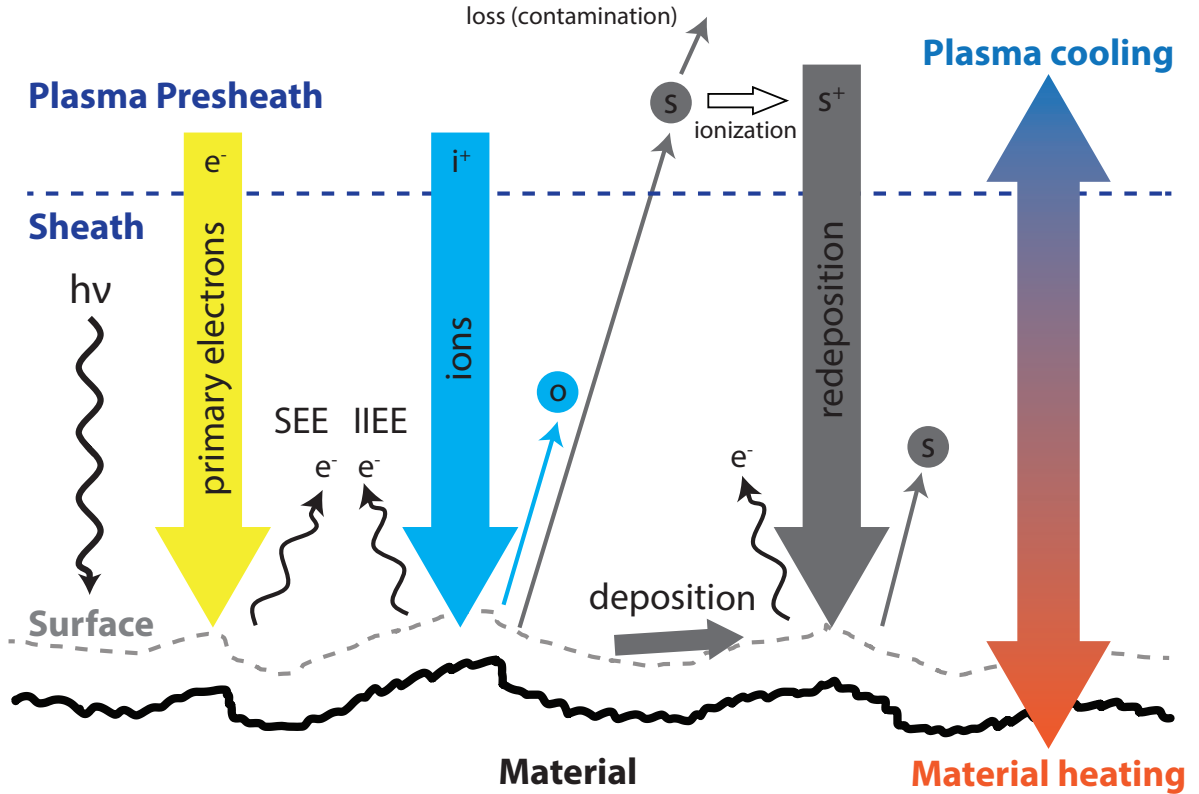


Figure 1.1: Interactions between plasma, surface, and sheath due to sputtering, deposition, redeposition, and SEE.

1.1 Motivation

Plasma material interactions have been observed to adversely affect the performance of plasma devices. Sputtering can limit the lifetime of conventional electric propulsion (EP)

thrusters and lead to contamination of fusion plasmas, lowering their performance. As primary electrons bombard the surface, depositing their energy and emitting slower secondary electrons, the plasma sheath potential decreases, resulting in an overall cooling of the plasma and decreased device efficiency (see figure 1.2).

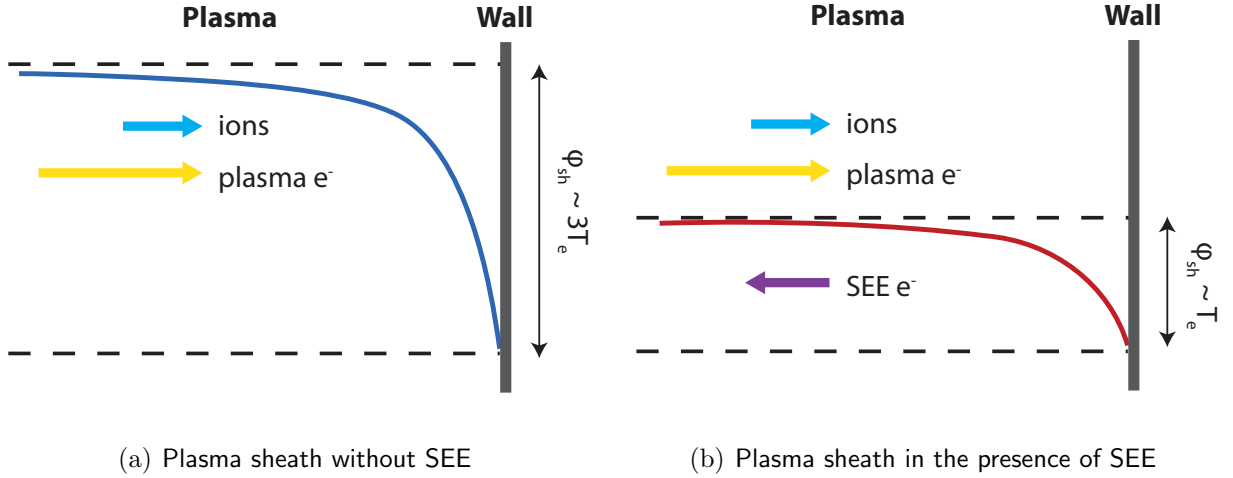


Figure 1.2: Secondary electron emission effects on plasma sheath potential.

1.1.1 Electric Propulsion

Electric propulsion devices, such as ion and Hall-effect thrusters, accelerate charged particles electrostatically or electromagnetically in order to achieve high exhaust velocities. This results in much higher specific impulse compared to conventional chemical thrusters. As seen from the rocket equation, high I_{sp} leads to significant reductions in the propellant mass required to achieve a given Δv

$$m_{prop} = m_o \left[1 - \exp \left(-\frac{\Delta v}{I_{sp}g} \right) \right] \quad (1.1)$$

where m_o is the initial (wet) spacecraft mass and $g = 9.8\text{m s}^{-2}$. Electric propulsion thrusters can enable high Δv missions typically not attainable with chemical propulsion, such as deep-

space missions and those with extended mission lifetimes with commercial and scientific objectives (e.g. GPS, satellite TV/radio, and Earth science). Thus, ensuring the longevity of these thrusters is vital to their viability and applicability. Two of the most common EP devices in use today are ion and Hall-effect thrusters.

Ion thrusters operate by producing electrons via a hollow cathode within the discharge chamber, as shown on figure 1.3. The electrons are accelerated by the anode (i.e. the discharge chamber walls) and collide with neutral gas atoms, which are injected into the chamber. Through these collisions, the propellant gas is ionized, and the ions are accelerated out of the thruster by the screen and accelerator grids. The grids form an electric field such that they are transparent to the ions but confine the neutral gas atoms inside the discharge chamber, while electrons are confined by a magnetic field (which is too weak to affect the ions). Finally, a neutralizer cathode ejects electrons away from the thruster to prevent charge buildup, which could cause arcing and damage the spacecraft.

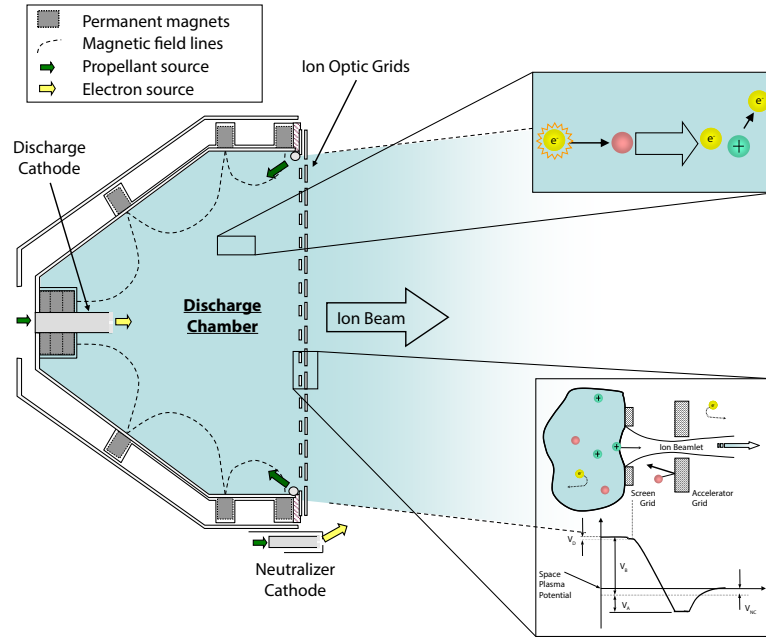
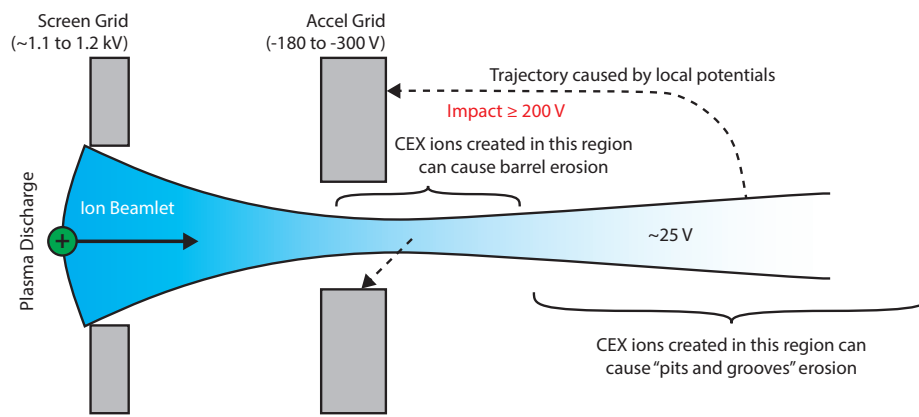


Figure 1.3: Ion thruster operation.

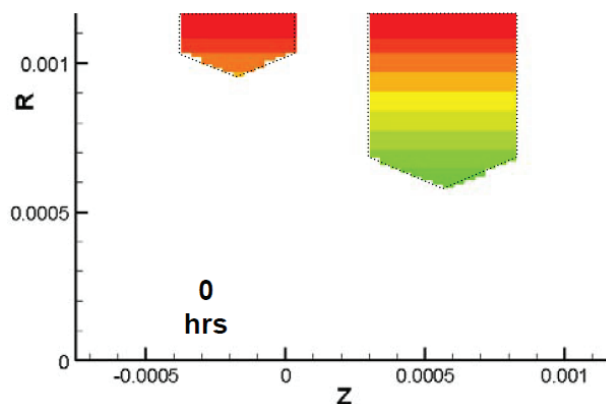
Brophy, Polk, and Rawlin identified 18 failure modes for the NASA Solar Technology Application Readiness (NSTAR) thruster, ten of which are caused by sputtering and erosion [32]. Charge exchange (CEX) collisions near and downstream of the accel grids between the emitted ions and neutral atoms that escape through the grids cause barrel erosion, as well as the formation of pits and grooves (see figure 1.4). As the grids erode, neutrals can more easily escape the discharge chamber, decreasing propellant utilization (a measure of how efficiently the propellant is ionized) and leading to more CEX collisions. Eventually, the grids are no longer able to confine the neutral gas and the ion thruster ceases to operate.

1.1.2 Fusion Devices

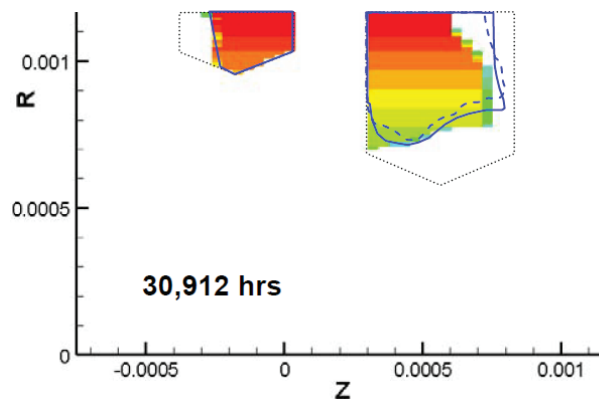
Similarly, erosion of the first wall and divertor (see figure 1.5) can limit component lifetimes in magnetic fusion reactors and sputtering can decrease the core plasma fuel density and fusion power [18]. The first wall surrounds the toroidally-shaped plasma (confined by strong magnetic fields) in order to shield external components from bombardment by the hot deuterium and tritium particles. The divertor, located at the bottom of the tokamak, collects energetic He particles and other impurities. In tokamaks, SEE increases the heat transmission to the wall and releases cold electrons into the scrape-off layer [16, 34]. Understanding PMI and its effects on the plasma may be key to improving the performance of current propulsion and fusion technologies.



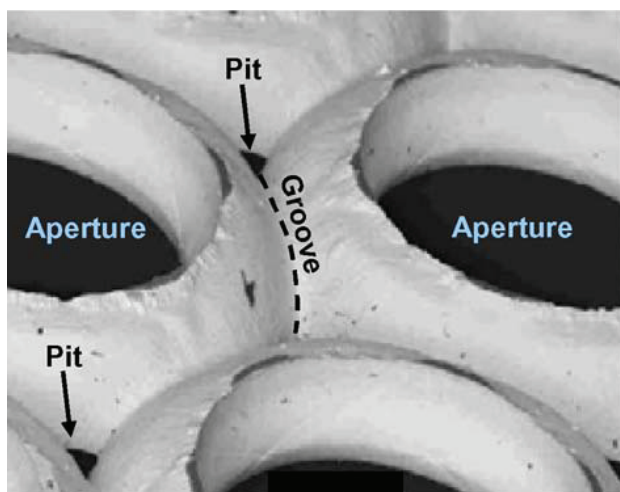
(a) CEX collisions in the ion beamlet cause erosion of the accel grid.



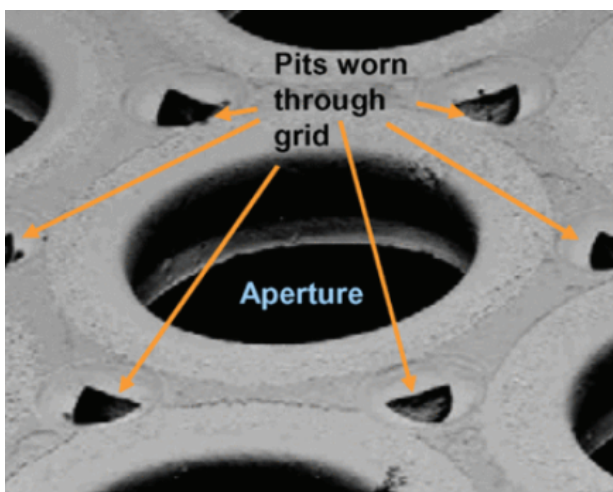
(b) Nominal grid.



(c) Simulation of grid erosion after 31,000 of operation (see Ref. [33]).



(d) Downstream grid erosion.



(e) Upstream grid erosion.

Figure 1.4: Erosion of the NSTAR ion thruster grids after 31,000 hours of operation.

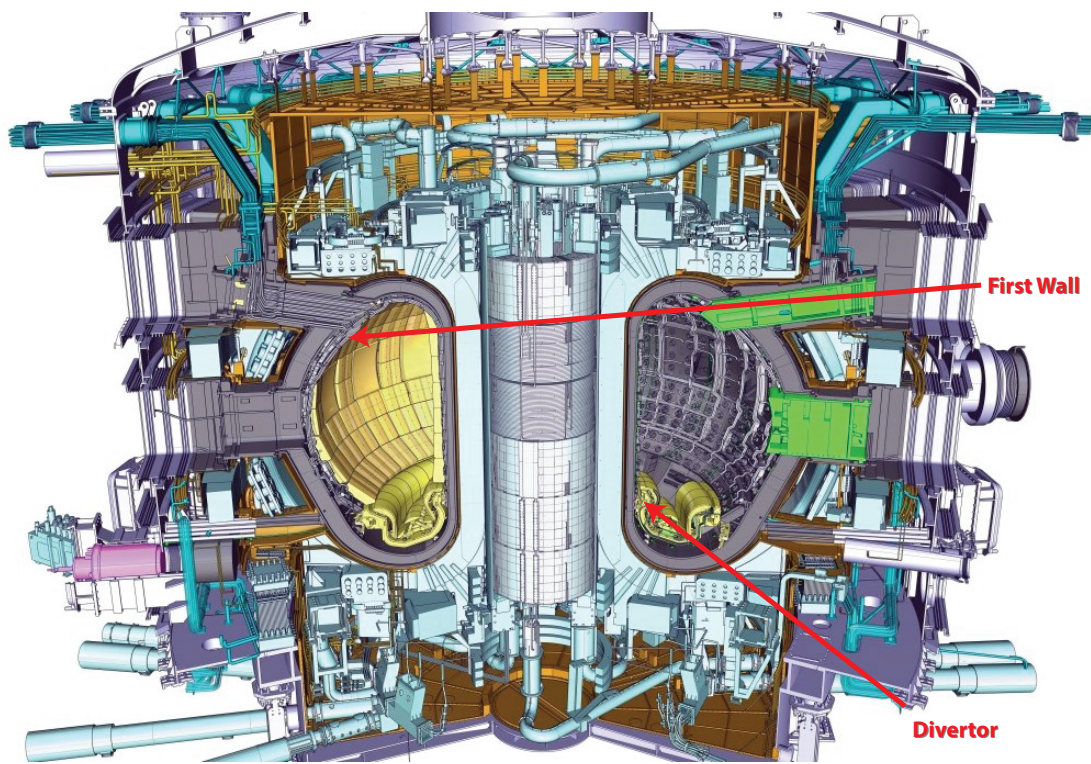


Figure 1.5: International Thermonuclear Experimental Reactor (ITER) schematic. Courtesy of www.iter.org

1.2 Thesis Objective and Approach

Previous work has been done to computationally simulate sputtering [35, 36] and SEE [37, 38, 39] for different thrusters and plasma-facing surfaces. However, there are no comprehensive models which couple the plasma, sheath, and material physics for low energy, low density devices (such as EP and laboratory plasmas). In addition, although the effects of complex surface texturing on PMI have been experimentally studied (i.e. fuzz, velvet, carpet), computational models have been limited to simulating simple surface patterns. The goal of this thesis is to address these needs.

To properly understand and simulate the complex, interconnected effects between the plasma and its bounding surfaces, varied physical phenomena must first be understood. The approach to accomplishing these objectives is:

- To develop analytical and computational models of PMI, such as sputtering, erosion, and electron emission.
- To understand how complex surfaces affect PMI through geometric trapping (i.e. by reducing the yield or changing the dependence of emission on incidence angle).
- To develop a coupled DC discharge plasma and PMI model in order to understand the effects of plasma parameters on PMI, and vice versa.

1.3 Dissertation Overview

Chapter 2 will focus on modeling and a discussion of results on sputtering. 2D and 3D simulations of sputtering from and erosion of textured surfaces will be presented, with analytical models used to supplement the simulation results. Validation of the sputtering model is presented in the appendix.

Chapter 3 covers modeling of SEE and the effects of surface texturing on it. Several

simple geometries are presented which simulate complex surface structures, such as velvet, carpet, and fuzz. These surfaces have been previously studied by other groups and have been used to improve the performance of plasma devices. In conjunction, these simulations will show the importance of properly and accurately modeling the surface's geometry when calculating the SEE yield and its dependence on incident conditions. Additional simulations of ion-induced electron emission (IIEE) from carbon velvet and tungsten fuzz are presented and discussed in the appendix section.

Chapter 4 presents work done with DC-ION, including improvements and modifications made to the code in order to simulate a canonical plasma column. Implementations of SEE and sputtering physics into DC-ION are discussed. Results and comparisons with experimental data are presented and discussed.

Finally, chapter 6 concludes this dissertation by summarizing the key results and contributions, and will propose future work necessary to continue this endeavor.

CHAPTER 2

Sputter-Deposition on Structured Surfaces

The UCLA Plasma Interactions (Pi) facility was developed to study the effects of surface architecturing on the sputtering and erosion of materials [40]. These materials are known to capture sputterants and therefore reduce the overall erosion rate [41]. In order to gain a better understanding of these processes and to guide experimental efforts, a view factor computational model was developed and validated. This computational model was applied to different surface configurations which are exposed to EP-like plasmas in order to investigate the dynamic interactions between the evolving surface and the plasma environment [20, 42]. Small-scale feature effects on net sputter yield through direct deposition of sputtered particles were examined, including surface patterning and micro-roughening. This was achieved through view factor modeling that accounts for the various off-cosine angular distributions of the sputtered particles that are known to occur at relatively low ion impact energies (~ 100 's of eV).

2.1 Theory

In a plasma, ions stream to the walls by accelerating through the sheath to velocities at or above the Bohm velocity, $v_B = \sqrt{kT_e/M}$. Energetic ions penetrate the surface and collide with wall atoms, imparting some of their energy onto the recoiling atoms. If these atoms gain enough energy to overcome the material's binding forces, they may escape the surface and be emitted as sputterants. The ratio of the sputterant flux to the incident ion flux is called the sputter yield [43].

Depending on the ion's incident energy, the sputtering events may be classified into one of three regimes: single-knockon, linear cascade, and spike regimes [43]. In the single-knockon regime, atoms only gain enough energy to possibly undergo a small number of collisions before being emitted. In the linear cascade and spike regimes, the recoiling atoms gain enough energy to generate secondary and higher generation recoils (see figure 2.1). The spike regime differs from the linear cascade regime by the higher density of recoiling atoms.

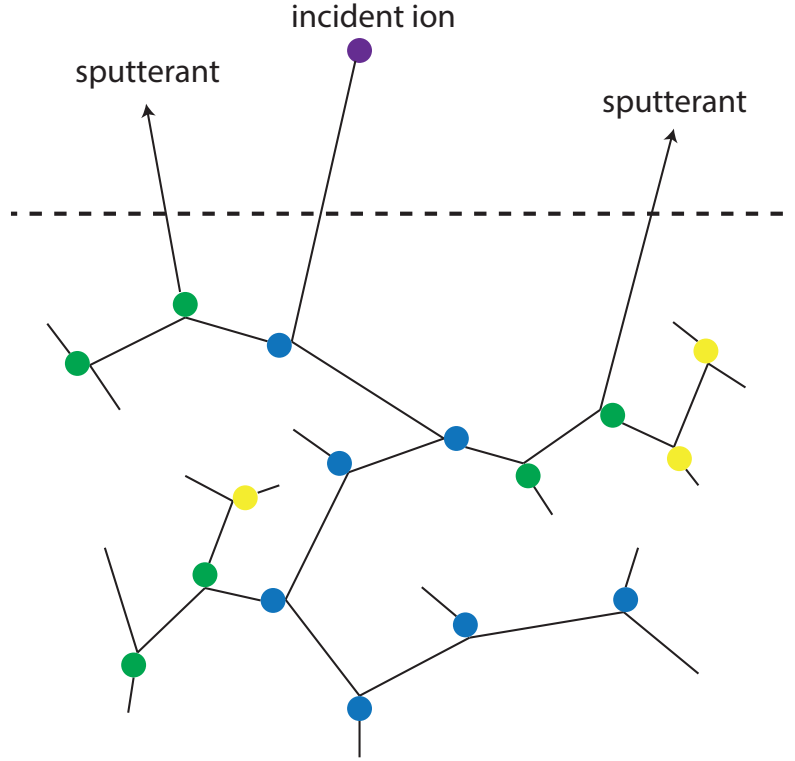


Figure 2.1: Sputtering of wall atoms due to recoils caused by incident ion collision cascade. Shown are primary, secondary, and tertiary recoils.

As the recoiling atom approaches the surface, the binding energy acts as a planar surface potential, decelerating the atom in the direction normal to the surface. This deceleration

causes the atom to be refracted as it exits the surface, as shown on figure 2.2:

$$\begin{aligned} E_1 \cos^2 \theta_1 &= E_0 \cos^2 \theta_0 - E_b \\ E_1 \sin^2 \theta_1 &= E_0 \sin^2 \theta_0 \end{aligned} \tag{2.1}$$

where 0 and 1 denote before and after emission and E_b is the surface binding energy [43]. Thus, if the energy normal to the surface is lower than the binding energy, the atom is incapable of sputtering.

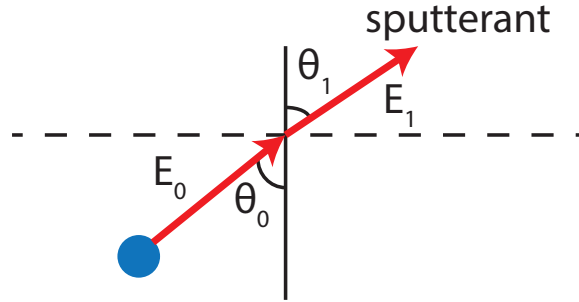


Figure 2.2: Atom being refracted by the surface binding energy.

Atoms struck by the incident ion near the surface are less likely to lose their energy to secondary and higher-generation recoil atoms and are more likely to have enough energy near the surface to overcome the binding force and be emitted. Furthermore, as ion incident energy increases beyond $\sim 10 - 100$ keV, the nuclear stopping cross section and stopping power increase, resulting in less energy being deposited near the surface as the ion is able to penetrate deeper into the material. Hence, the sputter yield initially increases with increasing incident energy, plateaus at the range indicated above, and then decreases past the keV range

[35]. The stopping cross section and power are given by

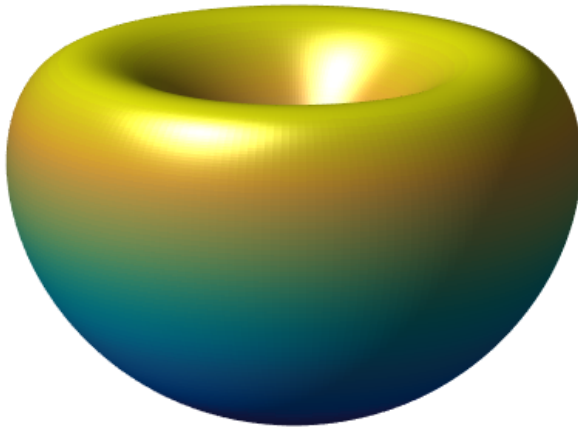
$$\begin{aligned}
S(E) &= \frac{1}{1-m} C_m \left(\frac{4M_1M_2}{(M_1+M_2)^2} \right)^{1-m} E^{1-2m} \\
C_m &= \frac{\pi}{2} \lambda_m a^2 \left(\frac{M_1}{M_2} \right)^m \left(\frac{2Z_1Z_2e^2}{a} \right)^{2m} \\
\frac{dE}{dx} &= -NS(E)
\end{aligned} \tag{2.2}$$

where m is proportional to E ($m = 1$ at high energies and ≈ 0 at low energies), λ_m is a dimensionless function of m , Z_1e and Z_2e are the nuclear charges, and a is the screening radius [43].

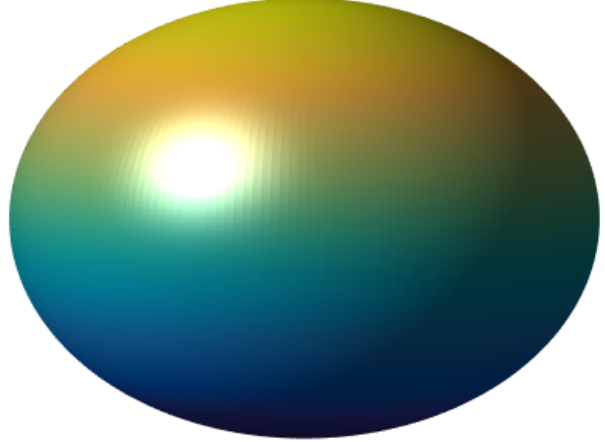
Similarly, the angle of incidence of the ions can affect the yield. Ions impacting the surface at the normal direction penetrate deeper and result in a lower probability of sputtering atoms. Near-grazing incidence angles (typically 80-90°) result in inefficient transfer of the ion's energy to the surface. Hence, the sputter yield increases with incidence angle up to a maximum value, θ_{max} , and then decrease back to 0 [35].

Not only does the yield depend on incident conditions, but the angular distribution of sputterants does as well. As shown on figure 2.3, as the incidence energy increases, atoms are sputtered at increasingly more cosine-like distributions. When the incidence angle increases, sputterants are emitted in a forward-biased distribution relative to the angle of incidence. These effects are in agreement with experimental measurements of the sputtering distributions for many different ion-material combinations [44].

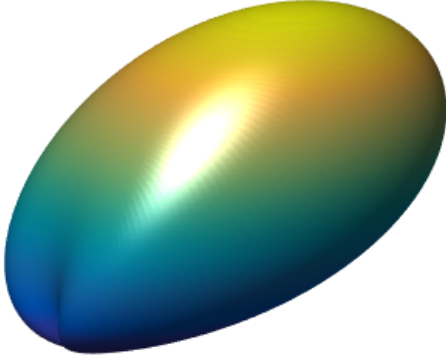
Because the sputtering yield, angular distribution, and their dependence on incident energy and angle are material-specific, the analytical and semi-empirical models will be reviewed in chapter 2.



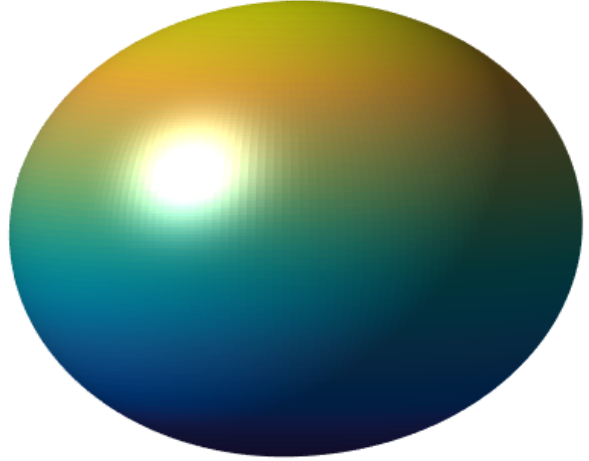
(a) Low incident energy and normal incidence.



(b) High incident energy and normal incidence.



(c) Low incident energy and high incidence angle.



(d) High incident energy and high incidence angle.

Figure 2.3: Sputtering angular distributions at different incidence conditions.

2.2 Model Overview

Previous sputtering models have relied on Monte Carlo methods to track the paths of sputterants [45, 46]. This is crucial for high density plasma cases, where sputterants are likely to ionize and redeposit onto exposed surfaces. For low energy, low density plasmas, the ionization mean free path of sputterants ($\lambda \approx 3$ cm for 2 eV Mo sputterants in a 10^{18} m^{-3} plasma) can be orders of magnitude longer than the sheath thickness (~ 10 's- 100 's of microns), and on the order of the device dimensions. Within the sheath, virtually all sputterants move

linearly. Some sputterants exit the sheath, ionize, and redeposit onto the surface, but at the low plasma densities studied ($10^{16} - 10^{18} \text{ m}^{-3}$), redeposition is negligible compared to sputtering erosion and deposition. For these reasons, a view factor approach proved to be attractive, since computational cost is reduced by an order of magnitude [47]. In addition, the code was paralellized using OpenMP to further decrease run time.

As shown on Fig. 2.4, the model takes plasma and surface geometry parameters as inputs and generates surface meshes. For each cell center, the sputter yield and view factor (accounting for cell-to-cell shadowing) are calculated. These calculations are repeated for all cell centers and the results are used to update the location of cell centers and nodes. This process is then iterated until the desired burn (or exposure) time is reached. The computational cost of this model is $\mathcal{O}(N_s N_d^2 N_t)$ for N_s cells sputtering onto N_d cells, with N_t time iterations (the N_d^2 term accounts for shadowing).

2.2.1 Sputtering Model

To model the sputter yield's dependence on ion incidence angle and energy, an empirical model established by Yamamura, Itikawa, and Itoh was used [48]. This model is based on empirical fits to parameters which are used to modify Sigmund's model [49]. Equations (2.3) have been previously used to predict Hall thruster lifetimes [50].

$$\begin{aligned}
\zeta &= 1 - \sqrt{\frac{E_{th}}{E}} \\
\frac{f}{f_s} &= 1 + 2.5 \frac{1 - \zeta}{\zeta} \\
\psi &= \frac{\psi_{1eV}}{E^{1/2}} \\
\theta_{opt} &= 90^\circ - 286\psi^{0.45} \\
\Sigma &= f \cos \theta_{opt} \\
\frac{Y(\theta_i)}{Y_0} &= (\cos \theta_i)^{-f} \exp[-\Sigma(1/\cos \theta_i - 1)]
\end{aligned} \tag{2.3}$$

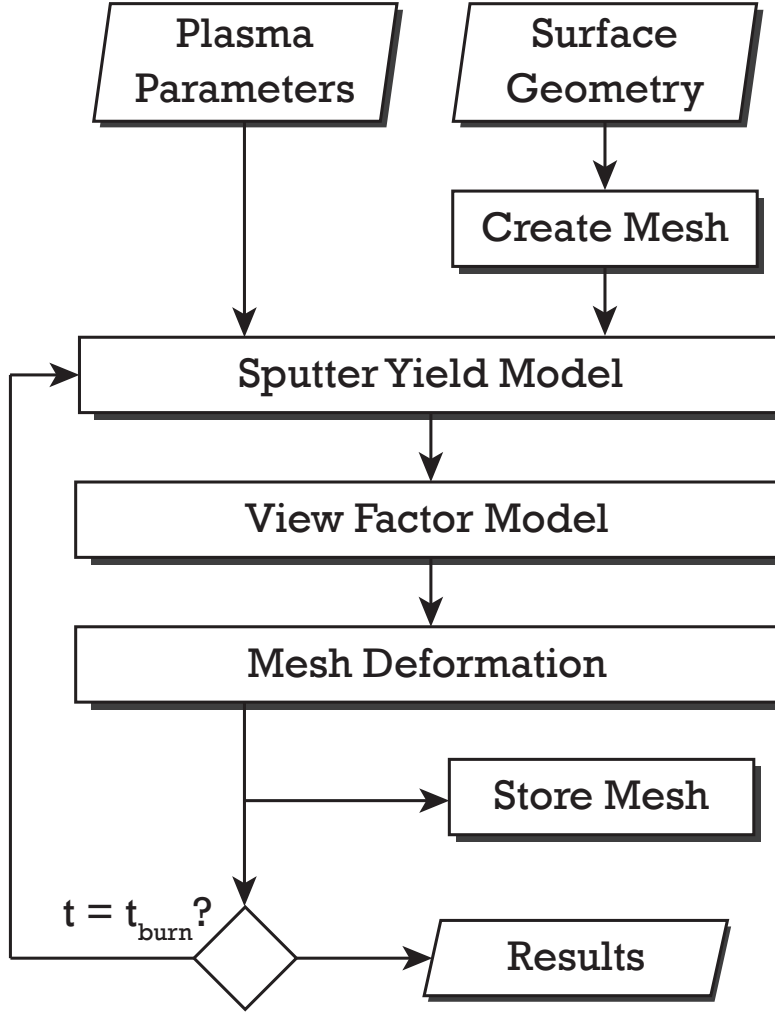


Figure 2.4: Sputtering-deposition view factor model flow chart.

Here, E_{th} , is the threshold energy, E is the ion incidence energy, θ_i is the ion incidence angle, Y is the sputter yield, and ζ , f , f_s , ψ , ψ_{1eV} , θ_{opt} , and σ are curve fit parameters which can be found in Ref. [48] for common ions bombarding on elementary target materials. For argon on nickel, $E_{th} = 27.66$ eV, $f_s = 1.73$, $\psi_{1eV} = 0.1353$, and $Y_0 = 0.545$. For xenon on molybdenum, $E_{th} = 63.45$ eV, $f_s = 1.85$, $\psi_{1eV} = 0.1465$, and $Y_0 = 0.28$.

For high energy applications, computational models such as The Transport of Ions in Matter (TRIM) can provide sputterant angular distributions. However, low energy ions relevant to electric propulsion (< 500 eV) are outside the range of validity of these models

[51, 52] and reliable measurements of these distributions are not well represented in the literature. Hence, a semianalytical model based on Zhang and Zhang's modifications to Yamamura's angular distribution model was used [53, 54].

$$S \propto \cos \theta \left(1 - \frac{1}{4} \sqrt{\frac{E_{th}}{E}} \left[\cos \theta_i \gamma(\theta) + \frac{3}{2} \pi \sin \theta_i \sin \theta \cos \phi \right] \right) \quad (2.4)$$

Equation (2.4) shows the dependence of the angular distribution, S , on the ion incident energy, E , the incident angle, θ_i , and the polar (θ) and azimuthal (ϕ) angles of the sputterants' velocity vectors. In this equation, Zhang and Zhang use E_{th} as a fitting parameter rather than the physical threshold energy (as in Eq. 2.3) to maximize agreement between their model and experimental data. The term γ is given by

$$\gamma(\theta) = \frac{3 \sin^2 \theta - 1}{\sin^2 \theta} + \frac{\cos^2 \theta (3 \sin^2 \theta + 1)}{2 \sin^3 \theta} \ln \left(\frac{1 + \sin \theta}{1 - \sin \theta} \right)$$

The denominators in this equation result in undefined values when $\theta \rightarrow 0$ and $\theta \rightarrow \pi/2$. Using L'Hopital's Rule, however, one obtains $\gamma(0) \rightarrow 16/3$ and $\gamma(\pi/2) \rightarrow 2$.

2.2.2 View Factor Model

The view factor, F_{i-j} represents the fraction of all particles sputtered from surface i that deposit onto surface j . To calculate F_{i-j} , the angular distribution from Eq. (2.4) is integrated as shown below

$$F_{i-j} = \frac{\int_{\phi_1}^{\phi_2} \int_{\theta_1}^{\theta_2} S(E, \theta_i, \theta, \phi) \sin \theta d\theta d\phi}{\int_0^{2\pi} \int_0^{\pi/2} S(E, \theta_i, \theta, \phi) \sin \theta d\theta d\phi} \quad (2.5)$$

where the limits of integration for the numerator, θ_1 , θ_2 , ϕ_1 , and ϕ_2 , are based on the nodes of cell j . Figure 2.5 summarizes this equation for an isotropic case (represented by the hemisphere).

The integral in the denominator is evaluated via the identity $\int_0^{2\pi} \cos \phi d\phi = 0$, reducing

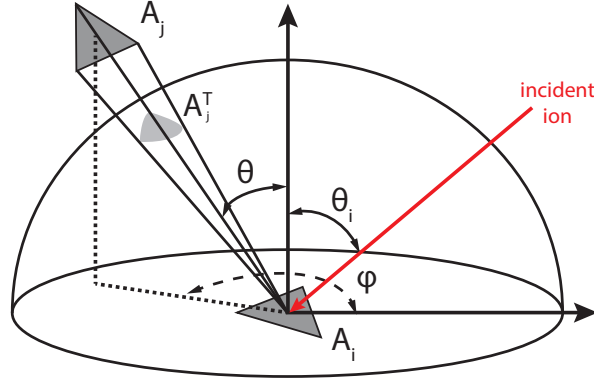


Figure 2.5: Representation of the view factor equation for an isotropic case. This diagram also defines the coordinate system used in the computational model.

the integral in the denominator to

$$2\pi \int_0^{\pi/2} \gamma(\theta) \cos \theta \sin \theta d\theta = 4\pi$$

Computing the integral in the numerator can be quite involved, especially for non-rectilinear meshes, since θ and ϕ are not independent of each other. For triangular meshes, assuming the solid angle subtended by the target surface is small, the angular distribution can be assumed constant, resulting in

$$F_{i-j} = \frac{S(E, \theta_i, \theta, \phi) A_j^T}{\pi(1 - \sqrt{\frac{E_{th}}{E}} \cos \theta_i)} \quad (2.6)$$

where A_j^T is the area of the spherical triangle projected by cell j . A simple algorithm for calculating the spherical triangle area can be obtained from Ref. [55]. For surfaces sputtering at normal incidence angle, the angular distribution can be approximated using a modified cosine distribution, $\cos \theta(1 - 2 \sin \theta)$, as in Ref. [40].

To ensure that sputterants are not double counted, i.e., that they do not deposit onto two cells at the same time, an algorithm that checks whether a cell is shadowed by any other cell was used. Many algorithms exist which can accomplish this task [56, 57], however,

these tend to be computationally expensive and are typically handled by graphics processing units (GPUs). Hence, emphasis was placed on minimizing the computational cost of this algorithm. For example, rather than checking whether a cell is shadowed by any other cell in the mesh, impossible cases can be discarded *a priori*, e.g. when the third cell is outside the field of view of the sputtering cell ($\phi \geq \pi/2$), or if the shadowing cell is behind the target cell (its distance from the sputtering cell is greater than the distance between the sputtering and target cells).

For simplicity, geometrical calculations were used to determine whether a cell is shadowed or not. In cases where symmetry allows, shadowing was detected in two dimensions to reduce computational cost. For this case, shadowing detection reduces to determining whether the segment representing the line of sight between the target (cell j) and the sputtering source (cell i) intersects the segment connecting the two nodes of a third cell k). For 3D cases, the algorithm should detect if the line of sight between source and target cells intersects the plane of the candidate shadowing cell. If this is the case, one must then determine if the intersection occurs within the dimensions of the shadowing cell (cell k). Sample algorithms for both cases can be found in Refs. [58] and [59]. These shadowing algorithms have been previously validated and found to agree favorably with more robust algorithms used in COMSOL (see Appendix B).

2.2.3 Mesh Deformations

Sputterant deposition causes a surface to grow, opposing erosion of the surface caused by its own sputtering. These two processes must be accounted for in order to properly track the evolution of the surface in time. The results from the view factor and sputter yield calculations were used to update the location of mesh cell centers, as in Eq. (2.7), and these displacements were interpolated to find the new locations of cell nodes. Inverse distance weighting is a simple technique to interpolate values for cell node location updating. Care must be taken so as to not artificially introduce (or leak) mass into (or out of) the system,

however.

$$\Delta \vec{r}_j = \frac{(\sum_i \Gamma_i Y_i F_{i-j} A_i - \Gamma_j Y_j A_j) m_t \Delta t}{A_j \rho_t} \hat{n}_j \quad (2.7)$$

Here, Γ is the incidence ion flux, Y is the sputter yield, A is the cell area, F_{i-j} is the view factor between cells i and j , m_t and ρ_t are the target mass and density, Δt is the time interval on which the cell is displaced by Δr , and $\hat{n}_j$ is the unit vector normal to cell j . In this equation, the first term inside the parentheses represents the flow rate of depositing particles from all other cells and the second term is the flow rate of particles sputtered from the surface. This equation assumes that the packing fraction of deposited material is the same as that in the bulk (as reflected by the target density).

Because of the simplicity of the interpolation step taken to update cell node locations, some mass will inevitably be leaked or introduced numerically. Hence, the difference between the change in mass calculated via view factors ($\Delta m_i^{calculated}$) and the actual change in mass due to deformation of the mesh (Δm_i^{actual}) must be tracked after each iteration, as in Eq. (2.8). The difference between predicted and actual system mass can then be reintroduced (or extracted) by updating mesh cells a second time. This process has the added benefit of smoothing out numerical noise. This recalibration step can be iterated until a desired tolerance is reached, however, it was found that doing so could result in nonphysical deformations. Thus, the mass was only recalibrated once, resulting in sufficiently accurate conservation of mass.

$$\Delta M(t) = \frac{\sum_{i=1}^N \Delta m_i^{calculated} - \Delta m_i^{actual}}{\sum_{i=1}^N \Delta m_i^{calculated}} \quad (2.8)$$

2.3 Simulation Configurations

The model was used to simulate sputtering on two surface configurations which have been previously tested experimentally. The first case corresponds to a triangular wave pattern etched via wire electric discharge machining (EDM) (see Fig. 2.6). The second configuration

simulated a local inhomogeneity protuberant over a nano-rod field, which was treated as a smooth surface for simplicity.

2.3.1 Triangle Wave Model

Plasma parameters were chosen to ensure that surface features were small relative to the sheath thickness and that sufficient mass erosion was observed per iteration. Table 2.1 summarizes the three studies conducted with the triangle wave model. Case I served as validation by direct comparison with Rosenberg and Wehner’s data [25]. Case II modeled surface evolution due to erosion and deposition from a steady plasma. Finally, case III investigated the effect of surface pitch (or triangle wave angle) on the net sputter yield.

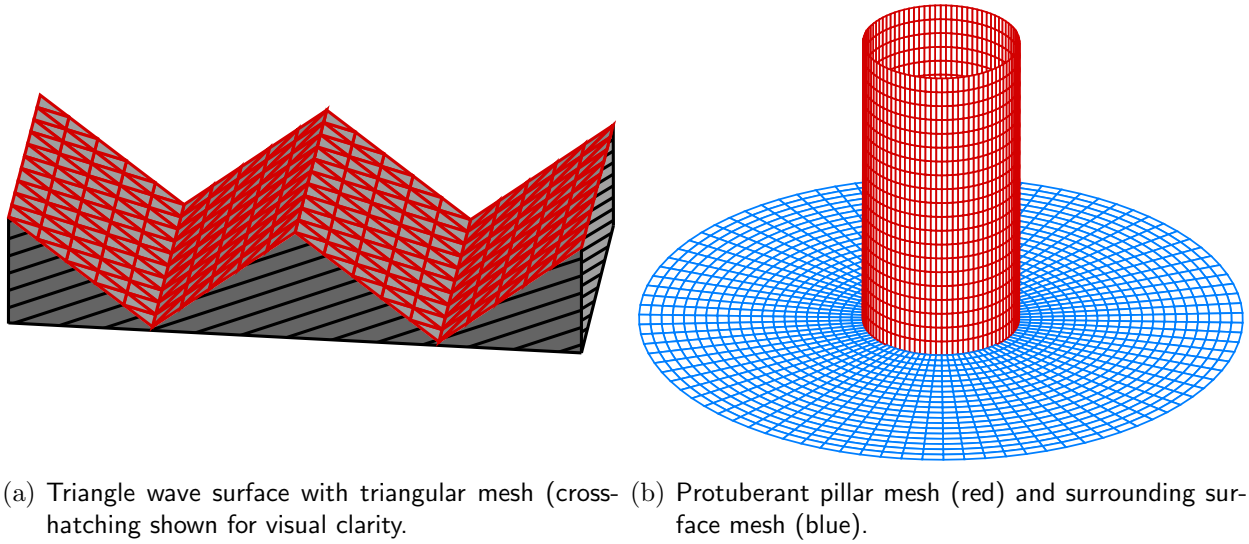
To simplify the problem and lower computational cost, the triangle wave pattern was only repeated once (peak to peak) and assumed to be infinitely long. Hence, surface evolution was tracked only in two dimensions, although the third dimension must be considered in the view factor calculations (see Fig. 2.6 a).

	Ion Energy (eV)	Pitch	Objective
Case I	75-400	38.7°	Validation
Case II	300	38.7°	Surface Evolution
Case III	75-400	0-75°	Pitch vs net sputter yield

Table 2.1: Triangle wave simulation test cases

2.3.2 Protuberant Pillar Simulation

The second configuration simulated experiments made on a sample similar to P/N 6 of Ref. [41] in the Pi facility (described in Ref. [40]). The 2 in diameter sample surface consisted of thick ($2 - 10 \mu\text{m}$) molybdenum-coated rhenium nano-rods fabricated through chemical vapor deposition (CVD). The sample was biased 200 V below ground. Although the plasma potential near the ion source was not measured, it ranged between cathode (-24 V) and



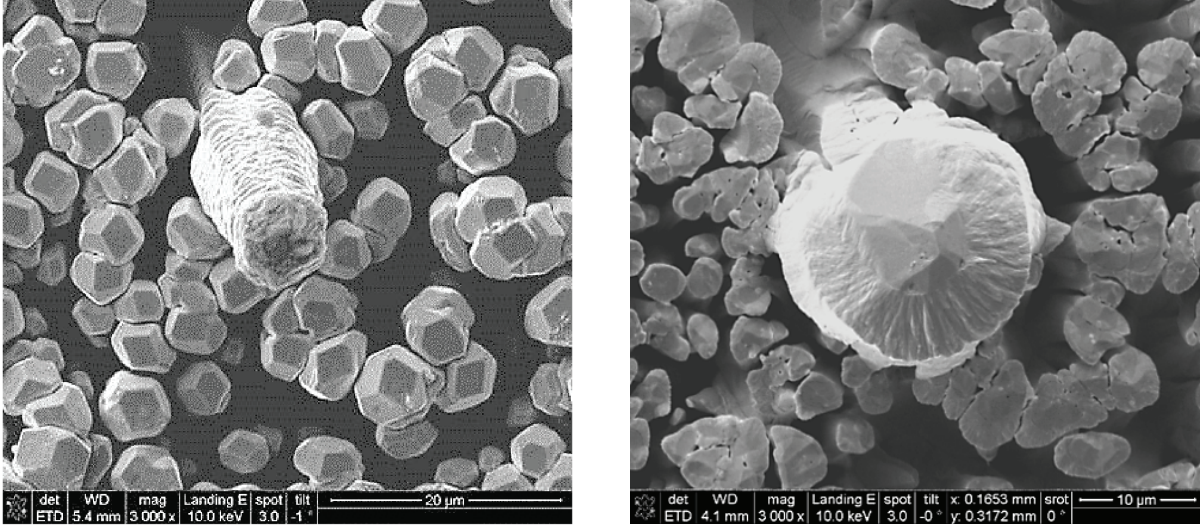
(a) Triangle wave surface with triangular mesh (cross-hatching shown for visual clarity). (b) Protuberant pillar mesh (red) and surrounding surface mesh (blue).

Figure 2.6: Representative meshes for sputtering models (not to scale).

anode (0 V) potentials to sustain discharge. After 120 minutes of exposure to the xenon plasma totaling an estimated ion dose of $(1.5 \pm 0.12) \times 10^{21}$ ions from an average ion current of 34.9 ± 1.5 mA, the sample lost 39 ± 6 mg of mass. Hence, the net sputter yield was calculated to be 0.155 ± 0.022 atoms/ion, assuming sputterants were purely Mo atoms (i.e. no Re was exposed). This represented a 32-44% reduction compared to a sputter rate of 0.228–0.277 atoms/ion as calculated using revisions made by Tartz et al. to Bohdansky's semi-empirical equations [60].

SEM images taken after the experiment revealed that while nano-rods receded due to sputtering erosion, localized protuberant sites grew radially to more than double their circumference (see Fig. 2.7). Although these locally perturbed structures only covered approximately 10% of the sample surface before exposure, they played an increasingly important role in trapping sputterants and reducing the erosion rate as they grew. To study the effects of these pillars on the sputtering and erosion behavior of these samples, a protuberant pillar was modeled and its radial growth due to local deposition was tracked. For simplicity, the pillar was assumed to be perfectly cylindrical and was surrounded by a smooth, flat surface. Estimates from stereo SEM images indicated that the cylinder is roughly 20 μm tall

with a 5 μm radius. Figure 2.6 b) shows the quadrilateral pillar and surface meshes (not to scale). For simplicity, both the pillar and the flat surfaces were assumed to erode axially at the same rate (hence, axial erosion was ignored). In addition, the ions were assumed to monoenergetically bombard the surface at 200 eV.



(a) Before exposure.

(b) After exposure.

Figure 2.7: SEM image of protuberant local inhomogeneity exposed to $7.6 \times 10^{23} \text{ m}^{-2}$ ion dose density. Pillar radius was estimated to be 4.25 μm initially, and 11 μm after the burn.

In order to validate the results for this case, a 2.5D analytical model was developed by deriving an expression to integrate Eq. (2.5) in three dimensions and evolving the cylindrical surface in 2D polar coordinates (taking advantage of azimuthal symmetry). The pillar was discretized into N_z rings, and for each ring, the simplified sputter distribution, $S(\theta) = \cos \theta(1 + 2 \sin \theta)$ (see section 2.2.2), was integrated along the pillar surface from $-\phi_m$ to ϕ_m , where $\phi_m = \sin^{-1}(r_p/r_c)$ and r_p and r_c are the radius of the pillar ring and distance to the sputtering surface ring, respectively. Equation (2.5) becomes

$$F_{i-j} = \frac{\int_{-\phi_m}^{\phi_m} \int_{\theta_1}^{\theta_2} \cos \theta (1 + 2 \sin \theta) \sin \theta d\theta d\phi}{7\pi/3} \quad (2.9)$$

where $\theta_j = \tan^{-1}(L/h_j)$, $j = 1, 2$, and L is a function of ϕ (see Fig. 2.8). This process was repeated to a far enough r_c distance for each time step until the desired burn time was reached. This analytical model did not account for shadowing between cells and erosion of lateral surfaces as they evolve and become exposed to the plasma. Hence, the more complete 3D model was still necessary to obtain accurate results.

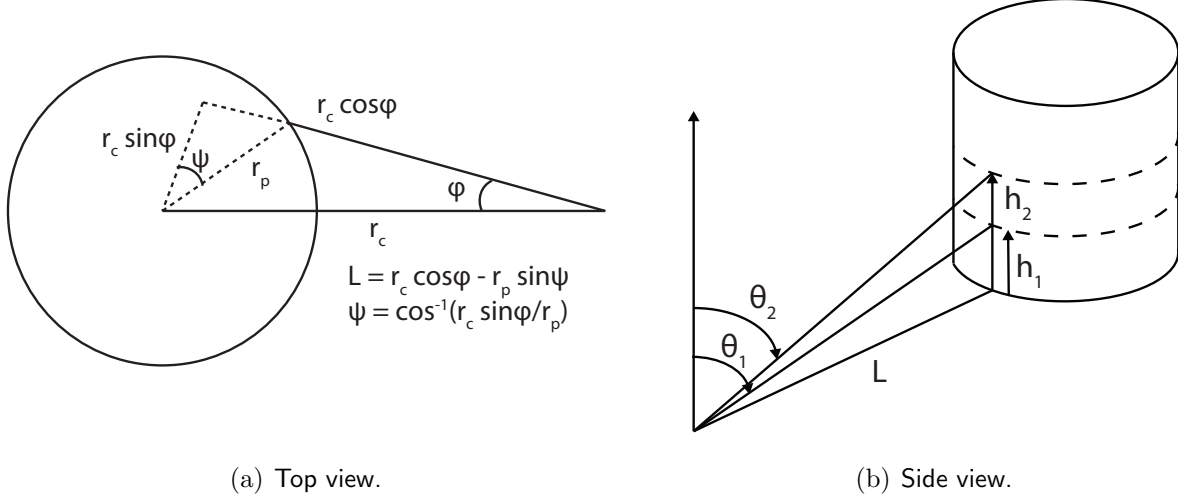


Figure 2.8: Analytical model diagrams

2.4 Results

Each major component of the model was validated by comparison with experimental data and computational simulations (see Appendix B). These validation tests isolated the sputter yield model, view factor calculations, and shadowing algorithms. Further validation was necessary to ensure that these model components worked in conjunction before applying them to the previously described simulations.

2.4.1 Triangle Wave Surface Results

This model was validated by comparison to data published by Rosenberg and Wehner in 1962 [25]. The model was applied to a surface with feature dimensions matching those used by Rosenberg and Wehner, and was used to estimate the net sputter yield at their tested conditions. The model was then applied to a similar configuration to observe the evolution of the surface as it is bombarded by plasma ions. Finally, the triangle wave pitch was varied to study the effects of aspect ratio on the net sputter yield.

2.4.1.1 Comparison with Rosenberg and Wehner's data

By applying a single iteration of the model to Rosenberg and Wehner's geometry, and using the calculated view factors for all cells in Eq. (2.10), the normalized net sputter yield was obtained (analogous to $Y_{threaded}/Y_{smooth}$ in Ref. [25]).

$$\bar{Y} = \frac{\sum_{m=1}^N \left(Y_m(\theta_i)(1 - \sum_{n=1}^N F_{m-n}) \right)}{NY_0} \quad (2.10)$$

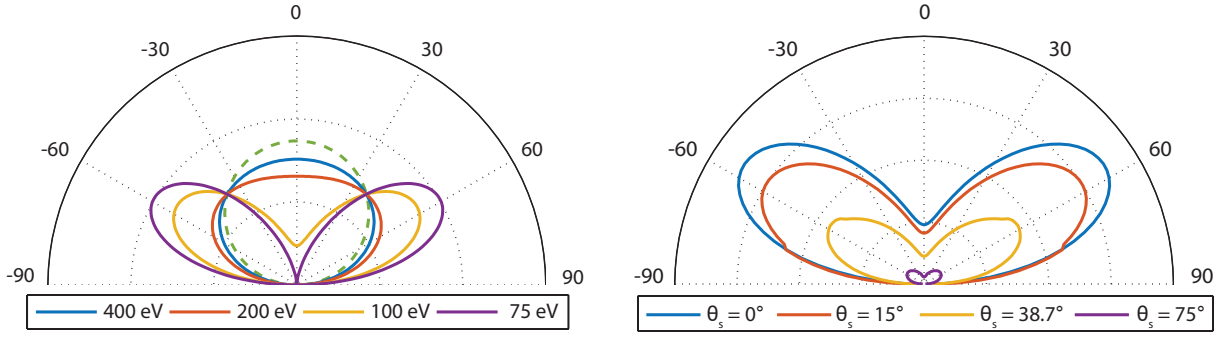
Here, $Y(\theta_i)$ is the sputter yield at ion incidence angle θ_i , N is the number of cells in the mesh, and Y_0 is the sputter yield at normal incidence. The term inside the outer parentheses represents the net sputter yield from cell m (i.e. the number of atoms not depositing on adjacent surface features per incident ion), which is then averaged over the entire surface and normalized by the normal incidence sputter yield.

There were two caveats to this validation effort, however: 1) there is an apparent lack of data on the angular sputterant distribution for low energy argon bombardment on nickel, and 2) Rosenberg and Wehner's data shows hysteresis attributed to micro-roughening of the threaded surface with sustained ion bombardment. These issues were addressed by employing qualitative approximations to the angular distributions at different energies and by perturbing the initial surface to simulate some micro-roughening.

The angular sputterant distributions shown on Fig. 2.10 a) were generated using Eq. (2.4) by setting the threshold energy, E_{th} , to 42 eV for the 75 eV incident ion energy case, and 50 eV for the 100, 200, and 400 eV cases. These distributions are heavily under-cosine at the lower energies and approach the cosine curve (dashed line) as the incidence energy increases. For comparison, Fig. 2.10 b) shows the sputterant angular distribution for different surface pitch angles. Figure 2.10 c) shows comparisons of the normalized net sputter yield with Rosenberg and Wehner's data. As expected, there was close agreement at 400 and 200 eV when micro-roughening was not yet significant. By perturbing the surface (cell centers) with a random number generator, closer agreement between the 100 and 75 eV results and Rosenberg and Wehner's roughened data were obtained. A roughness coefficient corresponding to the roughness peak height amplified the perturbation term and controlled surface micro-roughness. It was initially assumed that micro-roughening increased with time in Rosenberg and Wehner's experiments (i.e. traveling up the dashed line in Fig. 2.10 c) from low to high incident energies). However, to match the model's results with the experimental data, it was necessary to decrease the roughness coefficient at higher energies (from a roughness peak height of 2.6 μm at 75 eV ion incidence energy to 1.25 μm at 400 eV), which indicated a smoothing of the surface with prolonged exposure to the plasma. While this smoothing process is certainly plausible, no conclusions can be drawn without experimental verification. It is also noted that the surface not only roughens, but its aspect ratio decreases with time (as will be shown later). This process slightly increases the sputter yield for the higher energy cases (see Fig. 2.12 a), but does not completely account for the smoothing necessary to match with Rosenberg and Wehner's data.

2.4.1.2 Surface evolution results

The model was then applied to a hypothetical molybdenum sample (see Fig. 2.6 a). Triangle wave dimensions were reconfigured to 400 μm from peak to peak and 160 μm in height. The sample was biased to -300 V and exposed to an argon ion flux of $2.2 \times 10^{20} \text{ m}^{-2} \text{ s}^{-1}$. A



(a) Ar^+ -Ni angular distributions at normal incidence. (b) Macroscopic angular distributions from triangle-wave surface at several surface pitch angles. Cosine curve (dashed line) shown for reference.

Figure 2.9: Analytical model diagrams

threshold energy value of 150 eV was used in Eq. (2.4) to match angular distribution curves at 500 eV; this E_{th} value was expected to hold for sputtering at 300 eV. A mesh with 400 cells was used to track surface evolution, and 1000 triangular mesh cells were used in the perpendicular dimension for the view factor integration, Eq. (2.6). Burn time was set to 4 hours with 3 minute time steps used for each iteration to minimize artificial (numerical) mass insertion. A sputter yield at normal incidence of 0.55 atoms/ion, derived in Ref. [61] via semi-empirical equations, was used. The results, shown on Fig. 2.11, tracked the changes in the surface as ions eroded the material. As expected, the trough eroded much slower than the peaks due to increased deposition, leading to a flattening effect at the center. This is in sharp contrast with Bradley and Harper's theory of ripple evolution, which uses geometric arguments to predict higher ion energy deposition (and thus higher erosion rates) at troughs for near normal ion incidence angles [62], but neglects the decrease in erosion rate caused by deposition from nearby surfaces. Throughout the simulation, the relative difference in mass change, as calculated in Eq. (2.8) peaked early on at approximately 0.3% and stayed below 0.01% for most of the simulation.

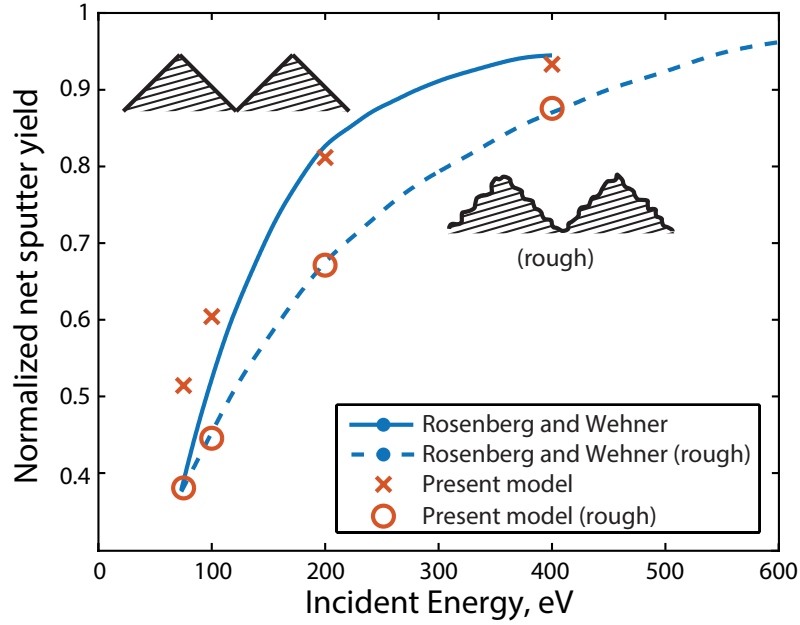


Figure 2.10: Normalized net sputter yield of patterned surface at different energies with and without micro-roughening, compared with Rosenberg and Wehner's data.

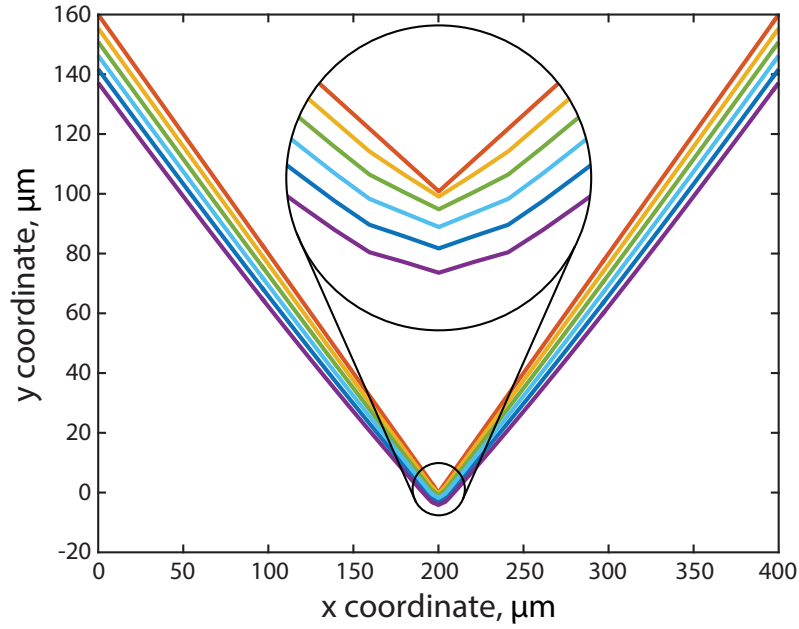


Figure 2.11: Results of triangle wave surface simulation through 4 hours of exposure. A Mo sample, biased at 300 V below ground, was exposed to a $2.2 \times 10^{20} \text{ m}^{-2} \text{ s}^{-1}$ argon plasma. Curves from top to bottom represent chronological surface profiles (top curve is the initial surface).

2.4.1.3 Effect of aspect ratio on sputter yield

The change in sputter yield due to varying surface angle (i.e. the angle between the horizontal and the surface edge) was also investigated for both smooth and micro-roughened surfaces. The results from these simulations are shown on Fig. 2.12. The micro-roughened surfaces were normalized by the sputter yield of the micro-roughened, 0° surface angle case (not normalized by the sputter yield of a smooth flat surface, which corresponds to the dashed line on Fig. 2.10 b). For comparison, the sputter yield of rough, flat surfaces normalized by the sputter yield of smooth, flat surfaces ranges from 0.65 to 0.99 for 75 eV and 400 eV, respectively.

Figure 2.12 a) shows that, for the lowest energies, a triangle wave surface always lowers the net sputter yield by trapping sputterants ejected from the troughs. At higher energies and near 45° incidence angles, there was a slight increase in the net sputter yield as compared to a flat surface because sputtering at higher energies is less forward-biased. At these higher energies, the increase in net sputter yield due to the incidence angle overcame the decrease in net sputter yield from trapping sputtered particles. Hence, patterning a surface does not guarantee a reduction in erosion, and can potentially result in increased erosion rates. As shown on Fig. 2.12 b), however, given an already roughened surface, patterned features decrease the net sputter yield for incidence energies below 400 eV (when compared to the sputter yield of the rough surface at normal incidence). Of course, comparing a patterned, micro-roughened surface against a flat, smooth surface, as is done on Fig. 2.10 b), also results in a decrease in the net sputter yield.

2.4.2 Protuberant Pillar Results

As discussed in section 2.3, the protuberant pillar model simulated erosion and deposition of a flat surface surrounding a cylindrical pillar, analogous to a field of nano-rods surrounding an overgrown pillar. In the model, a pure molybdenum sample was biased at 200 V and exposed

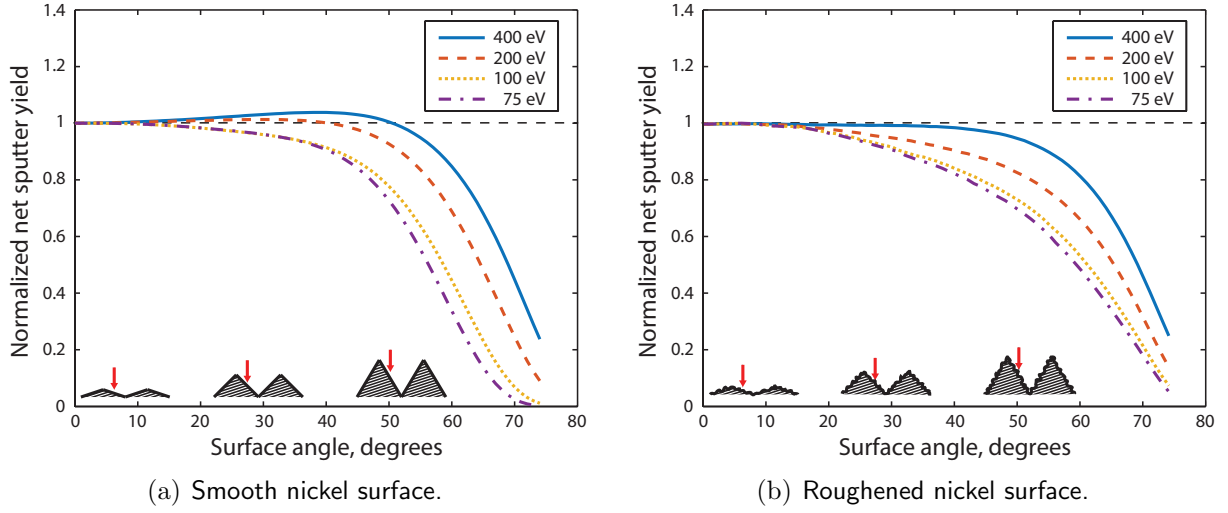


Figure 2.12: Normalized net sputter yield for argon ions at different incident ion energies and surface angles (complementary to ion incidence angle)

to xenon plasma, matching the UCLA Pi conditions reported in section 2.3. A sputter yield of 0.28 was obtained from Ref. [25]. The meshes, shown on Fig. 2.6 d), were constructed such that θ and ϕ were independent of each other when computing the integral in Eq. (2.5). As previously discussed, a modified cosine distribution was used instead of Eq. (2.4) to simplify numerical integration, since sputtering from the flat surface was at normal incidence angle only. As the flat, surrounding surface and the cylindrical pillar were bombarded by xenon ions, they eroded axially. Because the erosion rate of both the surface and pillar was similar in the direction inwardly normal to the surface, this produced a displacement of both meshes in that direction. Since there was no relative motion between the two surfaces, axial erosion was neglected (e.g. by imposing an opposing motion).

Sputterants from surrounding surfaces deposited onto the pillar, causing it to grow radially. As the pillar expanded, it shadowed the surface beneath it; these shadowed surfaces were no longer allowed to sputter, otherwise growth in the lower regions of the pillar would have been overestimated. Finally, as the pillar grew at different rates at different height levels, its lateral faces became exposed to the plasma. This resulted in sputtering of these faces and secondary deposition onto higher regions of the pillar. Although erosion of these faces

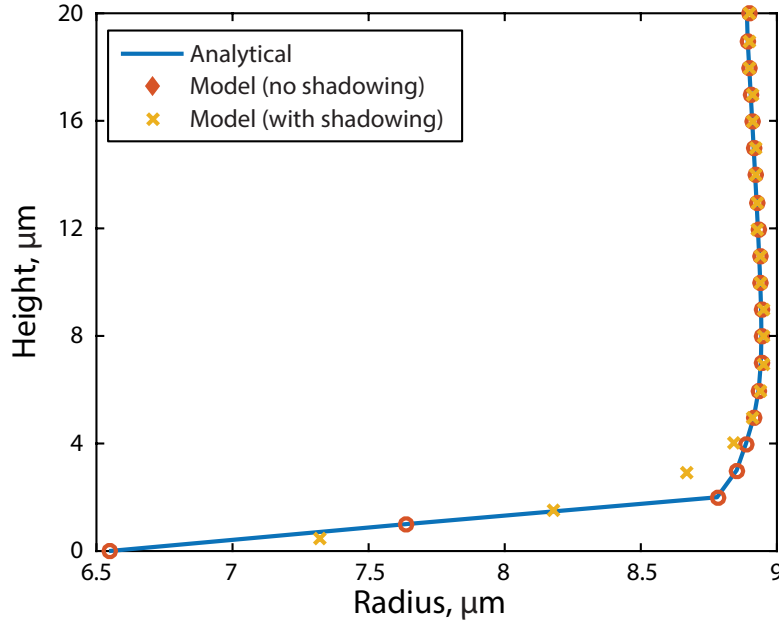


Figure 2.13: Comparison of analytical results and model (with and without pillar self-shadowing and lateral face erosion).

was accounted for in the model, secondary deposition was assumed to be unimportant.

2.4.2.1 Comparison with analytical model

The analytical model described in section 2.3 was compared with the full 3D model as well as the 3D model without cell-to-cell shadowing and erosion of lateral faces (a more analogous comparison, since the analytical model lacks these physics). Both models did account for shadowing of the sputtering surface as the protuberance grew, however. The results from these comparisons are shown on Fig. 2.13. Both versions of the model agreed acceptably well with the semi-analytical model, with differences in the lower region of the full 3D model due to the more realistic treatment of self-shadowing and lateral face erosion.

2.4.2.2 Comparison to SEM estimates

The model was again applied to the same geometry, this time accounting for shadowing between pillar mesh cells (in the view factor calculations) and erosion of lateral faces exposed to the plasma (i.e. no longer parallel to incident ions). These results were compared with estimates made using SEM images, such as those shown on Fig. 2.7. The results, shown on Fig. 2.14, extended the surrounding surface up to 1 mm away from the central pillar, and used 7,200 cells on the cylinder and 72,000 cells on the surface. Each ring of cells on the pillar and flat surface contained 360 cells. The surface was exposed to the plasma for 2 hours to match experiments, with 3 minute time steps taken each iteration, keeping the relative difference in mass change below 0.1% for most the simulation. Figure 2.14 b) shows the evolution process of the pillar surface in 2D polar coordinates:

1. At first, the region below 5 μm grew more rapidly because, being closest to the surface, the mesh cells there subtended a bigger area in the view factor calculation (see Fig. 2.5). Pillar mesh cells near the top were also more likely to be shadowed by lower mesh cells, so their growth slowed.
2. As the lower region grew increasingly faster than the higher regions, it became increasingly more exposed to the plasma and began to erode, slowing down its growth relative to other regions on the pillar.
3. As higher regions caught up and overtook the regions below a 5 μm height, they began to shadow the surface directly underneath, preventing sputtering from these surface cells. Because these surface cells were closest to the lower pillar cells (and thus the biggest contributors of deposition), growth in the lower region again decelerated. This process then lead to the final profile shown on Fig. 2.14 b) (curve furthest to the right).

Estimates from SEM images, shown on Fig. 2.7, agreed with the results from this computational model within experimental uncertainty. It was estimated that the pillar was initially

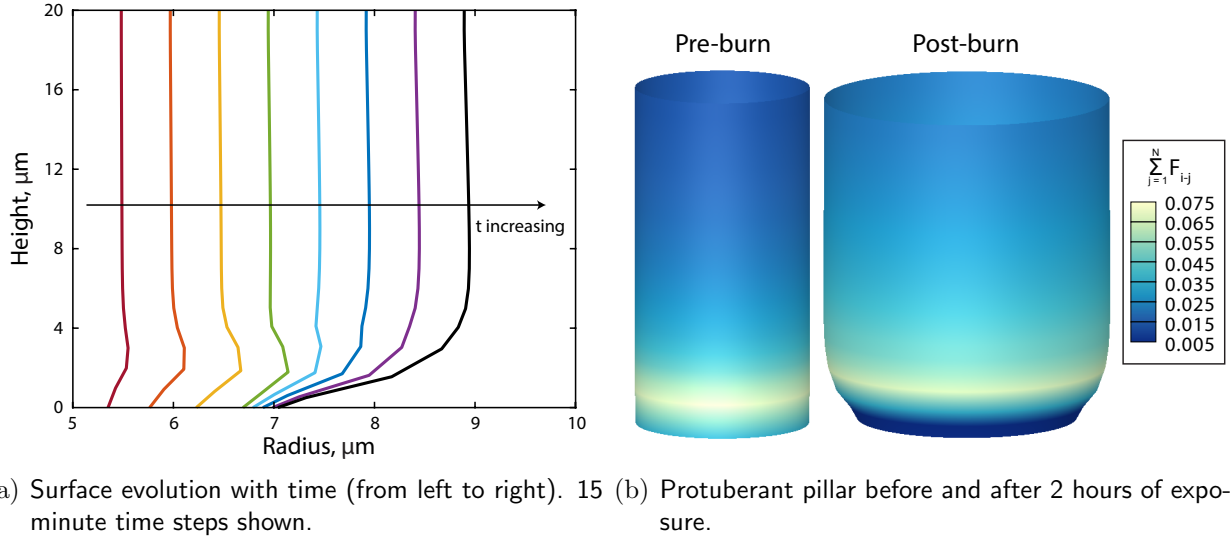


Figure 2.14: Protuberant pillar model results. Growth is due to deposition from sputtering surface (not shown).

4.25 μm in radius, and grew to 11 μm after 2 hours of exposure. Most of the disagreement is expected to come from the simplifications made to model the surrounding surface. The real surface was composed of dendritic rhenium nano-rods with molybdenum caps [41]. If rhenium was exposed after eroding the Mo coating off, the sputter rate would have increased and could have accounted for increased deposition onto and radial growth of the pillar. In addition, the pillar seems to taper off from base to tip, as shown on Fig. 2.7 a). Because the pillar base is hidden by the Re-Mo nano-rods, accurate estimates of the base radius were difficult with SEM images.

2.5 Discussion

Surface morphology (from micron-level surface roughness to 0.1 μm patterning) can strongly affect the net sputter yield of plasma-facing surfaces. In this chapter, I have presented an examination of the effects of both surface architecturing on sputter deposition and erosion using a computationally efficient view factor model. Model results for a nickel triangular wave surface in the presence of bombarding ion argon plasma agreed well with Rosenberg

and Wehner's data and extended their observations to different surface aspect ratios. Results from these tests showed significant decreases in normalized net sputter yield for all tested conditions (75, 100, 200, and 400 eV incidence ion energy for both smooth and roughened surfaces) when the triangle wave pitch angle increases beyond approximately 45° because for these cases, forward-biased sputtering favors deposition of sputterants into surrounding surfaces, counteracting erosion. For the higher incidence energy cases, however, it was found that smooth surfaces exhibited normalized net sputter yields above unity due to near-cosine (i.e. near-isotropic) sputtering distribution, indicating an increase in the erosion rate. Model results also agreed well with experimental data from the UCLA Pi facility for the sputter-deposition behavior of a molybdenum cylinder protruding from a surface in the presence of bombarding argon ions. The results captured the coalescence of sputterants at the protuberant site, which caused the cylindrical pillar to grow radially as observed in SEM images of the protuberance.

CHAPTER 3

Secondary Electron Emission from Textured Surfaces

A particle pushing model was developed to show that simple, repeating geometries can accurately and efficiently model SEE behavior of textured surfaces (see figure 3.4) [21, 63]. Most notably, a simple cage-like geometry was used to accurately simulate the SEE behavior for nano-structured tungsten fuzz. Modeling results are compared with computational and analytical results, as well as both historical and recent yield measurements, capturing distinct effects of the surface morphology on SEE and its dependence on incident angle.

3.1 Theory

As both ions and primaries (with sufficient energy to overcome the sheath potential) collide with electrons within the bounding walls, they may cause these electrons to be emitted from the surface, or in the case of electrons, may recoil and escape the surface [64]. For the energy range relevant to this work, the ion-induced electron emission (IIEE) yield is typically 10-100 times smaller than the SEE yield [65], so that phenomenon is neglected.

SEE can be categorized into three different types of secondaries based on their emission energy: elastically backscattered, inelastically backscattered, and true secondaries. Backscattered, or reflected, secondaries are simply recoiling primaries which may have a lower energy and travel in a different direction. True secondaries are surface electrons pushed out of the material by the primary. Primary electrons can also cause Auger electrons to be emitted, but these tend to be orders of magnitude fewer than other types of SEE and are grouped with inelastically backscattered electrons (see figure 3.1)

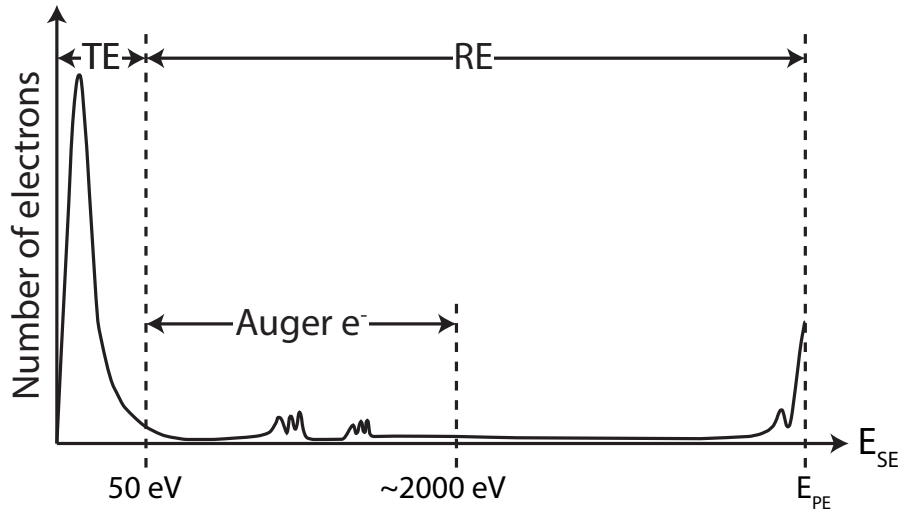


Figure 3.1: Energy distribution of electrons emitted from surface. Auger electrons are negligibly emitted and are grouped with inelastically backscattered secondaries.

Each type of secondary has its own yield, and the sum of their yields is the total yield (see figure 3.2). In addition, different types of secondaries are emitted with different angular and energy distributions. The yields and distributions are material dependent and will be reviewed in the next section.

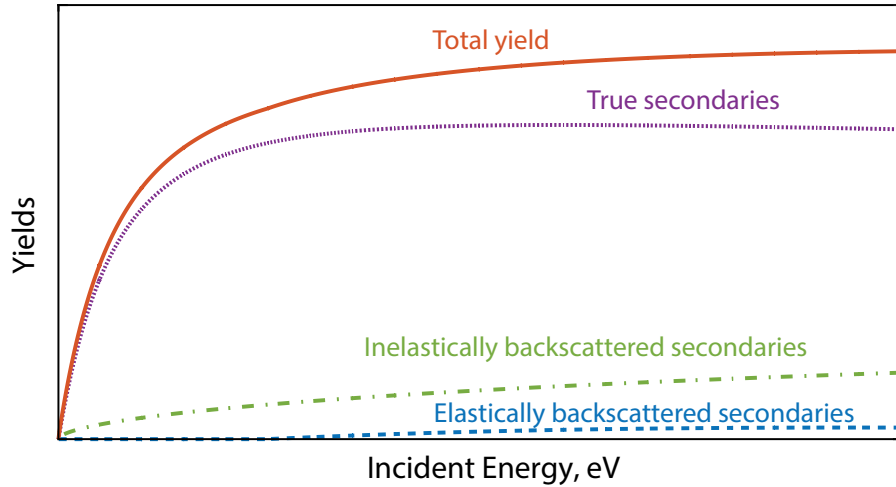


Figure 3.2: Typical yields for each type of secondary and total SEE yield.

One important feature of the the SEE yield to note is its trend with decreasing incident

energy at very low energies. Several measurements (and semi-empirical models based on these measurements) predict an increase in the yield or a decrease to a non-zero yield as the incident energy decreases to 0 [66, 67, 68, 69, 70]. However, as noted in Ref. [71], careful measurements of the yield at very low incident energies all show the SEE yield decreasing to 0. It is likely that contrary measurements were made by decelerating electrons with a retarding potential at the target rather than producing a collimated electron beam at low energy, thereby affecting the measurements [71]. Hence, as shown on figure 3.3, the yield should decrease at very low incident energies.

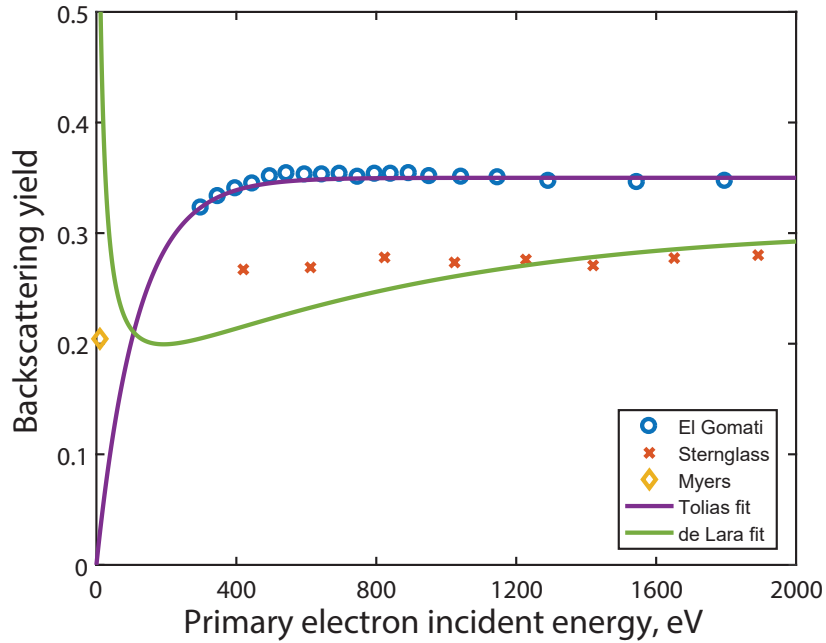


Figure 3.3: Backscattering yields from measurements (symbols) and models (lines). Careful measurements of the yield at low incident energy correctly show decreasing trends as the incident energy decreases to 0.

The effects of secondary electron emission on plasma and its sheath have been repeatedly studied and are well understood for simple cases. In 1967, Hobbs and Wesson analyzed how secondaries affect the potential profile near a wall due to the changes in electron flux caused by these secondaries. They found that the potential far from the wall is reduced by the SEE

yield and the energy flux to the wall increases [19]:

$$\begin{aligned} -e\phi_0 &\simeq kT \ln \frac{1 - \sigma}{\sqrt{2\pi m/M}} \\ Q &= n_0 v_0 \left(\frac{2KT}{1 - \sigma} + E - e\phi_0 \right) \end{aligned} \tag{3.1}$$

where σ is the total SEE yield and E the ion's initial energy. Evidently, lowering the emission of secondaries can sustain a higher plasma potential and reduce the energy lost to the bounding walls. Although this conclusion holds true for textured and other two-dimensional surfaces, Hobbs and Wesson's analysis is only true in 1D [19]. Because of the angular emission distribution's dependence on incidence energy and trapping in textured surfaces, the SEE effects on the sheath are not likely to be isotropic and could change the shape of the sheath and the incidence properties of plasma particles.

3.2 Computational Approach

The model simulates the interactions of incident primary electrons with the surface, and hence requires knowledge of material SEE properties, surface geometry, and electron incidence conditions (energy and angle). This paper focuses on accurately modeling textured surfaces to examine surface texturing effects on the SEE yield behavior (see figure 3.4). The following subsections detail the particle tracking, collisional and emission behavior, and geometric components of the model.

3.2.1 Electron Tracking

The model uses a Monte Carlo approach to push primary electrons towards the surface and then simulates the SEE behavior when a collision with the material is detected (see figure 3.5). Because the Debye length is larger than the surface layer, the electric and magnetic fields are assumed to be negligible near the surface. Hence, electrons travel linearly

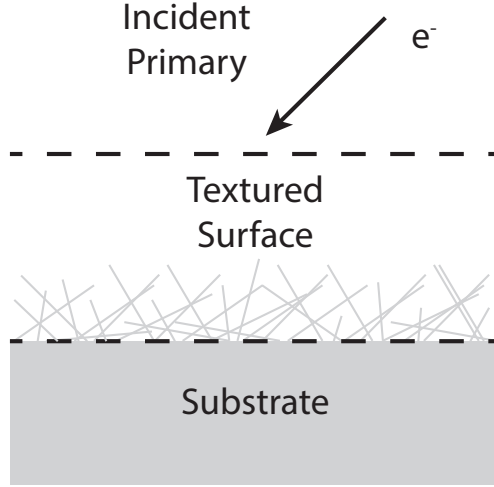


Figure 3.4: Regions defined by computational model. The focus of this paper is to accurately and efficiently model a representative geometry for textured surfaces.

until colliding with a surface. In addition, primaries and secondaries have mean free paths much larger than the surface feature scales, so their velocities change only after colliding with a surface.

At the low energies investigated herein, electron penetration depth into metals approaches a few nanometers and is therefore neglected. As primaries penetrate the surface, they collide with electrons to generate true secondaries or are inelastically backscattered, usually a small distance away from the point of collision. For the simulated conditions, this distance is small relative to fiber dimensions (for the worst case, primary electron penetration depth for tungsten is ~ 5 nm at normal incidence, compared to the 200 nm computational domain length) so inelastically backscattered and true secondaries are assumed to be emitted from the point of impact (see figures 3.6 c-d). Moreover, although primaries can inelastically backscatter while also generating true secondaries (see figure 3.6 a), in this model, incident electrons are assumed to be lost (or absorbed) when true secondaries are generated.

Primaries are seeded at the top face some distance above the fiber tops and secondaries

are only allowed to escape through this boundary. Electrons are reflected from the lateral boundaries (since the computational domain repeats infinitely in the lateral directions) and retained until they escape or are absorbed. Electrons are pushed linearly until a collision is detected geometrically by the intersection of the electron’s path segment and a fiber cylinder or the substrate plane.

Using empirical fits from Tolias [72] and de Lara et al. [70], a probabilistic model backscatters the primaries (elastically or inelastically) or removes them and generates a randomly calculated number of true secondaries (see section 3.2.2). These backscattered and true secondaries are then tracked through further collisions or until escaping through the top boundary of the computational domain. The algorithm limits the number of further secondary generations to two since additional generations were observed to negligibly affect the calculated true secondary yield in early runs of the model.

3.2.2 Secondary Electron Emission Treatment

Surfaces impacted by primary electrons emit secondaries through three different processes: elastic and inelastic backscattering and true secondary emission, as shown in figure 3.6. Elastically backscattered secondaries are reflected at the surface and retain their pre-impact energy. Inelastically backscattered secondaries, on the other hand, penetrate the surface and lose some energy before recoiling away from the surface. Finally, true secondaries are emitted due to collisions between primary electrons and near-surface atoms within the bulk. The respective yields for each type of secondaries are ε and η for elastic and inelastic backscattering and δ for true secondaries, and represent the ratio of the flux of each type of secondary to the flux of primaries. Each secondary population is treated independently in this model.

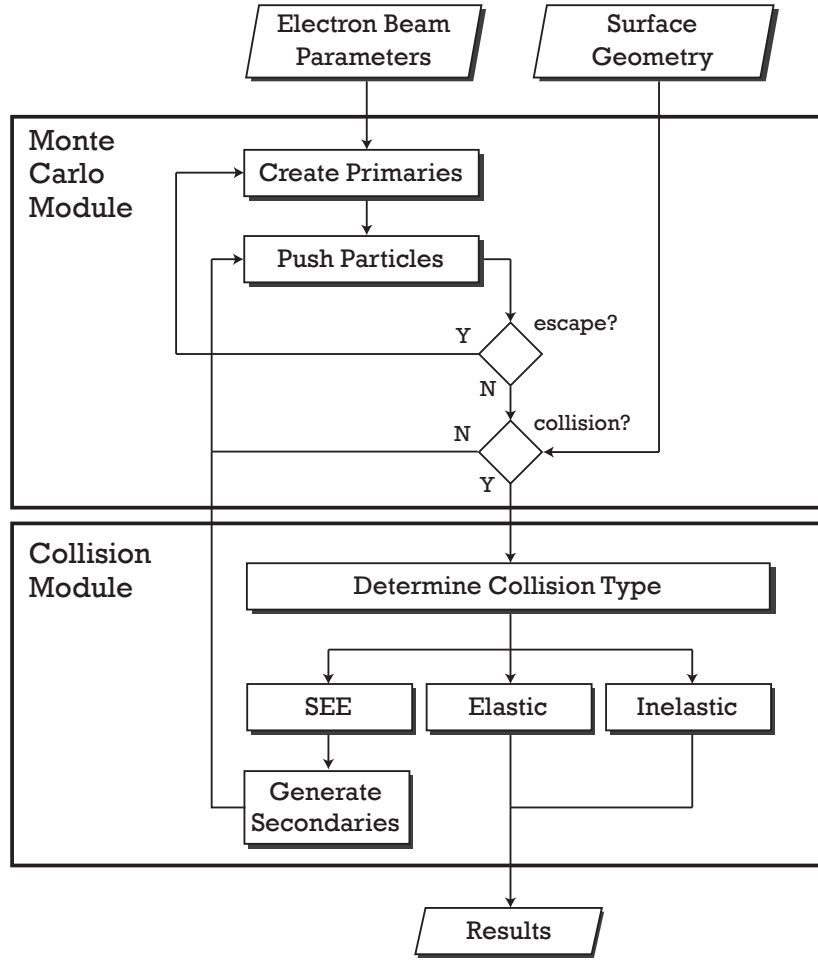


Figure 3.5: Secondary electron emission model flow chart.

3.2.2.1 Backscattered secondaries

Jonker has previously measured the angular distribution of “rapid” backscattered secondaries emitted from nickel at several incident energies and angles, showing that these secondaries are reflected preferentially at near incidence angles [73]. The spread in these distributions is likely due to the inclusion of inelastically backscattered secondaries and is neglected. Elastic backscattering is therefore modeled by retaining the electron’s incident energy (E_i) and reflecting the particle back through its original trajectory as shown in figure 3.6.

For inelastically backscattered secondaries, a uniform energy distribution, $50 \text{ eV} < E_{SE} <$

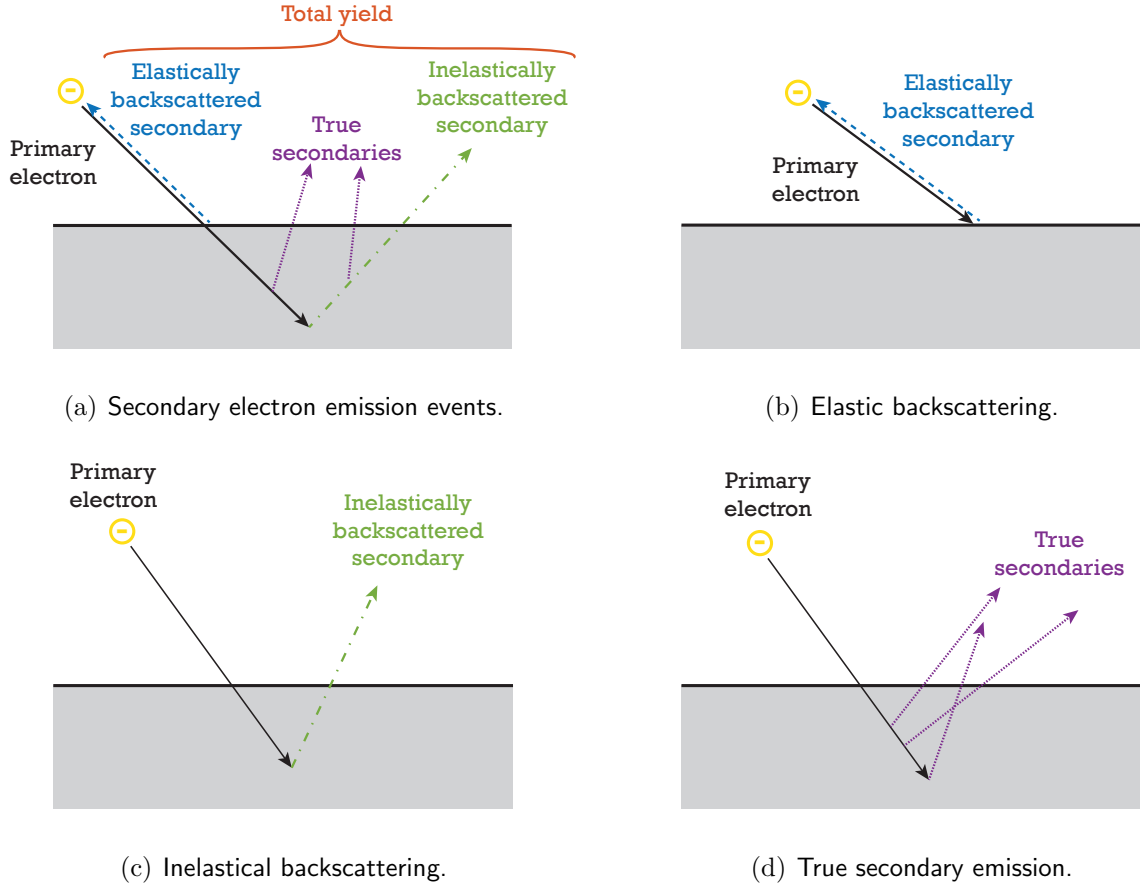


Figure 3.6: Secondary electron emission. Inelastic backscattering and true secondary emission are not mutually exclusive, but are separated in this model and assumed to occur at the primary electron's point of collision.

E_i , is assumed. Jonker's measured distributions for these secondaries are nearly cosine, with a slight bias toward the incidence angle [73]. For simplicity, a cosine distribution is used.

A probabilistic model developed by de Lara et al. [70] is modified using Tolias' empirical fits [72] to SEE yield data taken at low incident energies by El Gomati et al. [74]. This modification corrects the backscattering yield behavior to monotonically decrease at low incident energies, as discussed in Ref. [71]. The modified backscattering yields thus become:

$$\begin{aligned}
\eta(E_i) &= a (1 - b E_i) E_i^\gamma \exp \left(- \left(\frac{E_i}{c + d Z} \right)^\mu \right) \\
\varepsilon(E_i) &= f (1 - e^{-g E_i}) - \eta(E_i) \\
\eta(E_i, \theta_i) &= \eta(E_i)^{\cos \theta_i} \left(0.89 \frac{\eta(E_i)}{\varepsilon(E_i) + \eta(E_i)} \right)^{1 - \cos \theta_i} \\
\varepsilon(E_i, \theta_i) &= \varepsilon(E_i)^{\cos \theta_i}
\end{aligned} \tag{3.2}$$

where E_i and θ_i are the incident energy and angle and Z is the surface atomic mass number. The other parameters, a , b , c , d , f , g , γ , and μ , are fit values which can be found in Ref. [70] for η and Ref. [72] for ε . Each primary is backscattered as a single secondary, so the probability of backscattering is equal to the yield. Hence, a random number generator is used to determine what type of secondary is emitted after each collision (note that the probability of true secondary emission is $1 - \eta - \varepsilon$) [70].

3.2.2.2 True secondaries

For consistency, the true secondary model presented by de Lara et al. is used [70]:

$$\begin{aligned}
\delta(E_i) &= \delta_m \frac{s \frac{E_i}{E_m}}{s - 1 + \left(\frac{E_i}{E_m} \right)^s} \\
\delta(E_i, \theta_i) &= \delta(E_i) \frac{k + 1}{k + \cos \theta_i} \\
k &= 0.0027 Z + r
\end{aligned} \tag{3.3}$$

Here, δ_m is the maximum true yield, E_m is the incident energy at which δ_m occurs, s is a material-dependent parameter, and r accounts for surface smoothness [70]. These parameters can be obtained for specific surfaces by curve-fitting to experimental yield data from flat, clean samples.

When a collision results in the emission of true secondaries (with probability $1 - \varepsilon - \eta$),

the probability that n secondaries are emitted is calculated using a Poisson distribution such that the average number of secondaries emitted for all collisions equals the true secondary yield:

$$\begin{aligned} P_n &= \frac{\lambda^n \exp(-\lambda)}{n!} \\ \lambda &= \frac{\delta}{(1 - \varepsilon - \eta)} \end{aligned} \tag{3.4}$$

where $n = 0, 1, 2, \dots$ is the number of true secondaries generated and λ is the average number of true secondaries generated per impact [67, 70]. Each true secondary is assumed to be generated at the point of impact and follows a cosine angular distribution of emission independent of incident angle and energy [67, 75] and an energy distribution given by

$$f(E_{SE}) = \frac{E_{SE}}{(E_{SE} + W_f)^4} \tag{3.5}$$

where W_f is the material's work function [75, 76].

3.2.3 Geometry

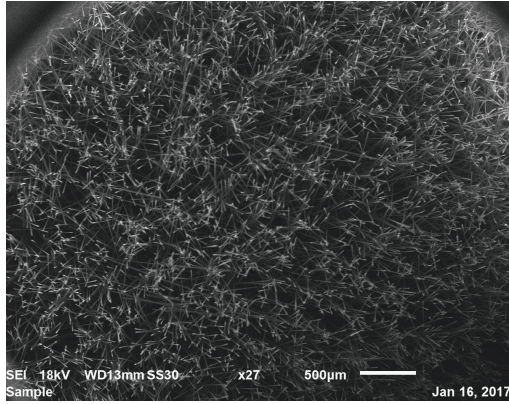
To examine what type of simple repeating geometry can be used to accurately and efficiently simulate the SEE behavior for the complex, chaotic geometry of velvet/carpet/fuzz, I utilized three different geometries, as shown on figure 3.7. A repeating, rectangular 3D section of the textured surface layer is used as the computational domain. The bottom face is treated as the solid, underlying substrate, and cylindrical fibers are positioned (in various configurations) at the corners of the domain. Three different geometries are employed to model different textured surfaces in this paper:

- A repeating lattice of vertical, cylindrical whiskers, analogous to carbon velvet, which is similar to the geometry used by Swanson and Kaganovich [39].
- A copper carpet, tested by Curren, Jensen, and Roman [77], is modeled as low aspect

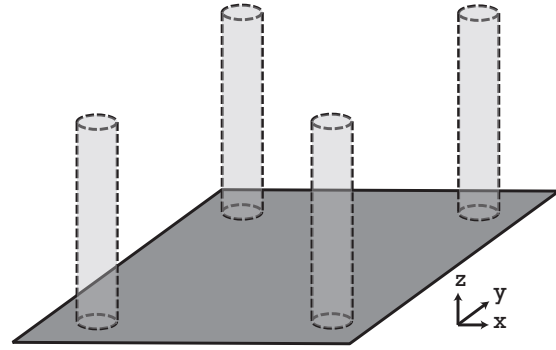
ratio, vertical, cylindrical fibers and tapered tops, centered at the domain corners.

- A plasma-generated tungsten fuzz, which Patino, Raitses, and Wirz studied in Ref. [24], is modeled as cylindrical fibers located at the substrate corners and connected by evenly distributed horizontal fibers in a cage-like geometry.

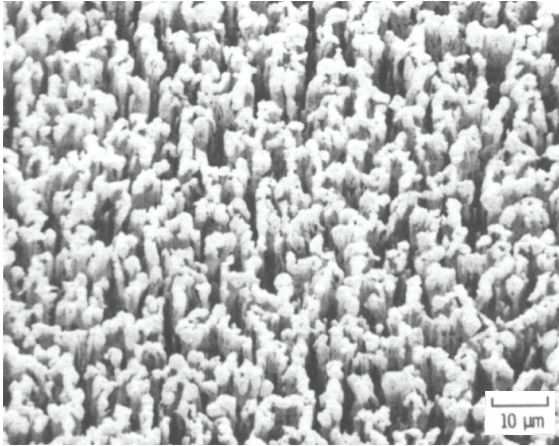
Figure 3.7 shows SEM images of the experimentally tested samples, as well as diagrams of the pillar, tapered fiber, and cage geometries used to model them.



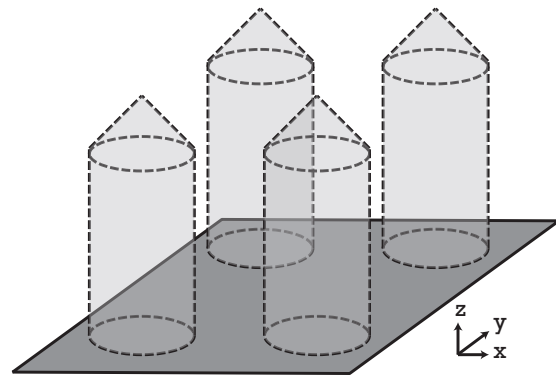
(a) Carbon velvet SEM image.



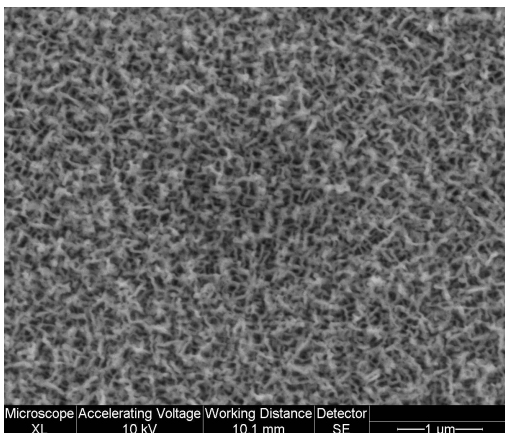
(b) Pillar geometry and computational domain.



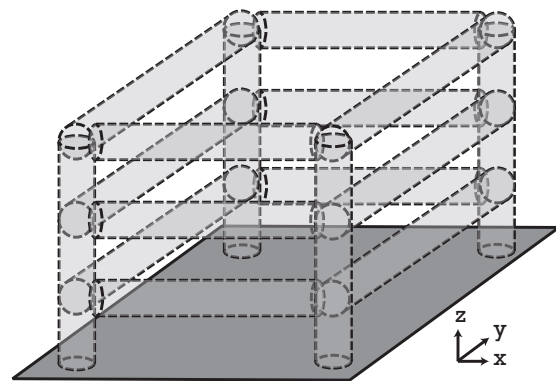
(c) Ion-textured copper (carpet) SEM image, reproduced from Ref. [78].



(d) Tapered fiber geometry and computational domain.



(e) Tungsten fuzz SEM image.



(f) Cage-like geometry and computational domain.

Figure 3.7: Fuzz geometries and SEM images. Note: all computational domains in this figure are representative and not to scale.

3.3 Results

Simulation results of the SEE yield were compared with measured and computed yields from various textured samples. The first is a carbon velvet modeled by Swanson and Kaganovich [39]; the second an ion-textured, oxygen-free, high-conductivity copper carpet from Ref. [[77]]; and the third a tungsten fuzz sample (see Ref. [24]) prepared at the MIT Plasma Science and Fusion Center, which occurs naturally when a heated tungsten surface (> 1000 K) is exposed to helium plasma with ion energies > 10 eV and fluxes $> 10^{20} \text{ m}^{-2} \text{ s}^{-1}$ (these conditions may occur in tokamaks that use tungsten as a plasma facing material).

3.3.1 Carbon velvet

To directly compare with Swanson and Kaganovich's model, the total SEE yield was modeled as:

$$\begin{aligned}\gamma(E_i, \theta_i) &= \gamma_{max}(\theta_i) \exp \left[- \left(\frac{\ln [E_i / E_{max}(\theta_i)]}{\sqrt{(2)}\sigma} \right)^2 \right] \\ E_{max}(\theta_i) &= E_{max0} \left(1 + \frac{k_s \theta_i^2}{\pi} \right) \\ \gamma_{max}(\theta_i) &= \gamma_{max0} \left(1 + \frac{k_s \theta_i^2}{2\pi} \right)\end{aligned}\tag{3.6}$$

The backscattering yields were obtained by multiplying the total yield by the fraction of elastically and inelastically backscattered secondaries as given in Ref. [39]. In addition, all secondaries were reflected with a cosine distribution, inelastically backscattered secondaries have a $0 \text{ eV} - E_i$ uniform energy distribution, and true secondaries were emitted with a Maxwellian energy distribution with $T = 5.4 \text{ eV}$.

As shown in figure A.4, the computed yield agrees well with analytical and simulation results from Swanson and Kaganovich for varying fiber aspect ratio ($A = h/r$) and packing density ($D = r^2/s^2$). For these simulations, the fiber radius, r , was kept constant while the fiber height, h , and separation distance, s , were changed. The models agreed especially well

when the aspect ratio and packing density were high. Most of the difference was likely due to the different approaches of each model; instead of using Monte Carlo to backscatter and emit secondaries, Swanson and Kaganovich tracked weighted macroparticles and changed their weight after each collision according to the total yield. Moreover, collisions in their model were detected using isosurfaces which coincide with the fibers rather than geometrically detecting the intersection of the particle's path with a surface. The analytical results are known to underestimate the yield because they do not account for tertiary electrons emitted by secondaries or the energy distributions of each type of emitted secondaries. Nevertheless, our model was capable of capturing the reversal of yield dependence on incidence angle as the aspect ratio increases past 100, which was analytically explained in Ref. [39].

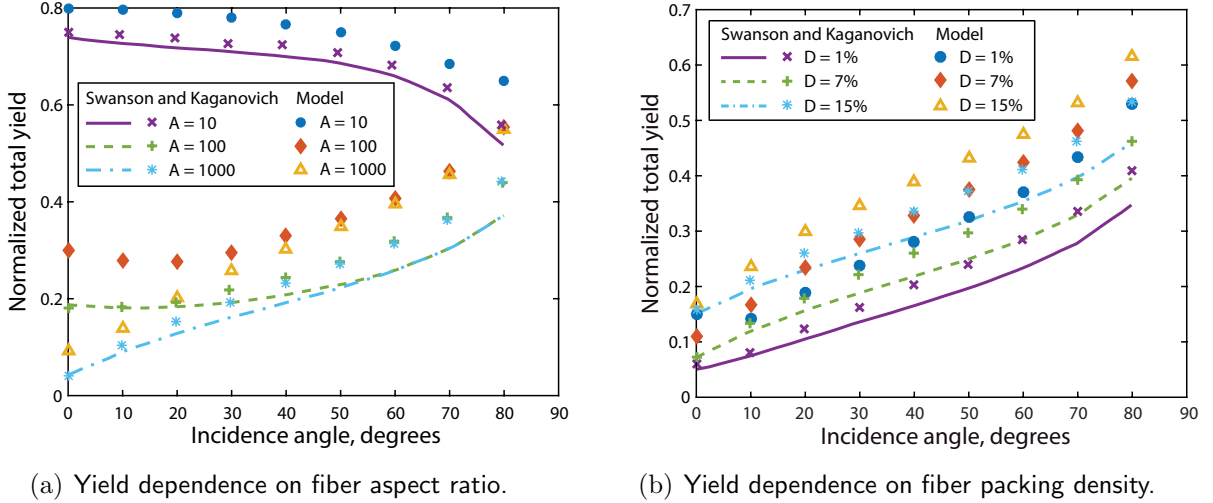


Figure 3.8: True secondary yield results from pillar geometry, compared with computational (symbols) and analytical (lines) results from Swanson and Kaganovich [39].

3.3.2 Copper carpet

The tapered fiber geometry closely resembles a repeating section of the copper carpet, as shown in figure 3.7. From the carpet image, I estimated an average taper angle (i.e. the angle between the fiber tip surface normal and the fiber axis) of 45° , however, I examined

the effects of this taper angle on the SEE results from the model. Measurements from the SEM image of the surface, along with estimates reported by Curren, Jensen, and Roman are summarized in table 3.1. The material-dependent fit values for copper were obtained by fitting to their flat copper data (see figure 3.9 a). Figure 3.9 b) shows the true secondary electron yield from the sample at 0° and 45° incidence angles for a 200 – 2000 eV energy range. In general, the computational results agree well with the trends and magnitudes from the experimental data, especially considering that roughening of fiber and substrate surfaces during the fabrication process was not considered.

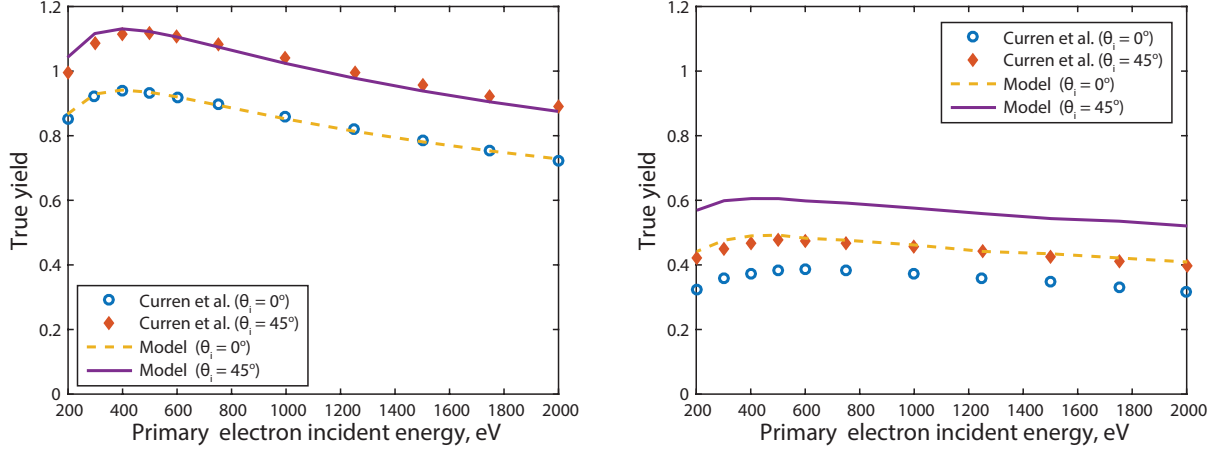
Fiber radius	350	nm
Fiber length	1500	nm
Fiber separation	1000	nm
Tip taper angle	45°	

Table 3.1: Copper carpet fiber dimensions

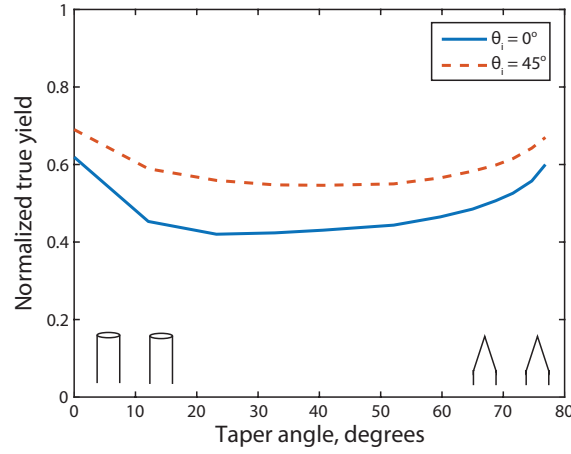
Because of the uncertainty in the taper angle estimates, a parametric study was carried out to gauge the effects of fiber tip tapering. These results are shown on figure 3.9 c) for a constant incident energy of 200eV and normalized by the true secondary yield from flat copper. This highlights the importance of accounting for fiber tapering in accurately modeling this particular textured surface. For example, flat-top fibers (0° taper angle) increase the SEE yield by $\sim 25 - 40\%$ as compared with 45° tapered fibers. Moreover, changing the taper angle by $\sim \pm 10^\circ$ from 45° affects the results by less than 4%, so precisely estimating the taper angle is not necessary in this range.

Although the true secondary yield at 45° incidence was almost 40% higher than at normal incidence for a flat copper surface (see equation 3.3 b), the fiber tips funneled electrons toward the substrate, resulting in increased trapping of secondaries and a reduction in the calculated/measured yield. These competing effects are evident in the non-monotonic trend of figure 3.9 c): as the fiber taper angle was increased, more backscattered secondaries were channeled to the substrate, reducing the yield up to a minimum at about 25° . Increasing

the taper angle further resulted in an increase in escaped secondaries because of the local increase in yield at the fiber tips (and because the tapered section of the fiber constitutes a larger fraction of the fiber in order to keep the radius and length constant). These effects were seen at both 0° and 45° incidence angles, although at normal incidence, the decrease in yield was more noticeable.



(a) True secondary yield from flat copper, compared (b) Comparison of true secondary yield results from tapered fiber geometry with copper fuzz data.



(c) Results from parametric study of taper angle (angle between fiber axis and tip surface normal).

Figure 3.9: True secondary yield results from tapered pillar geometry.

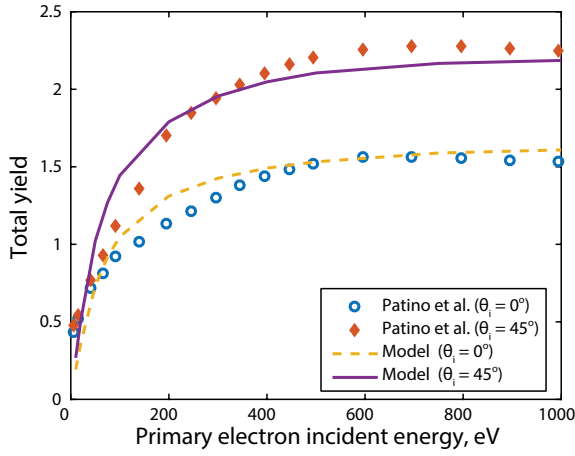
3.3.3 Tungsten fuzz

To examine nano-structured surfaces, the model was compared with recent experimental measurements of the yield from a well-characterized tungsten fuzz sample [21, 24]. This fuzz exhibits both vertical and horizontal fibers intertwined throughout the surface, so a cage-like geometry was used in our simulations. Table 3.2 summarizes the fiber dimensions measured from SEM images and figure A.5 a) shows curve fitting to flat tungsten yield data.

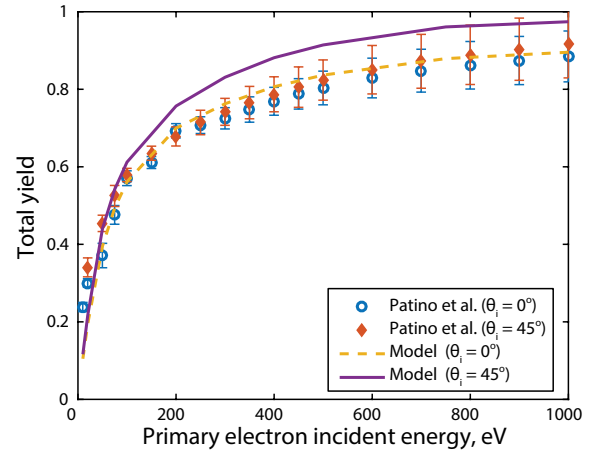
Fiber radius	12.5	nm
Fiber length	200	nm
Fiber separation	200	nm
Horizontal fibers	5	per side

Table 3.2: Tungsten fuzz fiber dimensions

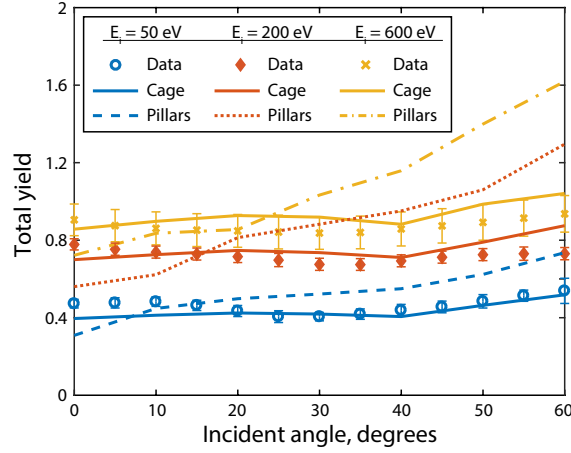
Comparing the fuzz results with experimental measurements shows good agreement in both trend and magnitude generally within the experimental error (see figure A.5 b). By examining figure A.5 c), we see that the yield is nearly constant across all incident angles. This independence is in contrast with earlier findings, where the yield monotonically increased with incident angle [77]. Our simulations show that this behavior is due to increased trapping of secondaries by the horizontal fibers, thus effectively eliminating the dependence of yield on incident angle.



(a) Total secondary yield from flat tungsten, compared with experimental data.



(b) Yield dependence on incident energy.



(c) Yield dependence on incident angle.

Figure 3.10: Total secondary yield results from cage geometry.

3.4 Discussion

The results of this paper show that the behavior of SEE from several common textured surface geometries can be accurately and efficiently modeled with relatively simple geometric constructs. Results were compared to and agreed with calculated and measured yield data from geometrically dissimilar carbon velvet, copper carpet, and tungsten fuzz surfaces, as well as new data of the independence of yield on incidence angle for tungsten fuzz presented in

this paper. Most importantly, the model captured contrasting surface effects on the yield's dependence on incidence angle between the different surface configurations via geometric modifications, showing its flexibility in simulating textured surface SEE. The model was able to simulate the reversal in the yield's dependence on incidence angle as the fiber aspect ratio increased past 100 for velvet geometries and the critical effect of fiber tip taper angle for carpet geometries. This study also showed that yield is independent of all incident angles for nano-structured fuzz geometries; a behavior that is unique in comparison to many other textured surfaces. Our simulations showed that this independence is primarily due to trapping of secondary electrons by the horizontally-oriented fibers in such a geometry. Therefore, this effect is expected to also be found for similar geometries, such as foam materials.

CHAPTER 4

DC-ION Plasma Model

Thruster miniaturization has shown promise in delivering high ΔV and inclination change capabilities to CubeSats and other SmallSats [79, 80, 81, 82, 83, 84]. Accurate computational models of such electric propulsion devices can significantly speed up the iterative design process, reduce the cost of (or enable) lifetime testing, and uncover physical processes vital to improving performance and efficiency. Electric propulsion devices such as the Miniature Xenon Ion (MiXI) thruster and the Magnetically Shielded Miniature (MaSMi) Hall thruster have utilized computational models (DC-ION and Hall2De, respectively) to inform design decisions and converge on a final design [5, 85, 86, 87].

Computational thruster models have been so far validated by comparisons with experimentally measured performance data, such as thrust, specific impulse, and mass utilization. However, recent plasma parameter mapping techniques allow extended validation of these models by comparison with plasma density, potential, temperature, etc. [88, 89, 90, 91]. In this work, DC-ION simulations are qualitatively validated against MiXI plasma mapping measurements. Recent improvements to the model are discussed which are necessary for capturing small density structures in the plasma.

Section II will briefly overview DC-ION and its subcomponents, and section II discusses improvements made to memory management, mesh resolution, and magnetic field modeling. Section IV then compares simulation results to plasma density maps for the MiXI (3-Ring) configuration, and section V concludes with closing remarks.

4.1 DC-ION Model Overview

DC-ION is a hybrid discharge model originally developed to aid in the design of the MiXI thruster. DC-ION successfully matched performance data for the NASA Solar Technology Application Readiness (NSTAR) thruster and accurately predicted MiXI's performance. It combines view factor, particle-in-cell (PIC), and fluid sub-models to track the neutral, primary (high-energy) electron, and ion and plasma (thermalized, low-energy) electron densities, respectively. Figure 4.1 summarizes the structure of the algorithm, which is well suited for plasma physics modeling within ion thrusters.

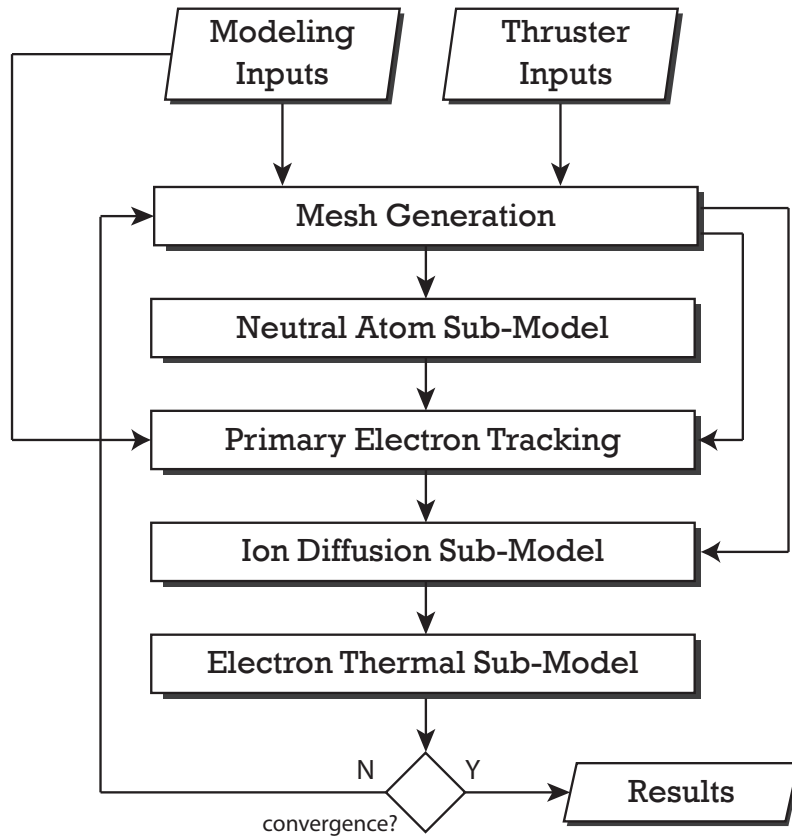


Figure 4.1: DC-ION model flow chart.

Plasma species densities are computed over an internal, orthogonal, 2D mesh (though other types of meshes could also be used). A boundary mesh is also constructed to incorpo-

rate geometric effects of the discharge chamber, cathode, and grids. The model takes initial guesses on various densities and temperatures as inputs, and ramps up the operating conditions for a specified number of iterations in order to prevent large density gradients between iterations. Similarly, mixing between iterations is used to reduce noise primarily from the PIC sub-model. The algorithm is iterated until reaching steady state, which is detected by tracking the convergence of neutral gas and ion beam calculations of the discharge propellant efficiency.

In the following subsections, the neutral view factor, primary electron PIC, diffusion, and electron energy sub-models will be described in some detail. A more detailed review of the model can be found in Ref. [47]. A discussion on improvements made to the model will be subsequent to the model description.

4.1.1 Neutral sub-model

Neutral atoms are tracked with a computationally-efficient view factor model which traces neutral flux contributions due to recombination and neutral gas sources onto internal mesh cells in 2.5D, as shown on figure 4.2. A similar model has been previously used to successfully simulate thermal transport [92]. Geometric protrusions (for instance due to cathodes and grid flanges) can shadow other surfaces and are accounted for in the view factor calculations. Along each ray, neutral "loss" due to ionization collisions reduces the flux contribution onto each cell. Similarly, grid neutral transparency can reduce the flux by a prescribed percentage.

The view factor between every boundary mesh cell is used to calculate the flow of neutrals from each cell using continuity,

$$Y_h = \sum_m V_{mh} Y_m (1 - \zeta_{o,m}) + \sum_s V_{sh} Y_s + Y_{rh} \quad (4.1)$$

where Y is the flow (in atoms/s), V is the view factor, ζ_o the grid neutral transparency, and

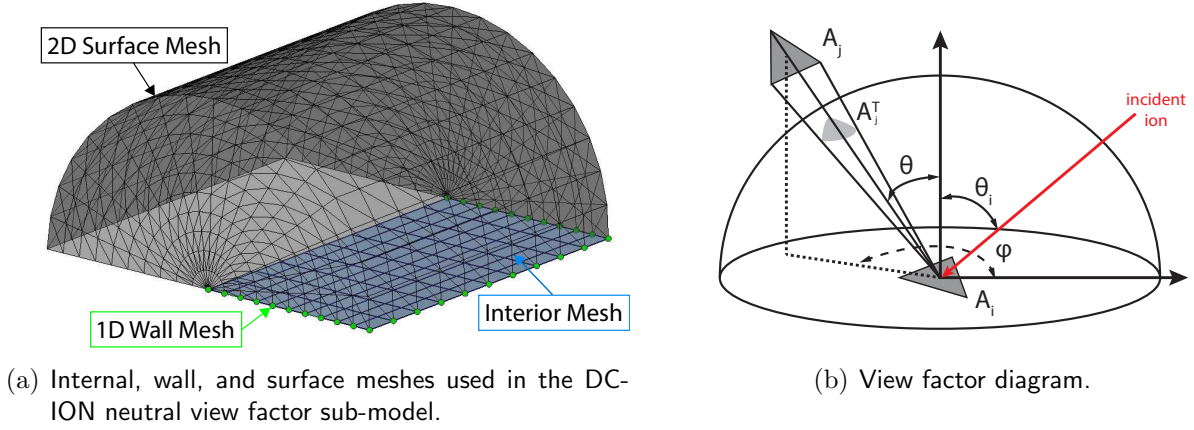


Figure 4.2: Overview of neutral gas submodel.

the subscripts represent cells h and m , source s . The resulting matrix is solved numerically for the flows Y . These flow values are then used to solve for the neutral density on each internal mesh cell using momentum conservation,

$$n_k = 4 \sum_m V_{mk} (1 - \zeta_{o,m}) \frac{\Gamma_m}{\bar{C}_m} + \sum_s \frac{\Gamma_{sk}}{\bar{C}_s} \quad (4.2)$$

where n_k is the density on internal mesh cell k , Γ is the neutral flux (in atoms/s/m²), and $\bar{C}$ the thermal velocity. The neutral flux from the wall is obtained by dividing the flow by the wall area, and the flux from sources is calculated assuming a cosine distribution,

$$\Gamma_{sk} = Y_{sk} \frac{\cos \theta_{sk}}{\pi \Delta_{sk}^2}$$

Here, θ_{sk} and Δ_{sk} are the angle and distance between the source and the center of mesh cell k , respectively.

Finally, the discharge propellant efficiency is calculated as

$$\eta_{ud[Gas]} = \frac{\dot{m}_d - \dot{m}_{loss}}{\dot{m}_d} = 1 - \frac{\sum_h Y_h \zeta_{o,h}}{\sum_s Y_s} \quad (4.3)$$

Equation 4.3 is compared with equation 4.8 in order to detect steady-state convergence.

4.1.2 Primary Electron Tracking

Because high energy primary electrons are primarily responsible for ionization of the neutrals, they are kinetically treated using a PIC method. The Boris method is the prevalent technique for particle tracking in plasma models due to its second-order accuracy and computational efficiency. Because the Boris method is a leap-frog technique which necessitates time symmetry between position and velocity half-steps, it is limited to constant time step iterations. In ion thruster magnetic fields, where the field strength varies greatly between the near-cusp and low-field regions, the Boris method may require a large number of short time steps to preserve accuracy throughout the particle's path. Adaptive time stepping is often used to speed up particle pushing in the low-field regions and maintain accuracy in the near-cusp regions, but this leads to a failure to conserve the total energy, as shown on Ref. [93] and figure 4.3.

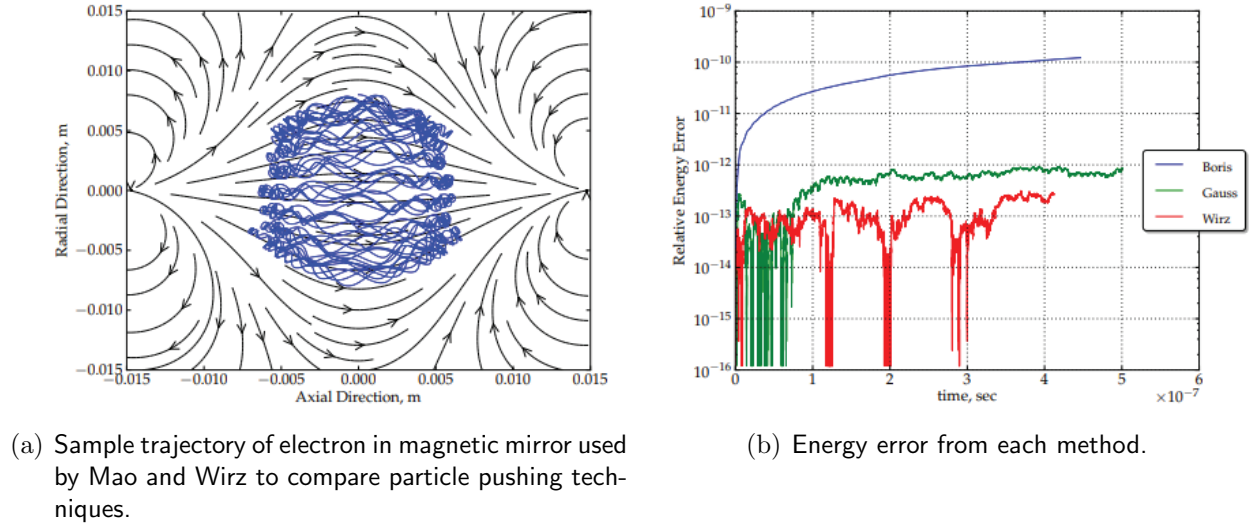


Figure 4.3: Wirz particle tracking method validation. Figures reproduced from Ref. [93].

To take advantage of adaptive time stepping, a modified predictor-corrector method pushes the particle on a coordinate system based on the local magnetic field line is used (henceforth referred to as the Wirz method). Similar to the Boris method, this scheme provides second-order accuracy and partitions the electric field push in two (before and after

the magnetic field), but it also perfectly conserves the angular momentum of the particles. In addition, because the position and velocity are aligned on the temporal grid, the method does not require constant time stepping. The method is summarized in figure 4.4; a more thorough review of the Wirz method can be found in Ref. [93].

Sample particle tracks of primary electrons in NSTAR obtained using the Wirz method are shown on figure 4.4. Performance and accuracy comparisons between the two methods are made in this work and can be found in section 4.3.

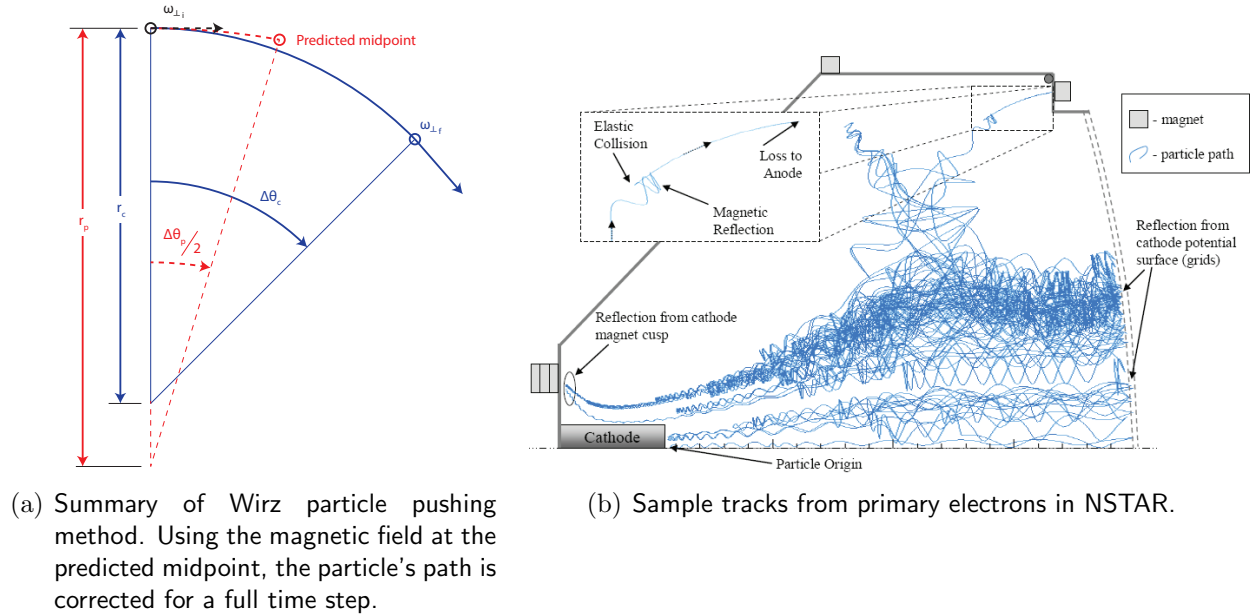


Figure 4.4: Overview of Wirz particle tracking method and sample tracks.

As the primary electrons are pushed, they may experience collisions with neutrals, ions, or plasma electrons, resulting in ionization, excitation, double ionization, or Spitzer particle-field slowing. Primary electron recombination and ion excitation collisions are neglected because they are at least an order of magnitude slower than the Spitzer particle-field slowing time [47]. Using the probability of each type of collision, the total primary electron current before and after each time step can be calculated,

$$J_{p,f} = J_{p,i}(1 - P_{iz})(1 - P_{ex})(1 - P_{rx})(1 - P_{an}) \quad (4.4)$$

where P is the probability of ionization, excitation, relaxation, or anomalous resistance, and i and f represent the initial and final primary electron currents, respectively. The anomalous resistance is described in Ref. [94]. After each time step, the closest internal mesh cell is populated with a primary electron density given by

$$\Delta n_p = \Delta t \frac{J_{p,f} + J_{p,i}}{2} \frac{V_{cell}}{e} \quad (4.5)$$

4.1.3 Diffusion sub-model

The diffusion model couples continuity and momentum conservation equations for ions and electrons via the electron-ion collision term. The resulting equation, assuming that the plasma is an ideal gas at steady or quasi-steady state, stationary diffusive plasma conditions, ion temperatures one-half to one order of magnitude smaller than electron temperatures (see Ref. [47]), and Simon short-circuiting (so that $E_\perp \approx 0$ [95]), the diffusion equation becomes

$$\dot{n}_i = -\nabla \cdot \left(\underline{\underline{\mathbf{M}_i}} \nabla(nT_i) + \underline{\underline{\mathbf{M}_e}} \nabla(nT_e) \right) \quad (4.6)$$

where $\dot{n}_i$ is the ion generation rate, n is the plasma density, T_i and T_e are the ion and electron temperatures, and the ion and electron mobility tensors are given by

$$\begin{aligned} \underline{\underline{\mathbf{M}_i}} &= \begin{bmatrix} M_i & 0 \\ 0 & M_i^\perp \end{bmatrix} = \begin{bmatrix} \frac{\mu_e \mu_{ii} + \mu_i \mu_{ei}}{\mu_e + \mu_i} & 0 \\ 0 & \frac{\mu_e \mu_{ii}^\perp + \mu_i \mu_{ei}^\perp}{\mu_e + \mu_i} \end{bmatrix} \\ \underline{\underline{\mathbf{M}_e}} &= \begin{bmatrix} M_e & 0 \\ 0 & M_e^\perp \end{bmatrix} = \begin{bmatrix} \frac{\mu_e \mu_{ee}^\perp + \mu_i \mu_{ee}}{\mu_e + \mu_i} & 0 \\ 0 & \frac{\mu_e \mu_{ee}^\perp + \mu_i \mu_{ee}^\perp}{\mu_e + \mu_i} \end{bmatrix} \end{aligned}$$

These mobility equations are modified to include the non-classical "Bohm mobility," $M_B^\perp$ which accounts for the B^{-1} perpendicular diffusion observed in fully ionized regions. This

leads to an effective electron mobility given by

$$\underline{\underline{\mathbf{M}_e}}_{eff} = \begin{bmatrix} M_e & 0 \\ 0 & \frac{\nu_{e-o}}{\nu_{e-o} + \gamma_{nc}\nu_{e-i}} M_e^\perp + \frac{\gamma_{nc}\nu_{e-i}}{\nu_{e-o} + \gamma_{nc}\nu_{e-i}} \frac{k}{16eB} \end{bmatrix} \quad (4.7)$$

where ν are collision frequencies, B is the magnetic field strength, and γ_{nc} is a non-classical diffusion parameter which controls the relative effects of classical and Bohm diffusion. It was found that $\gamma_{nc} \approx 1/4$ best matches experimental NSTAR and MiXI data.

The ion generation rate in equation 4.6 is calculated using the results from the primary electron tracking sub-model,

$$\begin{aligned} \dot{n}_i &= \dot{n}_i^p + \dot{n}_i^s \\ \dot{n}_i^p &= \frac{\sum (J_{p,i} - J_{p,f}) P_{iz}}{(P_{iz} + P_{ex} + P_{rx} + P_{an}) V_{cell}} \\ \dot{n}_i^s &= K_{iz}^s n_o n_s + K_{iz}^{+s} n_i n_s \end{aligned}$$

The first iteration of DC-ION requires an initial guess for the slow (plasma) electron density, n_s , as an input, and is subsequently calculated from quasi-neutrality. Equation 4.6, modified by the effective electron mobility in equation 4.7, is solved numerically along the internal mesh using a packaged sparse matrix solver. Plasma electron density is then obtained from quasi-neutrality using the calculated values of the primary electron and ion densities on each internal mesh cell center.

Finally, in order to track convergence of the model, the propellant utilization is calculated by

$$\eta_{ud[Gas]} = \frac{\dot{m}_d - \dot{m}_{loss}}{\dot{m}_d} = \frac{J_B m_i}{e \dot{m}_d} \quad (4.8)$$

where J_B is obtained from the total flux of ions (including single and double ions) entering the ion optics sheath.

4.1.4 Electron Thermal sub-model

The plasma electron temperature is obtained via energy conservation by obtaining an estimate of the electron flux using an effective potential.

Combining electron continuity with momentum conservation,

$$\dot{n}_e = \nabla \cdot \Gamma_e = \nabla \cdot \left(-\underline{\underline{\mu_e^*}} n \mathbf{E} - \underline{\underline{\mu_e^*}} \nabla (n T_e) \right)$$

$$\underline{\underline{\mu_e^*}} = \frac{e}{m_e(\nu_{e-i} + \nu_{e-o})} \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{1+\Omega_e^2} \end{bmatrix}$$

where Ω_e is the electron Hall parameter. Defining an effective potential, $\psi = T_e \log(n/n_c) - \phi$, where n_c is a reference density, this equation reduces to

$$\dot{n}_e = \nabla \cdot \underline{\underline{\mu_e^*}} n \nabla \psi \quad (4.9)$$

This equation is coupled with boundary conditions at the cathode, magnetic cusps, and between the cusps to obtain the effective potential everywhere on the internal mesh (see Ref. [47]).

Following Braginskii's analysis [96], the electron energy conservation equation can be combined with Ohm's law to obtain

$$\frac{\partial}{\partial t} \left(\frac{3}{2} n k T \right) + \nabla \cdot \left(\frac{5}{2} k T \Gamma + \mathbf{q} \right) = Q_c \quad (4.10)$$

where $\mathbf{q}$ is the electron heat flux as derived in Ref. [96] and Q_c is the change in energy density due to inelastic collisions, given by

$$Q_c = -(\dot{n}_i^s \epsilon_c) |_s + \sum_w (\dot{n}_w \epsilon_w) |_p$$

Here, the first term is the product of the ionization rate due to plasma electrons and the

energy loss per plasma electron ionization event due to inelastic conditions. The second term represents the sum over all primary collisions w and ϵ_w is the average energy of plasma electrons created by process w . Equation 4.10 assumes that $Q_c \gg \dot{n}mu^2/2$ and Q_{el} (i.e. energy density changes due to elastic collision) is negligible. This equation is then numerically solved as a sparse matrix throughout the internal mesh.

4.2 DC-ION Improvements

Several changes are made to the code in order to decrease computational cost, increase modeling capabilities, and improve accuracy. The modifications were first tested with MiXI simulations in order to gage their benefits over the previous version of DC-ION. These improvements are discussed in the following subsections.

4.2.1 Efficient Memory Management

Previously, DC-ION used a separate module to define all derived types (analogous to classes in C++) and create all variables that are passed between the sub-models, functions, and subroutines. This was inefficient because each time function was called, it duplicated every variable, requiring more memory. Because these variables were static data, the model was limited to 2 GB of memory [97]. Switching to 64-bit architecture increases the memory limit for dynamic (allocatable) data, but has no impact on the limit on static data [97]. Hence, the model was limited in the internal mesh density by the static data limitations.

To ameliorate this problem, derived types are still defined in a separate module, but each function only declares the necessary variables relevant to that function. This change resulted in an increase in the internal mesh density from 17×17 to 160×80 . Further improvements in memory management can be made by making large arrays dynamically allocatable, which has a data limitation of 8 TB for 64-bit applications [97].

4.2.2 Matrix Solver Implementations

Reducing static memory use allows for refined meshing, but this can slow down the model significantly, especially in the neutral view factor sub-model. This is because solving for the neutral density requires numerically solving an $N \times N$ matrix and accounting for collisions along each view factor ray.

To decrease computational run time, Intel’s Math Kernel Library (MKL) Linear Algebra Package (LAPACK) is used. LAPACK improves computational time by parallelizing the work through several CPU threads and using optimized algorithms. In addition, the sparse matrices that are solved in the diffusion and thermal sub-models use MKLs Parallel Direct Sparse Solver (PARDISO) to further decrease computational run time. Together, efficient memory management and parallelized, high-performance matrix solving packages allow very fine meshes to be used in DC-ION.

4.2.3 Magnetic Field Solver Additions

Finally, to improve accuracy in the primary electron tracking sub-model, two new options were added to the magnetic field solver module: an analytical solution for permanent block magnets, and a Helmholtz magnetic field solver.

4.2.3.1 Permanent Block Magnet Solution

The equations, derived by Engel-Herbert and Hesjedal, are given by [98, 99]

$$\begin{aligned}
B_x &= \frac{\mu_0 M}{4\pi} \sum_{k=1}^2 \sum_{l=1}^2 \sum_{m=1}^2 s_{klm} \log \left(y_l + \sqrt{x_k^2 + y_l^2 + z_m^2} \right) \\
B_y &= \frac{\mu_0 M}{4\pi} \sum_{k=1}^2 \sum_{l=1}^2 \sum_{m=1}^2 s_{klm} \log \left(x_k + \sqrt{x_k^2 + y_l^2 + z_m^2} \right) \\
B_z &= -\frac{\mu_0 M}{4\pi} \sum_{k=1}^2 \sum_{l=1}^2 \sum_{m=1}^2 s_{klm} \frac{x_k}{|x_k|} \frac{z_m}{|z_m|} \tan^{-1} \left(\frac{|x_k| \cdot y_l}{|z_m| \cdot \sqrt{x_k^2 + y_l^2 + z_m^2}} \right)
\end{aligned} \tag{4.11}$$

where μ_0 is the permeability of free space, M is the magnetization (in the z direction), $s_{klm} = (-1)^{k+l+m}$, $x_k = x + (-1)^k W/2$, $y_l = y + (-1)^l L/2$, $z_m = z + (-1)^m H/2$, and W , L , and H are the corresponding block magnet dimensions.

This analytical solution is more accurate than the corrected dipole approximation previously used [47], especially near the cusps. In addition, the field is solved in three dimensions and accounts for asymmetries in the magnetic field in the azimuthal regions between block magnets. A comparison of the MiXI (3-Ring) magnetic field using the permanent block magnet analytical solution and Maxwell results is shown on figure 4.5. Note that DC-ION uses 8 block magnets (as does MiXI) for each equivalent ring magnet in Maxwell.

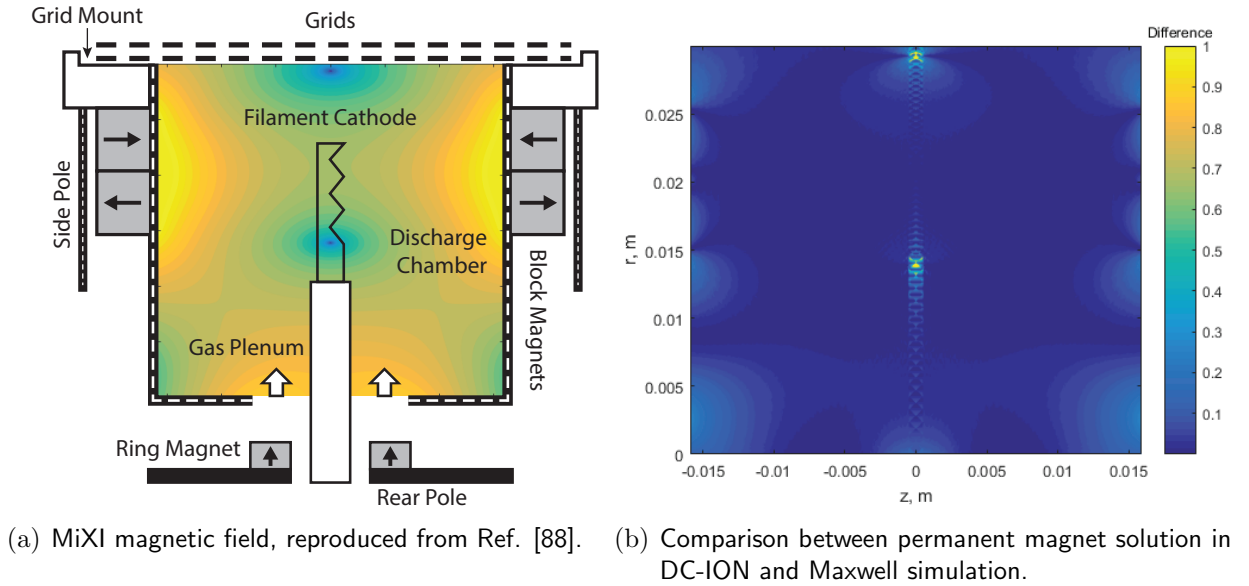


Figure 4.5: Permanent magnet solver validation.

4.2.3.2 Helmholtz Field Solver

While the permanent block magnet solver is instrumental in accurately simulating MiXI and other ion thruster configurations, it is inadequate for obtaining the magnetic field from electromagnet coils. The plasma column experiment used current loops in a Helmholtz configuration to generate a uniform axial field. Although an analytical solution exists for

current loops, this solution requires integration over small sections of the loop and can be computational costly [100]. Equations for the magnetic field from a Helmholtz coil are given in Ref. [101]:

$$\begin{aligned}
B_r(r, z) &= \frac{\mu_0 N I \left(z + \frac{R}{2}\right)}{2\pi r \left[(R+r)^2 + \left(z + \frac{R}{2}\right)^2\right]^{\frac{1}{2}}} \left[-K_1 + \frac{R^2 + r^2 + \left(z + \frac{R}{2}\right)^2}{(R-r)^2 + \left(z + \frac{R}{2}\right)^2} E_1 \right] \\
&\quad + \frac{\mu_0 N I \left(z - \frac{R}{2}\right)}{2\pi r \left[(R+r)^2 + \left(z - \frac{R}{2}\right)^2\right]^{\frac{1}{2}}} \left[-K_2 + \frac{R^2 + r^2 + \left(z - \frac{R}{2}\right)^2}{(R-r)^2 + \left(z - \frac{R}{2}\right)^2} E_2 \right] \\
B_z(r, z) &= \frac{\mu_0 N I}{2\pi \left[(R+r)^2 + \left(z + \frac{R}{2}\right)^2\right]^{\frac{1}{2}}} \left[K_1 + \frac{R^2 - r^2 - \left(z + \frac{R}{2}\right)^2}{(R-r)^2 + \left(z + \frac{R}{2}\right)^2} E_1 \right] \\
&\quad + \frac{\mu_0 N I}{2\pi \left[(R+r)^2 + \left(z - \frac{R}{2}\right)^2\right]^{\frac{1}{2}}} \left[K_2 + \frac{R^2 - r^2 - \left(z - \frac{R}{2}\right)^2}{(R-r)^2 + \left(z - \frac{R}{2}\right)^2} E_2 \right]
\end{aligned} \tag{4.12}$$

where R is the Helmholtz radius, r, z are the radial and axial coordinates, N and I are the number of loops and the current passing through them, and K_1 , K_2 , E_1 , and E_2 are the complete elliptic integrals of the first and second kind with moduli given by

$$\begin{aligned}
h_1^2 &= \frac{4Rr}{(R+r)^2 + \left(z + \frac{R}{2}\right)^2} \\
h_2^2 &= \frac{4Rr}{(R+r)^2 + \left(z - \frac{R}{2}\right)^2}
\end{aligned}$$

A comparison of the results from the analytical solution and Maxwell simulations is shown on figure 4.6.

4.2.4 Argon Collision Rate Constants

Changing the neutral gas species from xenon to argon in DC-ION requires modifying the collision cross section equations. These equations are obtained semi-empirically; for DC-

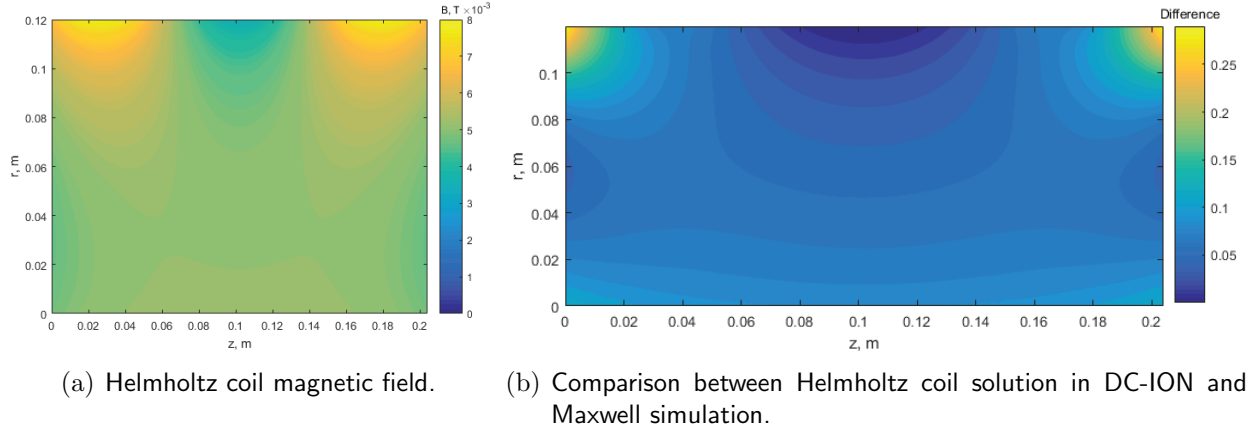


Figure 4.6: Helmholtz coil magnetic field solver validation.

ION, the curve fits for inelastic, elastic, and total momentum exchange collisions, as well as for ionization and excitation, respectively, are obtained from Ref. [102].

$$\begin{aligned}
 \sigma_{il} &= 4\pi a_0^2 \left[M_{il}^2 \frac{R}{E} \ln \left(4C_{il} \frac{E}{R} \right) \right] \\
 \sigma_{el} &= 4\pi a_0^2 \left[A_{el} \frac{R}{E} + B_{el} \frac{R^2}{E} + C_{el} \frac{R^3}{E} + \dots \right] \\
 \sigma_{tot} &= a_0^2 \left[A_{tot} \frac{R}{E} + B_{tot} \frac{R}{E} \ln \left(\frac{E}{R} \right) + C_{tot} \frac{R^2}{E} \right] \\
 \sigma_{iz}^i &= \frac{1}{EE_i} \left[A \ln \left(\frac{E}{E_i} \right) + \sum_{j=1}^N B_j \left(1 - \frac{E_i}{E} \right) \right] \\
 \sigma_{ex} &= \frac{1}{F(G+E)} \ln \frac{E}{E_{ex}}
 \end{aligned} \tag{4.13}$$

where $R = 13.6$ eV is the Rydberg constant, a_0 is the Bohr radius, and E the electron energy in eV. For argon, $M_{il} = 2.255$, $C_{il} = 0.8114$, $A_{el} = 231$, $B_{el} = -324$, $C_{el} = 0$, $A_{tot} = 800.9$, $B_{tot} = 63.9$, $C_{tot} = -1018$, $F = 25.19 \times 10^{-20} \text{ keV}^{-1} \text{ m}^{-2}$, $G = 23.6$ eV and argon ionization energies, E_i , are shown on table 4.1. These equations are shown on figure 4.7.

Collision rate constants can then be obtained from these cross sections knowing the

Constant	Ar ⁺	Ar ²⁺	Ar ³⁺
A	2.532	2.086	1.170
B_1	-2.672	1.077	0.843
B_2	2.543	-2.172	-2.877
B_3	-0.769	0.809	1.958
B_4	0.008	—	—
B_5	0.006	—	—

Table 4.1: Argon ionization constants, taken from Ref. [102], in units of $10^{-23} \text{ eV}^2 \text{ m}^2$

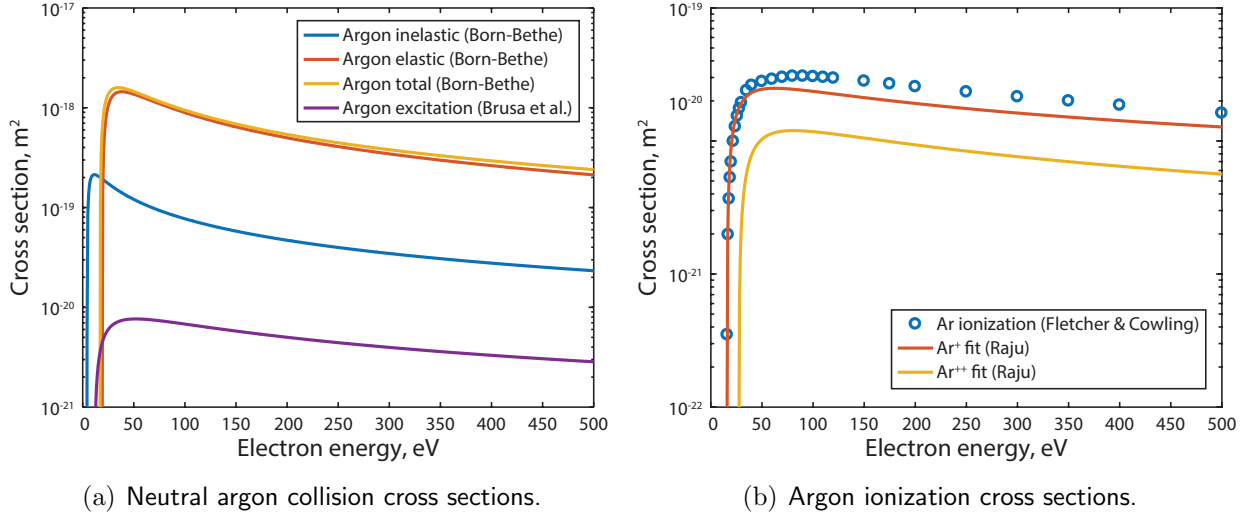


Figure 4.7: Ar cross section curve fits, obtained from Ref. [102]

velocity distribution $f(v)$,

$$K(v) = \int_0^\infty v f(v) \sigma(v) dv \quad (4.14)$$

The electron velocity distribution of the electrons is assumed to be that of an accelerated

half-Maxwellian, given by

$$\begin{aligned}
f_{HM}(\alpha) &= \frac{2}{\int_{\alpha_0}^{\infty} e^{-x^2} dx} \alpha (\alpha - \alpha_0) e^{-\alpha^2} \\
\alpha &= \sqrt{\frac{V_p + 3T_p}{T_p}} \\
\alpha_0 &= \sqrt{\frac{V_p}{T_p}}
\end{aligned} \tag{4.15}$$

Hence, $K = K(V_p, T_p)$. The rate constant is fitted numerically using polynomial of V_p for several values of α_0 . These rate constant values are then interpolated to obtain an approximate result. The polynomial curve fits used for each type of collision can be found in Appendix C.

4.3 MiXI Simulations

With the improvements discussed in the previous section, DC-ION is used to simulate the MiXI thruster configuration and these results are compared with experimental density mapping data from Refs. [88, 89]. These results are then compared with analogous simulations using the previous version of DC-ION to show the improvements in accuracy achieved in this work. A comparison between the accuracy and computational efficiency of the Boris and Wirz particle tracking methods is also presented. Finally, convergence studies are carried out that justify the modeling parameters (mesh density and number of primary electrons tracked) used in obtaining accurate results.

4.3.1 Density Mapping Validation

DC-ION density mapping results for primary electrons and ions are compared with experimental data in figure 4.8. The differences seen near the downstream region are believed to be caused by the use of a slotted plate needed for probing (see Refs. [88, 89]) rather than

the ion optics modeled by DC-ION. In addition, experimental errors, disturbances due to probing, and numerical errors due to mixing and PIC noise introduce further differences. Regardless, the model is able to capture the arching structure of the primary electron density indicative of electron confinement near the magnetic cusps and successfully predicts the primary electron density qualitatively.

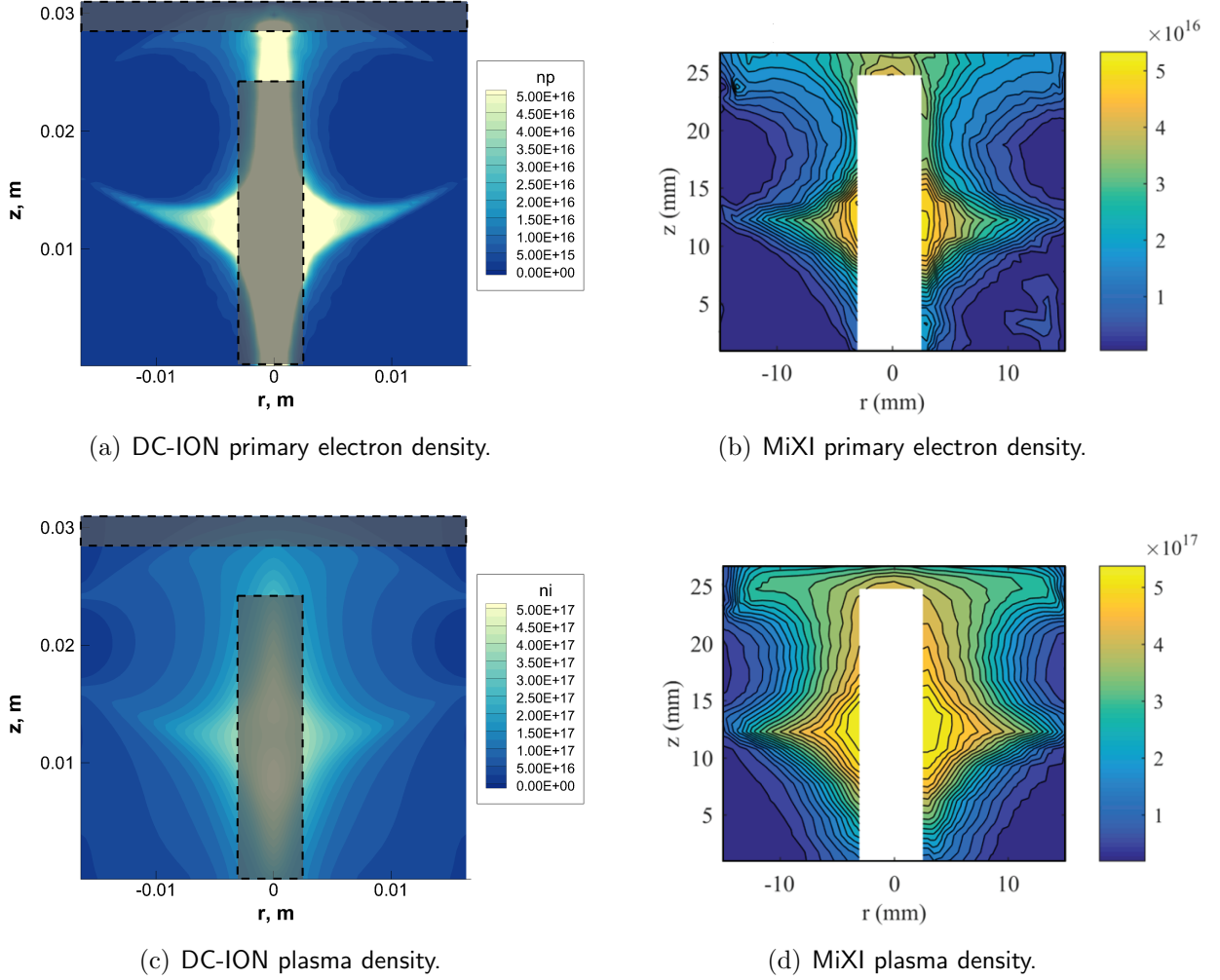


Figure 4.8: Qualitatively, the improved version of DC-ION presented in this work matches the observed density maps. Some differences in the downstream region are due to difficulties in simulating slotted plate used in experiment. Shaded boxes indicate regions the probe was unable to access.

4.3.2 Improvements in Modeling Results

The primary electron density is also simulated using the previous version of DC-ION for comparison purposes. Figure 4.9 shows the primary electron density using a 17×17 mesh, 100 primary electrons, and a dipole approximation for the magnetic field corrected near the cusps (see [47]). Because the mesh cell scale length is much greater than the density gradient scale length, the model is incapable of capturing density structures near the cusps. On the other hand, the improvements made to DC-ION allow it to capture the small density structures shown in the mapping data near the cusps. The model resolves the arching structure indicative of primary electron magnetic confinement correctly.

4.3.3 Wirz vs. Boris Methods

The primary electron densities obtained by changing from the Wirz to the Boris method are compared in table 4.2. For this comparison, constant time stepping was used for the Boris method, while the Wirz method is allowed to adapt the time step relative to the local magnetic field strength. Initial comparisons between the two methods showed comparable run times, with the Wirz method taking 1 hour and 2 minutes and the Boris method taking 1 hour and 10 minutes. However, the Boris method failed to properly capture the primary electron density near the cusps. The results using extremely small time stepping with the Boris method, detailed in table 4.2, were more accurate, but took almost 12 hours to complete. This comparison highlights the advantages of using adaptive time stepping and shows that the predictor-corrector technique is more accurate when the magnetic field has large gradients in small volumes.

4.3.4 Convergence Studies

With DC-ION qualitatively validated, a convergence study is carried out to ensure that appropriate modeling parameters are chosen which attain reasonable accuracy while main-

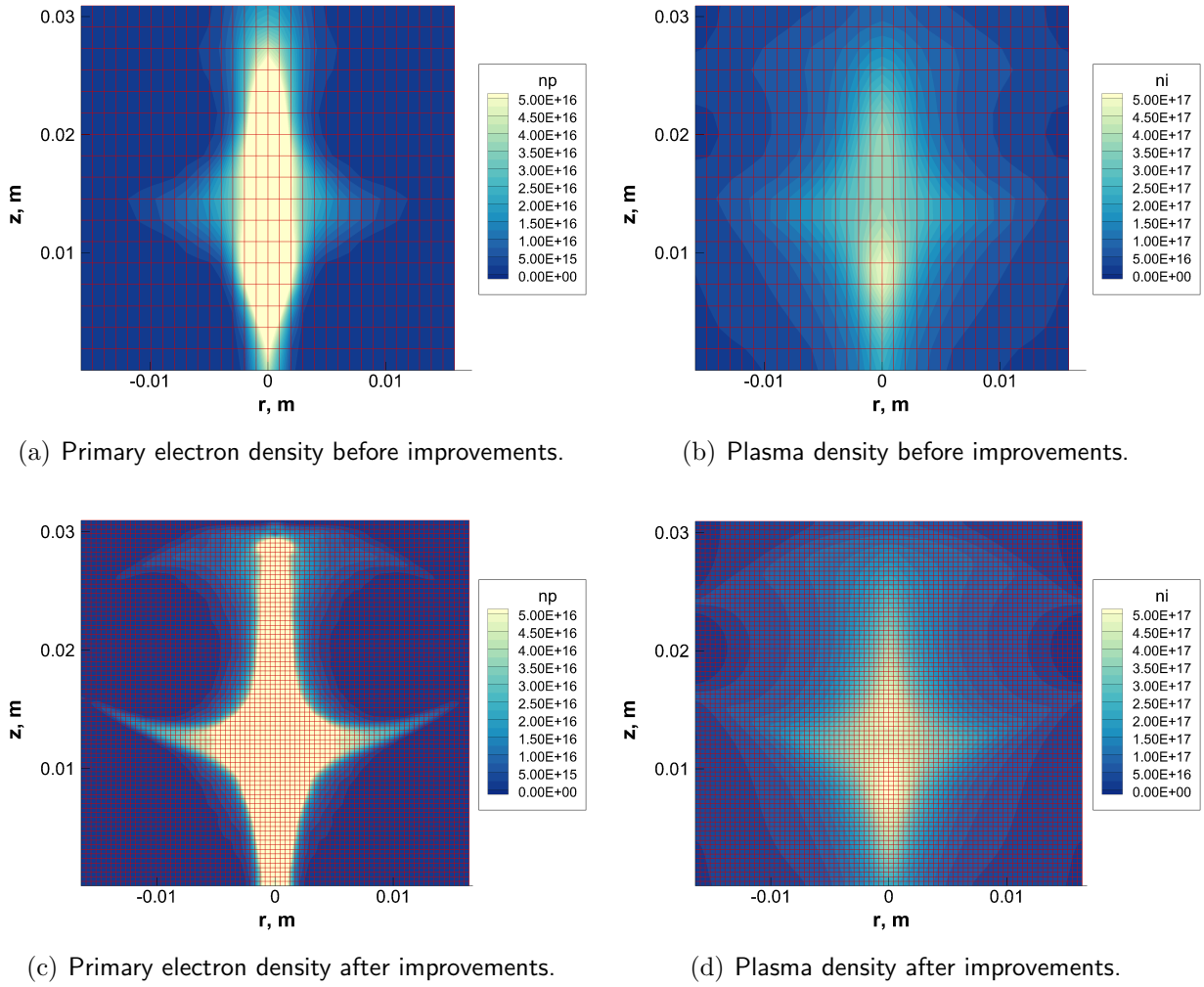


Figure 4.9: Side by side comparison of results before and after improvements to DC-ION.

PIC Method	Run Time (h:mm)	Initial step size (μ m)	Max no. of steps
Wirz Method	1:02	500	50,000
Boris Method	11:45	10	100,000

Table 4.2: Comparison of DC-ION run times using Wirz method (with adaptive time stepping) and Boris method (using constant time stepping) while attaining the same level of accuracy.

taining relatively low computational run time. The contour plots in figure 4.10 show the relative difference in plasma (left) and primary electron (right) densities compared with results from a 160×80 simulation for various mesh densities. The relative difference in primary electron density tends to be high, but only in low density regions where ionization is not likely to occur. The comparisons show that a mesh of 80×40 cells is sufficiently precise.

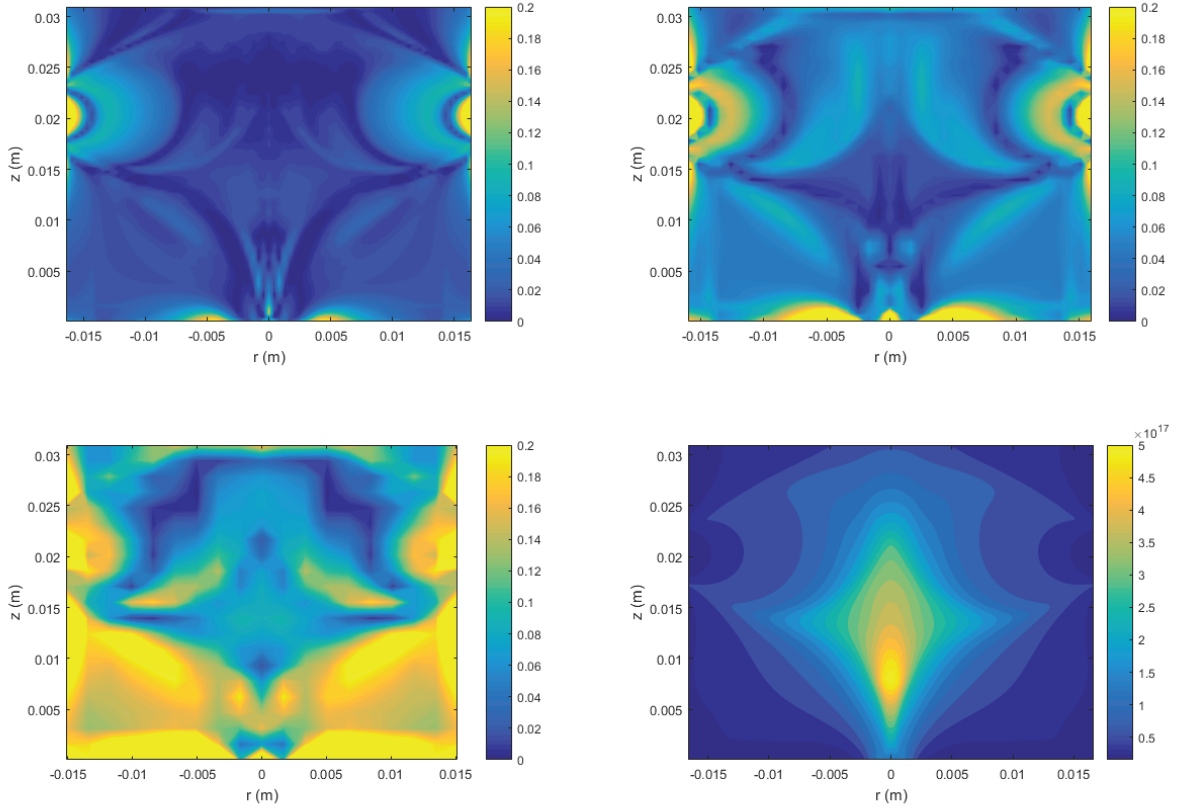


Figure 4.10: Convergence study for mesh density. Primary electron and plasma density differences calculated vs 160×80 mesh case for 80×40 (top left), 40×20 (top right), and 20×10 (bottom left) mesh cases. Plasma density shown for reference (bottom right).

Similarly, a convergence study is carried out to ensure that enough primary electrons are tracked to obtain accurate primary electron densities. Figure 4.11 shows that 200 primary electrons are sufficient to minimize the relative difference where the density is significant and ionization is likely to happen.

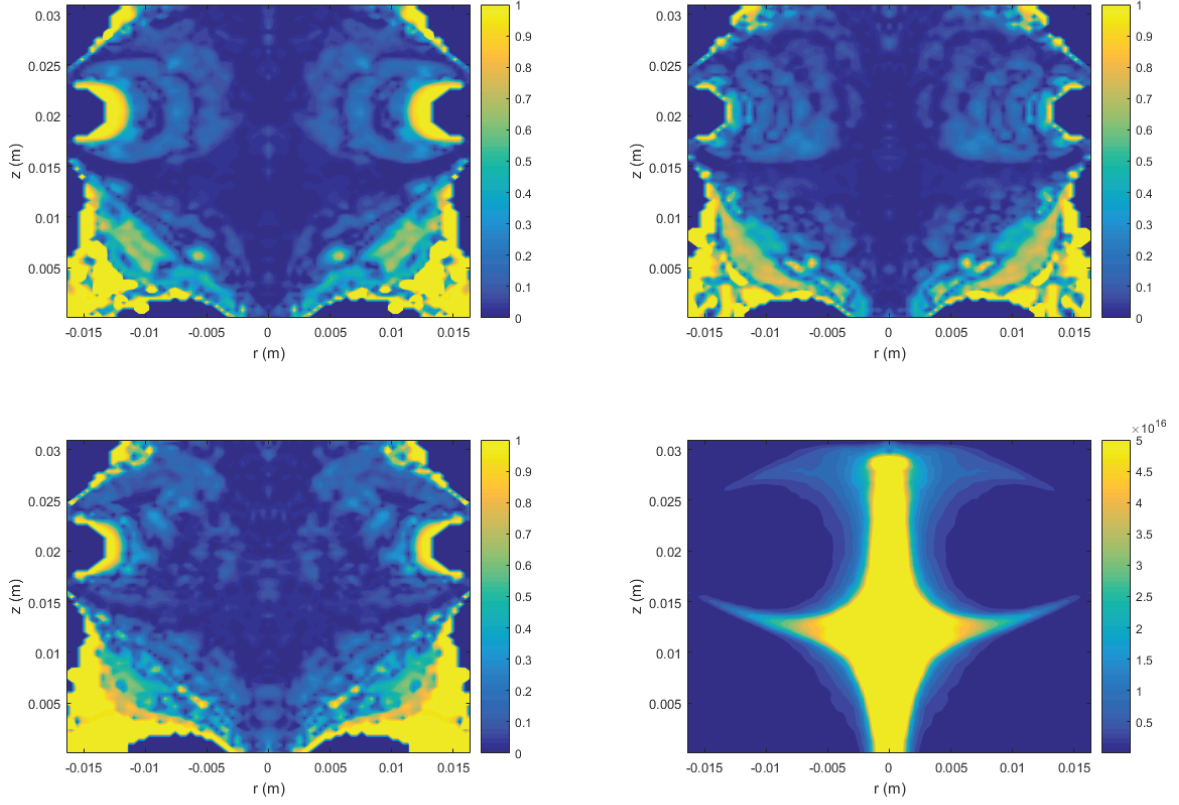


Figure 4.11: Convergence study for the number of primary electrons used. Primary electron density differences for 400 (top left), 200 (top right), and 100 (bottom left) primary electrons calculated vs. 800 primary electron case. Primary electron density shown for reference (bottom right). Note that errors are high only in regions of low primary electron density.

4.4 Ring Cusp Test Discharge Simulations

Because DC-ION was originally developed as an ion thruster model, its capabilities had to be tested to simulate DC discharge laboratory plasmas. The Ring Cusp Test Discharge (RCTD) was a simple experiment with three ring cusps that emulated an ion thruster's magnetic environment. This setup was used to baseline Langmuir probe theories and tip orientations and to map the plasma properties to facilitate validation of computational models.

The RCTD used a 5 mil tungsten wire coil as the cathode source, heated to under 2.4 A and 12 V. Xenon was used to backfill the entire vacuum chamber, and the primary electrons

were confined via three ring-magnets comprised of fifteen discrete samarium cobalt block magnets held in place by thin iron strips. The ring-magnets alternated in polarity to produced three magnetic field cusps at 1.2 kGauss. A radially oriented probe was axially swept along a 2 mm gap between the black magnets. Figure 4.12 shows the RCTD experimental setup.

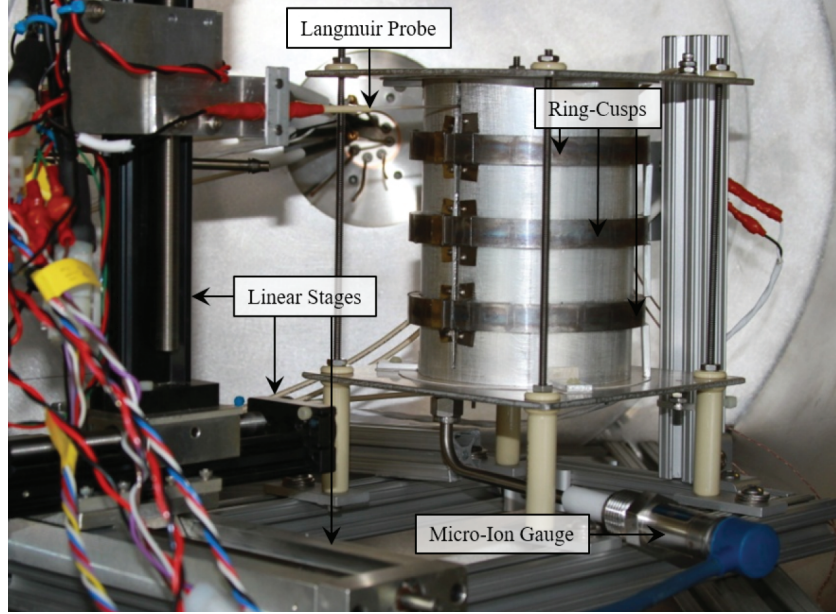


Figure 4.12: Ring cusp test discharge experimental setup (courtesy of Ref. [103]).

Simulation results agreed with experimental data taken by Dankongkakul and Wirz [103]. The primary electron density predicted by DC-ION follows the magnetic cusp structure, as observed in the experimental measurements. The plasma density results also agree qualitatively and are accurate to within experimental error and modeling uncertainty. These results show that DC-ION is capable of simulating a DC discharge plasma with the modifications and improvements outlined in the previous sections.

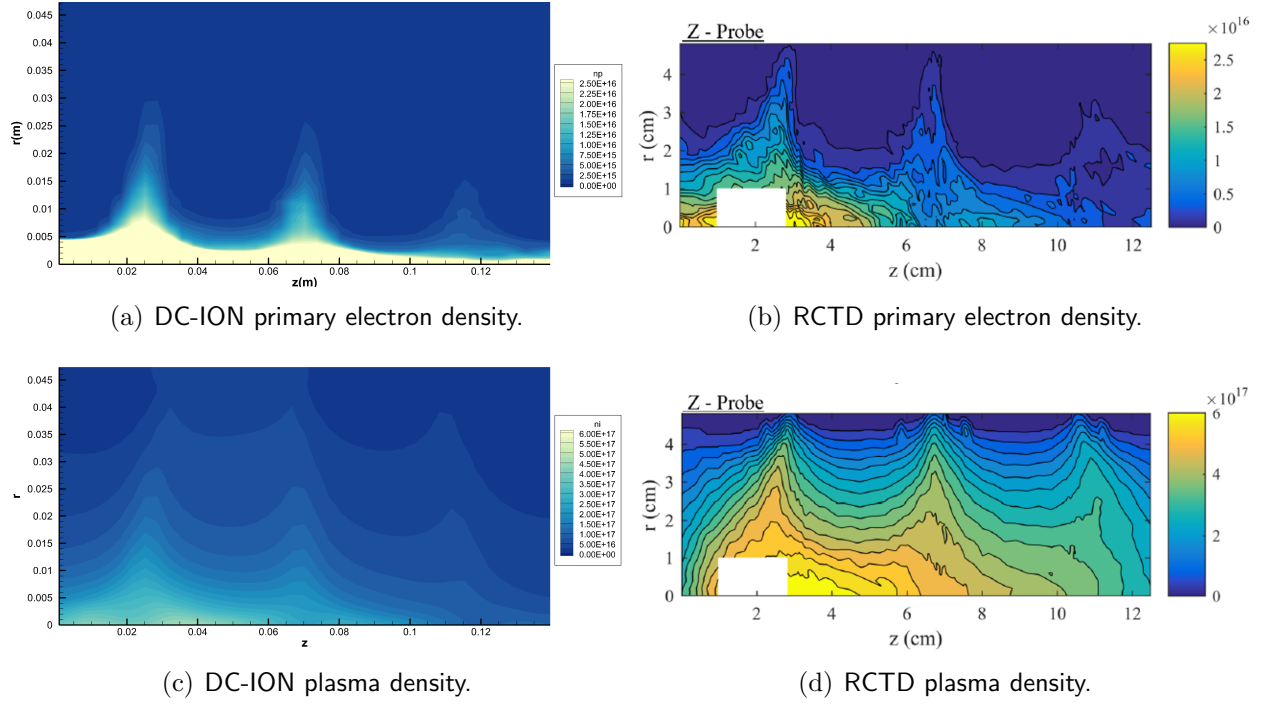


Figure 4.13: Ring cusp test discharge simulation results and comparison with experimental data from Ref. [103].

4.5 Plasma Column Simulations

With the modifications and improvements made to DC-ION, a canonical plasma column simulation was carried out to determine what effects surface structuring has on PMI, and how these effects in turn modify the plasma. The simulation results were compared with probe measurements from a plasma column experiment, which is detailed in the following subsection. The SEE physics discussed in chapter 3 were implemented into DC-ION, and the anode surface was changed (both experimentally and computationally) to interrogate plasma and PMI changes based on surface structure.

4.5.1 Plasma Column Experiment

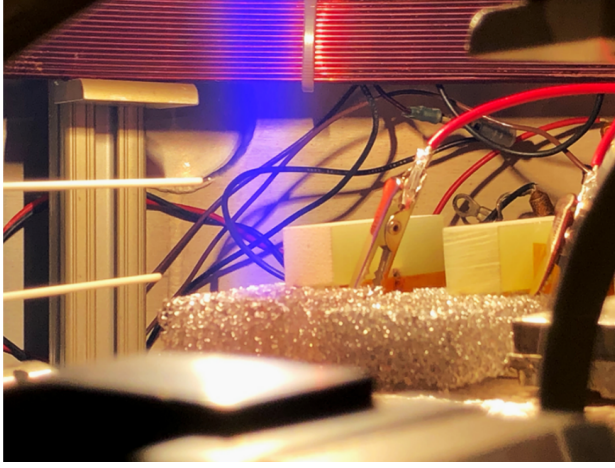
A cylindrical, DC discharge plasma column was set up inside the UCLA PLasma-Metamaterial Interactions facility by thermionically emitting electrons from a tungsten filament into argon

between two electrodes. The cathode filament was held at ground potential and supplied with 2.2 A, the anode aluminum target was biased to 55 V, and the vacuum chamber was pumped to maintain a background pressure of 2 mTorr. The electrons were confined by an axial magnetic field from a Helmholtz coil, measured to be approximately 56.5 G. Two cylindrical Langmuir probes were used to sweep out radial distributions of the plasma properties near the anode (approximately 20 mm away) and at the midplane. The anode surface was swapped using a planar stage between flat aluminum and two aluminum foams with porosities of 10 and 40 pores per inch (PPI). The current collected at the anode was 0.3 A for the slab and 0.45 A for the two foams. Figure 4.14 shows a diagram of the experimental setup, along with radial profiles of the plasma density in the near-anode and midplane regions for all three anode surfaces tested. These data show that the plasma density is not substantially affected far from the anode, but increase significantly due to reduced SEE in the presence of a foam surface.

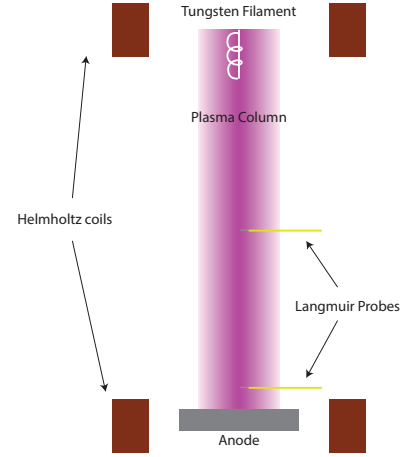
4.5.2 Plasma Column Simulation Results

The plasma column experiment discussed in the previous subsection was simulated using the new version of DC-ION. Secondary electron emission effects on the plasma were considered through the primary electron particle tracking module. As primary electrons impact the anode surface, the backscattering and true secondary electron emission yields are calculated to determine the collisional event outcome. When a backscattering event occurs, the angular and energy emission distributions discussed in chapter 3 are used to update the particle's velocity. The low energy true secondary electrons are accounted for in the plasma electron diffusion calculations. The effects of SEE on the plasma sheath are also accounted for through boundary conditions for the primary electrons. When near the anode, the primary electrons are decelerated by the plasma sheath potential drop. This effect is decreased in the presence of a low SEE surface, such as foam.

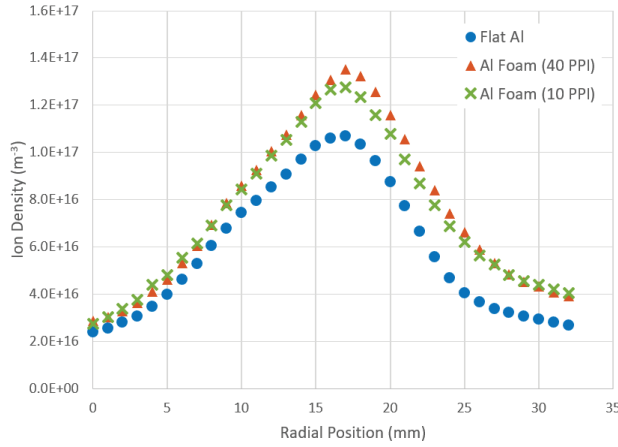
Tracking the path of primary electrons penetrating the foam layer was found to be pro-



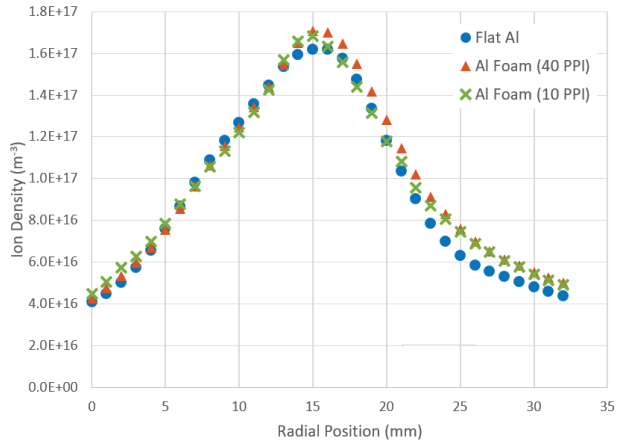
(a) Plasma column incident on aluminum foam anode surface.



(b) Diagram of plasma column experiment.



(c) Near-anode plasma density.



(d) Axial midplane plasma density.

Figure 4.14: Plasma column experiment.

hibitively inefficient because the length scales between the plasma column and the foam layer differ by several orders of magnitude. For computational simplicity, the SEE yield from the foam surfaces is estimated a priori to be reduced by approximately 50%, in agreement with preliminary experimental measurements using a quartz crystal microbalance (QCM). Because the foam is volumetrically porous, sputtering has not been observed to affect the SEE yield with sustained ion bombardment, hence, erosion is also not considered in these simulations.

The results from these simulations are compared with the experimental data and shown on figure 4.15. DC-ION successfully captured the increase in the plasma density near the anode due to the reduction in the SEE yield from the foam's surface structure, as predicted. This is because the suppression of SEE by capturing low energy emitted electrons in the foam pores maintains a high primary electron current to the wall, preventing a drastic reduction in the sheath potential drop, and allowing the high energy electrons to ionize the neutral gas near the anode.

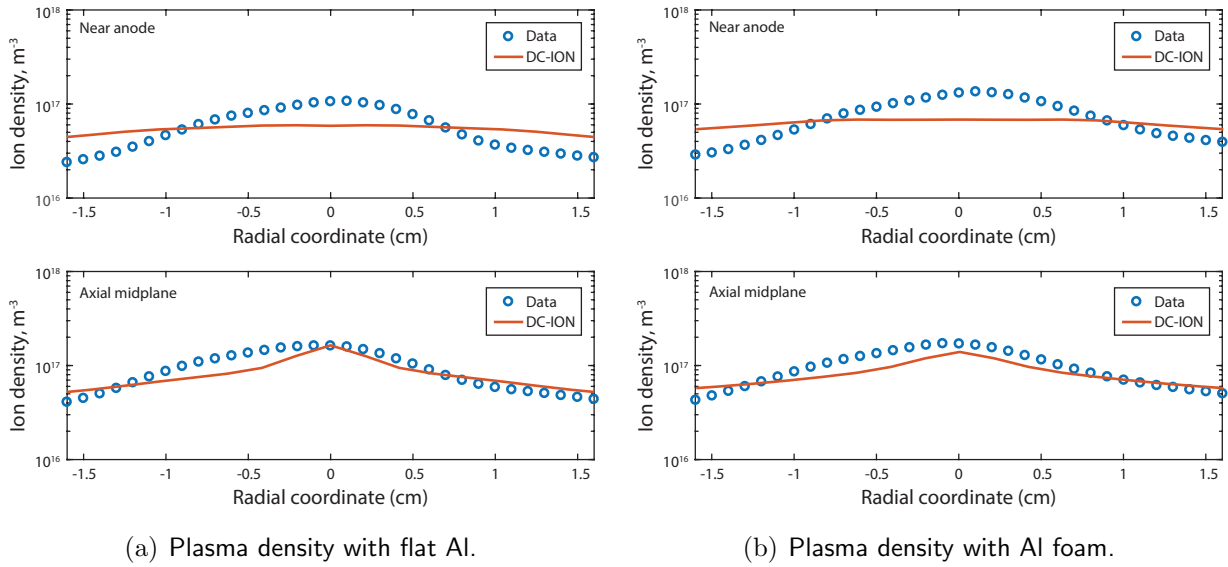


Figure 4.15: DC-ION simulation results compared with plasma column experimental measurements.

4.6 Discussion

The modifications discussed in this chapter significantly improved the capabilities of DC-ION, as well as the accuracy of the model's plasma and primary electron density predictions. Improved memory management and high-performance matrix solver implementation allowed the internal mesh to be substantially refined. The magnetic field solver was improved using analytical permanent magnet and Helmholtz coil solutions which increased the accuracy of

the primary electron tracking and ion diffusion sub-models, particularly near block magnet cusps. In addition, the ability to use adaptive time stepping through the Wirz method allowed for accurate and computationally efficient tracking of primary electrons for all plasma simulations. DC-ION was qualitatively validated with plasma and primary electron density mapping data for MiXI (3-Ring) and the Ring Cusp Test Discharge, capturing the correct density structures observed in these experimental data.

Finally, DC-ION was used to simulate the effects PMI on a canonical plasma column, and the results were compared with experimental measurements. The model successfully simulates the increase in the plasma density near the anode surface when aluminum foam is used for the target anode. This is due to the geometric suppression of SEE by the foam, reducing the effects of SEE on the potential drop and the electron energy loss to the anode, maintaining high ionization rates in the bulk region.

CHAPTER 5

Future Work

Although the modeling campaigns undertaken were successful, many improvements and further studies have been identified and are suggested as future work in the following sections.

5.1 Temporal Surface Evolution

The sputtering model tracks surface changes by moving the mesh commensurate with how much mass is emitted and deposited onto each mesh cell. This capability can be used to track the evolution of a structured surface as it erodes with sustained ion bombardment. The accuracy of this process can be validated by exposing a simple surface, such as the threaded surface discussed in chapter 2, to a constant ion flux and performing profilometry analysis in-situ to physically measure the surface topology. These data can then be compared with the computational results.

Tracking the evolution of a foam surface is crucial in showing that the foam can extend the lifetime of EP devices. Computationally modeling the evolution of the foam after thousands of hours of ion bombardment, and how erosion affects SEE and sputtering suppression after prolonged exposure to ions, is a viable design tool for plasma facing surfaces.

5.2 Angular and Energy Electron Emission Distribution

Tracking the direction at which the electrons escape the computational domain in the SEE model can provide important information about the SEE behavior of structured surfaces.

Accurately tracking the path of emitted electrons is important for determining the effects of SEE on the sheath when considering two dimensions. Preferential emission of secondary electrons due to a porous surface’s structure could result in two-dimensional sheath effects, which would then affect ion bombardment incident conditions, and result in sputtering hotspots as ions are concentrated on a surface region.

5.3 DC-ION PMI Modeling

DC-ION’s computational efficiency could be further improved by implementing dynamic memory allocation and further optimizing code parallelization to reduce computational time. Beyond that, the techniques used in this work to implement PMI physics into DC-ION could also be improved to more accurately simulate the interactions between the plasma and the foam (or other structured) surface. Currently, the SEE yield for the foam is estimated a priori based on experimental measurements, but the yield could be calculated in real time by using the primary electron incident conditions as inputs into the SEE model and running it between iterations to update the yield value. In addition, the secondary electrons are currently introduced back into the model through the ion and plasma electron fluid diffusion equations, but their paths could also be tracked as a separate species to observe how they interact with the plasma itself. Finally, the plasma diffusion sub-model can be modified to address the unique geometry and diffusion mechanisms of plasma columns. These improvements could lead to better simulation results for the plasma column model.

CHAPTER 6

Conclusion

The work presented herein has significantly contributed to the understanding of plasma-surface interactions and the effects of surface structure on the interplay between PMI and plasma properties. The sputtering model allowed for accurately modeling of the hysteresis of yield measurements from a threaded surface due to surface micro-roughening caused by ion bombardment; showed that the net yield can potentially increase in certain surface structuring configurations for moderately high incident energies; and confirmed that protuberant pillar growth due to deposition critically affected the net yield from a molybdenum nano-rod sample. The SEE model was used to simulate yield from complex surfaces through simple, repeating geometric models of textured surfaces such as velvet, carpet, and fuzz. These results showed the varying dependence (or lack thereof) of the SEE yield on the incidence angle, which is significantly sensitive to the surface geometry. These PSI models will be integrated into DC-ION, along with other modifications and improvements, in order to study the effects of PSI on a plasma column (and vice versa) and how surface structuring affects these interactions. DC-ION was improved and modified to simulate a DC plasma column, and the results were compared with experimental measurements for both a flat aluminum and an aluminum foam anode. The model successfully captured the increase in the plasma density observed in the experiment due to the suppression of secondary electron emission by geometric capturing of emitted electrons by the foam. Together, these results confirm that structured surfaces are viable candidates for improving the performance and longevity of current plasma devices, from electric propulsion to high-temperature fusion devices, as well as enabling future technologies, such as the Z-pinch thruster concept, which harnesses

fusion-like plasmas and will require plasma-robust surfaces.

Appendix A

Ion-Induced Electron Emission from Textured Surfaces

The emission of electrons from bounding surfaces due to bombardment of ions and primary electrons can significantly affect the plasma sheath, and in turn, the interactions between the plasma and surface. Because emitted electrons enter the plasma at low energies, they decrease the sheath potential, which causes high electron energy loss through the sheath from the plasma. From the material's perspective, this causes increased wall heating but a reduction in the ion incidence energy. Hence, the sputtering, secondary electron emission (SEE), and ion-induced electron emission (IIEE) yields are affected[8, 19, 104, 105]. This in turn can impact the performance of a wide range of plasma devices, from electric propulsion devices [9, 10, 11] to tokamaks [15, 16, 17].

To suppress the effects that electron emission and sputtering have on the plasma, textured surfaces have been shown to trap emitted electrons and sputterants, decreasing the yield [20, 21, 25, 77]. In particular, carbon velvet and tungsten fuzz have been shown to reduce electron emission as compared to flat surfaces of the same material, which can improve the performance of miniature Hall thrusters (on which magnetic shielding is challenging) and fusion devices [8, 39, 106]. However, experimental and modeling work has focused on secondary electron emission and largely neglected ion-induced electron emission (IIEE), which can be a significant contributor to electron emission at high energies or for small ions (such as helium).

The SEE model discussed in chapter 3 is used to study IIEE by changing the emission physics to match those of ion-induced electron emission. Figure A.1 schematically shows

this approach. Incident particles are pushed until colliding with a surface, a number of electrons are generated at the point of collision, and once all incident ions have been lost, the emitted electrons are tracked until escaping or being absorbed by a neighboring surface. Unlike the SEE model, the incident ions and emitted electrons are assumed to be absorbed after impacting a surface, and secondary electrons are neglected due to the low incidence energy of electrons emitted by ion bombardment.

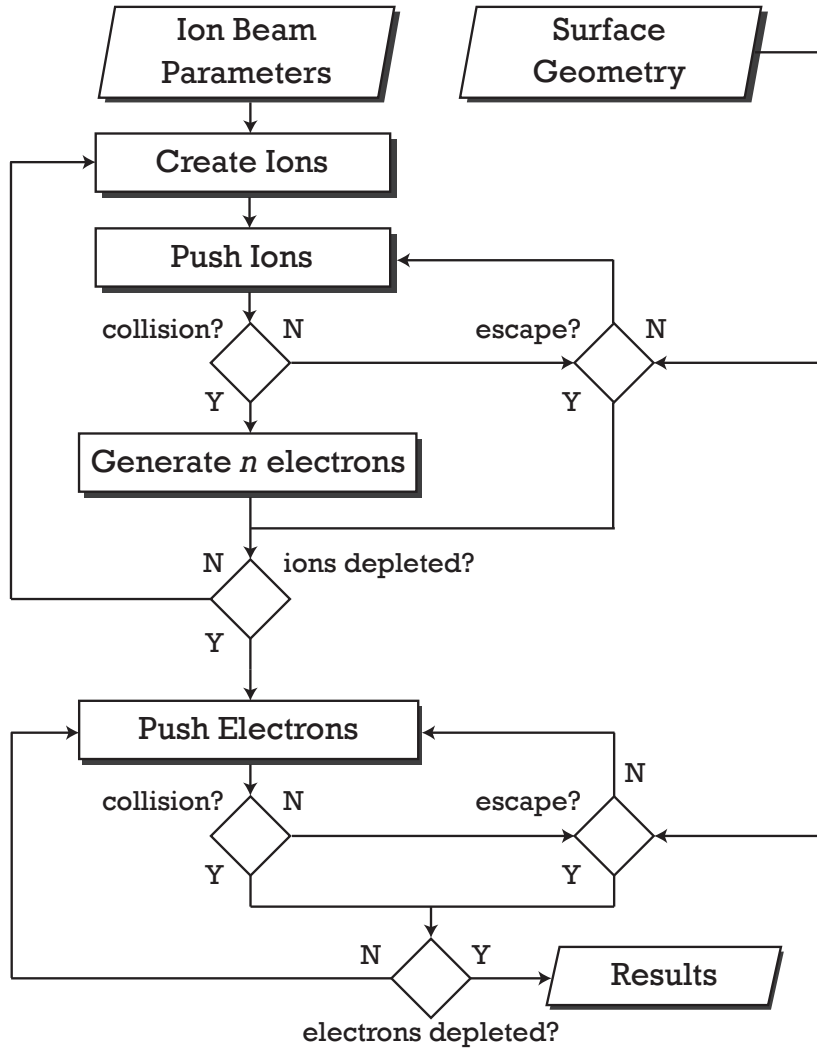


Figure A.1: Flowchart for IIEE model

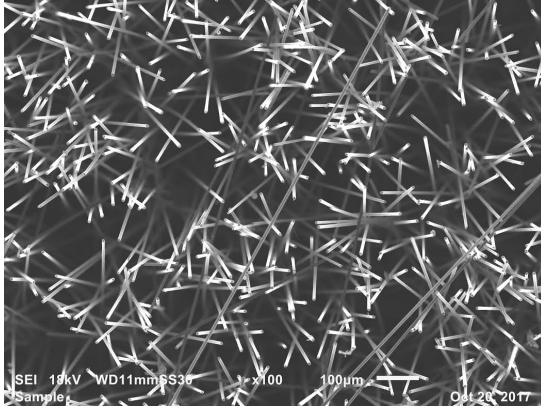
Accurately representing the textured surface is paramount to successfully predicting ge-

ometric effects on the electron emission yield. Vertical pillars have been previously used to parametrically study yield suppression from carbon velvet, however, new SEM images show two distinct apparent geometries when viewed from the top and profile directions, as shown on figure A.2. Looking from the top, the surface can be modeled as sparsely distributed slanted fibers, approximately 50 μm apart at about 30° , on average, to the substrate. From the profile view, it is estimated that the fibers are approximately vertical and closely packed, with a separation distance of about 14 μm , near the substrate. Both geometries are studied in this work. For simplicity, for the slanted fiber geometry, the reference plane is rotated so that the substrate and particles are angled while the fibers are held vertical in the model.

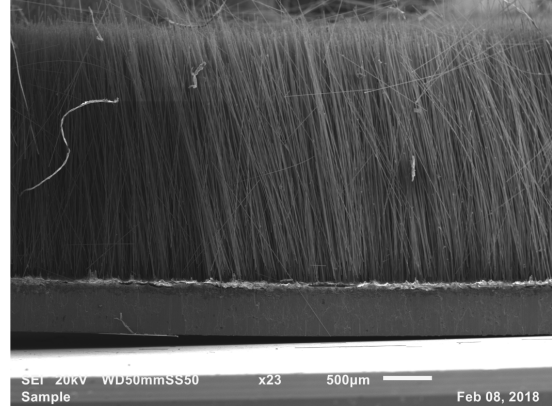
Tungsten fuzz has been modeled as a cage-like geometry, which accurately captured the reduction in the SEE yield, as well as the independence of the yield on incidence angle [21, 39]. The tungsten fuzz geometry is modeled with this same geometry of interlaced horizontal and vertical fibers, as discussed in more detail in Ref. [21].

As shown on figure A.3, the emission of electrons due to ion bombardment is typically categorized into potential and kinetic emissions, which depend on different mechanisms to eject the electrons [107]. While potential emission relies on resonance or Auger neutralization, kinetic emission occurs through direct transfer of energy through collisions. Several approximations have been suggested for the yield from each type of electron emission [107, 108]. However, because surface geometry effects on the electron emission yield is agnostic to the ejection mechanism, the two types of emission are not differentiated in this work. Hence, the total emission yield at normal incidence is obtained semi-empirically by fitting exponential terms, as will be discussed later. The yield is then corrected for the incidence angle by dividing by the cosine of the incidence angle, $\gamma(\theta_i) = \gamma(0^\circ)/\cos(\theta_i)$.

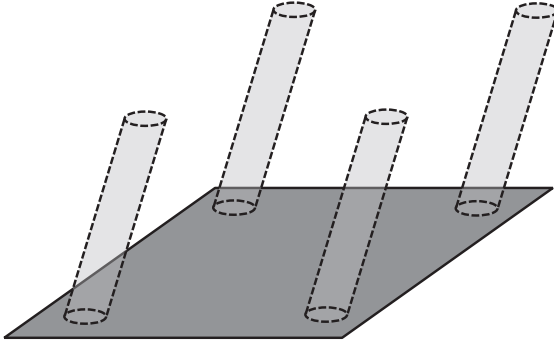
When ions collide with surfaces, emitted electrons are seeded with random emission energies and directions. These emission characteristics must satisfy an angular cosine distribution and an energy distribution dependent on ion and surface properties and incident energy and direction. At the incident energies studied in this work, the electrons are predominantly



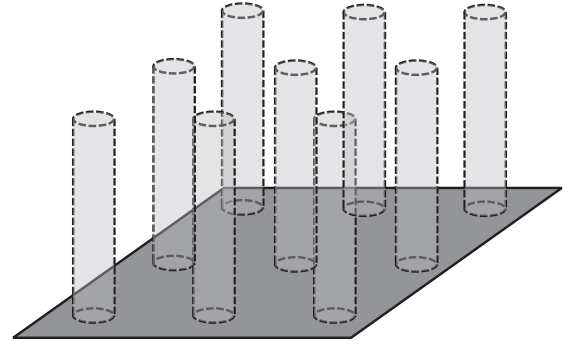
(a) C velvet top view.



(b) C velvet side view.



(c) 30° slanted fiber geometry.



(d) Vertical fiber geometry.

Figure A.2: C velvet SEM images and corresponding representative geometries.

emitted at energies well below 50 eV, with the most probable energies in the 2 – 4 eV range. Thus, secondary electron emission is neglected and the model becomes independent of the emission energy. For simplicity, all electrons are assumed to be emitted with an energy of 3 eV in the model.

When an ion impacts a surface, the number of electrons that are emitted is calculated using a Poisson distribution with the yield set as a distribution average. More complex distributions, such as Polya and others empirically derived, have a negligible effect on the results, since the emitted particles would still average to the yield over a large number of incident ions [107, 109].

$$P_n = \frac{\gamma^n e^{-\gamma}}{n!}$$

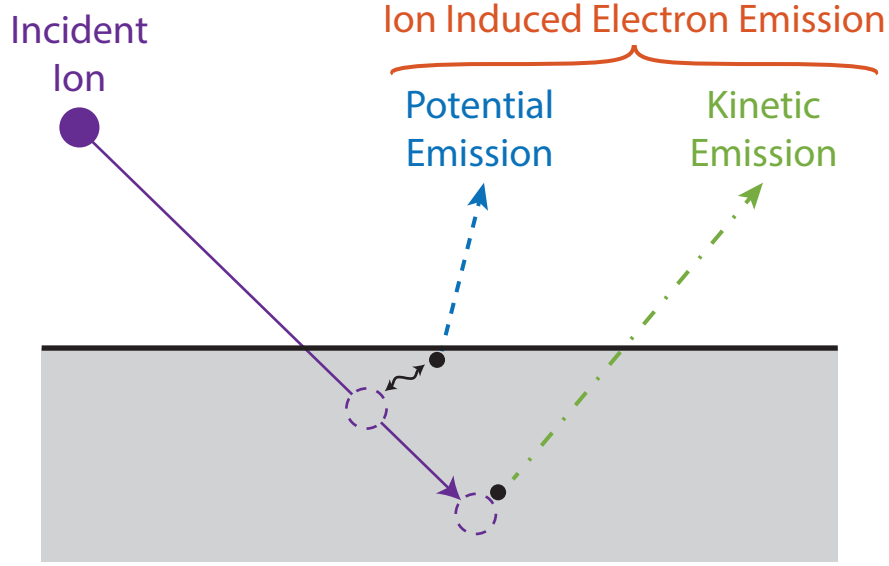
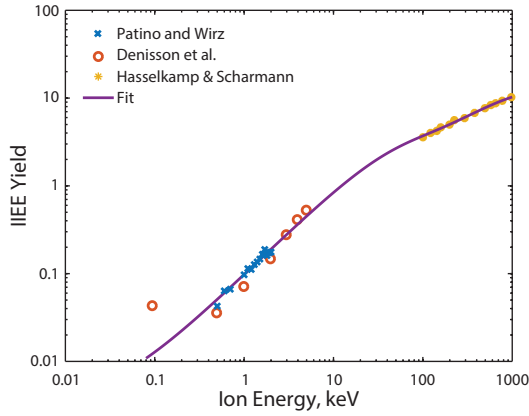
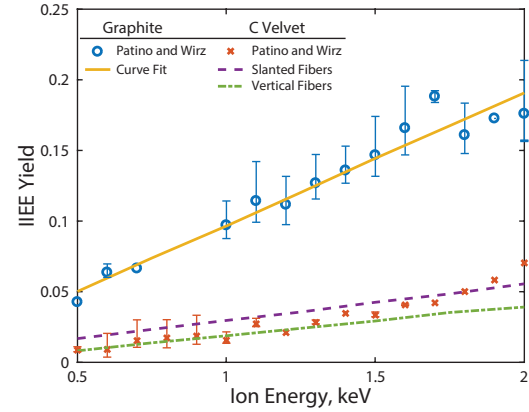


Figure A.3: Ions incident on a surface penetrate it, causing near-surface electrons to recoil. Electrons that gain enough energy normal to the surface escape and are emitted.



(a) Xe^+ bombardment on flat graphite.



(b) Xe^+ bombardment on C velvet.

Figure A.4: Comparison of IIEE model results with data.

The model is first validated using data from Patino and Wirz [110]. The fibers are measured to be approximately $2.6 \mu\text{m}$ long, with a 6.8 nm diameter. The IIEE yield from flat graphite is obtained by least squares curve fitting to Xe^+ on C yield data, as shown on

figure A.4 a)[110, 111, 112]:

$$\gamma = 12.45 - 10.11e^{\frac{-E_i}{649\text{keV}}} - 2.34e^{\frac{-E_i}{29\text{keV}}}$$

where E_i is the ion incident energy, in keV. Using this fit, figure A.4 b) shows the results of modeling the carbon velvet as both slanted and vertical fibers (as shown on figure A.2. The results from both geometries agree well with the data, with the slanted fibers case resulting in a higher yield, as expected.

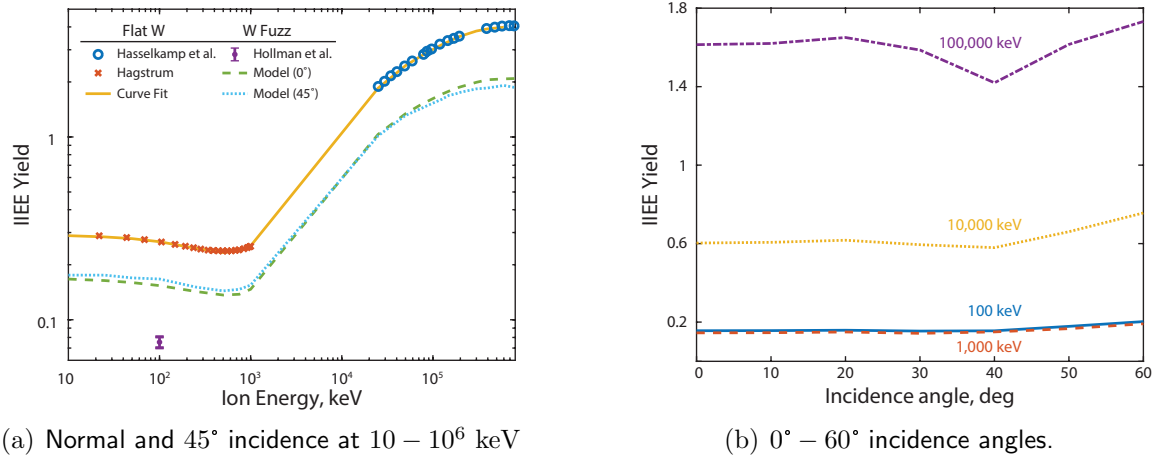


Figure A.5: Curve fitting and simulation results for IIEE from He^+ on W

Similarly, flat tungsten data from Refs. [65, 113] is fitted using exponential terms, resulting in the relationship

$$\gamma = 4.03 - 2.22e^{\frac{-E_i}{127\text{keV}}} - 1.68e^{\frac{-E_i}{16.2\text{keV}}} + 0.17e^{\frac{-E_i}{441\text{eV}}}$$

Figure A.5 compares this fit with the experimental data for flat tungsten at normal incidence. In addition, the IIEE yields from tungsten fuzz for different incident angles are shown, along with an estimated yield from Hollman et al. [31] In that work, the yield was approximated by assuming a reduction in the SEE yield taken from the literature and fitting the calculated

current to experimental measurements. In contrast, the reduction in the IIEE yield from the model agrees with results from Ref. [21] (for SEE yield reduction from W fuzz).

Because the decrease in the yield is due primarily to trapping (which is a geometric effect) and the angular distribution of the emitted particles (which is primarily cosine for both SEE and IIEE) is the same, this agreement in the reduction is expected. Moreover, the results from the present model also show that the IIEE yield from W fuzz is independent of incidence angle because of trapping by the horizontal fibers, as was explained for SEE in Refs. [21, 106]]. Figure A.6 shows that the increase in IIEE yield with incidence angle is balanced by a roughly equal increase in trapping by the horizontal fibers, thereby eliminating the dependence of the yield on incidence angle for fuzz.

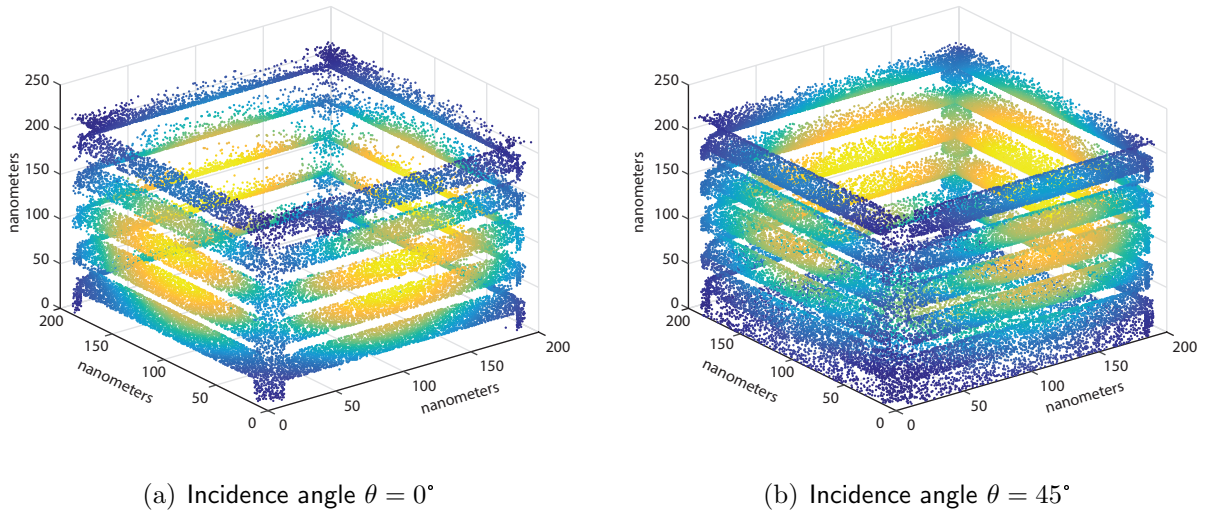


Figure A.6: Emitted electron collision heatmaps. The emission yield from the cage-like geometry is maintained independent of incidence angle by increased trapping at higher incidence angles, as seen in the higher density of collisions on b).

The model accurately simulates the reduction in the ion-induced electron emission yield from textured surfaces due to trapping of emitted electrons. The mechanisms that lead to this effect have been clearly shown to be strongly dependent on the surface's geometry and is agnostic to the emission physics. The first empirically-derived yield curves are formulated

for flat graphite and tungsten for a wide range of ion incidence energies. Simulations of emission from carbon velvet using slanted and vertical fiber surface representations agree well with experimental data within the expected error and modeling uncertainty. The nano-scale tungsten fuzz results show that the reduction in the yield is independent of incidence angle, as was previously observed for SEE. Understanding the IIEE characteristics from these surfaces will help improve the performance of EP devices and tokamaks (where self-generated nano-scale W fuzz has been observed to naturally form). Furthermore, other complex surfaces, such as foams and micro-architected dendritic surfaces (such as micro-spear or capped nodule texturing), can be simulated with this model and could prove to be candidate surfaces for plasma devices [23, 114].

Appendix B

View Factor Model Validation

Before applying the model to micro-architected surfaces as discussed in chapter 2, the sputtering model was validated by comparing to experimental data, fitted data, and computational results. Furthermore, the view factor and shadowing algorithms were validated against COMSOL simulations.

Zhang and Zhang’s modified sputter yield model was compared to curve fits used by Zoerb et al. of the form [115, 116]

$$Y(0^\circ \leq \theta \leq 90^\circ) = \sum_{i=1}^6 C_i \cos^i \theta \quad (\text{B.1})$$

As shown on Fig. B.1 a-c), the model agreed well with these curve fits when E_{th} was set to a value of 150eV (independent of incidence energy or angle) for argon ions bombarding molybdenum. Note that Zoerb et al. were unable to match their curves exactly with the data used to find the coefficients C_i (see Refs. [[115, 116]]). For instance, near $\theta = 0^\circ$, the slope of the fit approaches 0, whereas the data continues to decrease (similar to the present model’s curve). In summary, although the two curves did not perfectly match, the trends certainly agreed.

Figure B.1 d) shows comparisons of Yamamura, Itikawa, and Itoh’s sputter yield model with data and computational results from the literature [48, 115, 117]. Again, the present model matches well with trends from literature. Note that the results from ACAT, a Monte Carlo computational model, is expected to mispredict sputter yield at low incidence energies

[52]. In addition, Zoerb's sputter yield results assume azimuthal symmetry for simplicity[115, 116], resulting in overprediction of the sputter yield for $\theta_i > 45^\circ$.

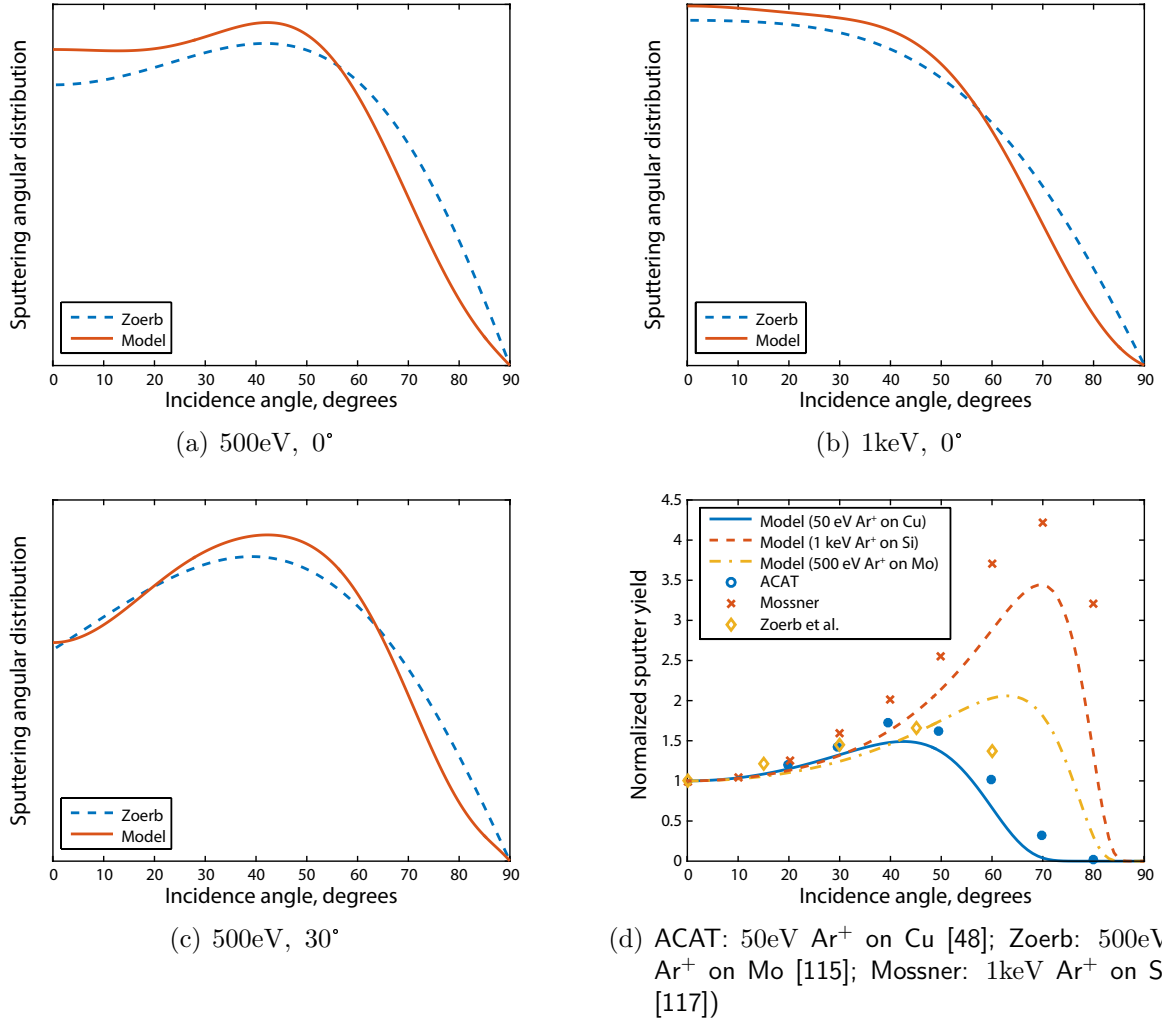


Figure B.1: Comparison of Zhang and Zhang's modified sputter yield model with fits from Zoerb et al. for argon ions bombarding molybdenum and Yamamura, Itikawa, and Itoh's sputter yield model with data and results from the literature

Similarly, the view factor and shadowing models were validated, in this case by comparison with test cases simulated using COMSOL. In order to directly compare with COMSOL, which uses view factor calculations via its radiation module, the ambient view factor had to be calculated ($f_A = 1 - f$) and the sputtering distribution was replaced by a cosine distribution, corresponding to what COMSOL uses for radiation. As shown in figure B.2 a

peak-to-peak section of a triangle wave (V-shaped) surface was used to test the approximation made in Eq. (2.6). The results along the centerline, shown on figure B.2 b), displayed close agreement except near the intersection. This was to be expected, however, as the assumption that the integrand is constant within the cell area was invalid for adjacent cells. The relative difference at this intersection was only about 10%. It should also be noted that both COMSOL and the present model extended at least an order of magnitude further in the axial direction than the height or width of the V-shaped geometry such that the infinitely-long assumption was reasonable.

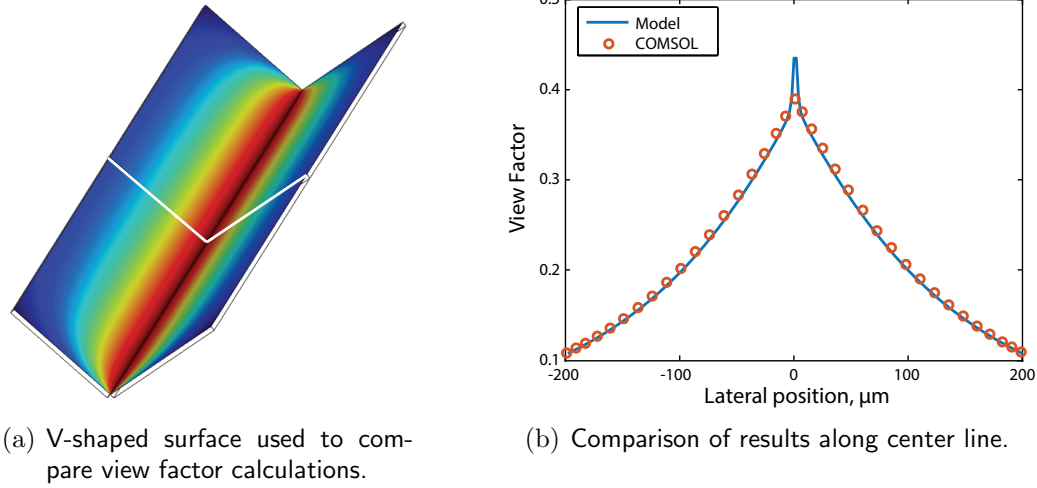
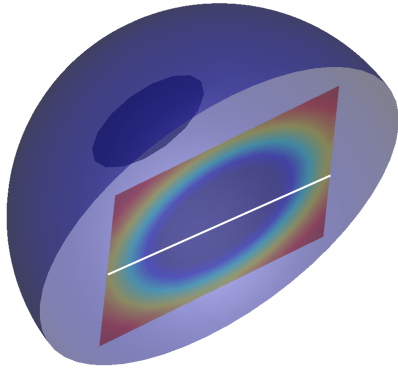
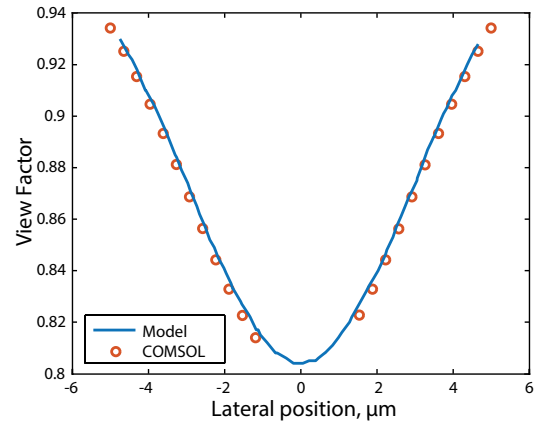


Figure B.2: Comparison of present model's view factor calculations (using a cosine distribution) with COMSOL's radiation results.

Lastly, the shadowing model was tested against COMSOL. Once again, the ambient view factor was calculated, and a cosine distribution was assumed. For this test, a sputtering/radiating surface was shadowed by a disk a short distance away from the quadrilateral. As shown on figure B.3 a), an “ambient” hemisphere was used in our model to capture sputterants so that the ambient view factor could be calculated. Figure B.3 b) shows a comparison of results along the centerline of the quadrilateral. As expected, there was close agreement between both simulations.



(a) Sputtering sample shadowed by disk and surrounded by sputterant-collecting hemisphere.



(b) Comparison of results along center line.

Figure B.3: Comparison of present model's shadowing algorithm (using a cosine distribution) with COMSOL's radiation results.

Appendix C

Argon Collision Rate Constant Curve Fits

The rate constant integrals, discussed in chapter 4, are curve fitted using polynomials for several values of α . In DC-ION, several $K(\alpha, V_p)$ values are calculated for different α in terms of V_p , and the rate constant is then interpolated for each type of collision. The polynomial equations used for each collision type are shown below.

C.1 Inelastic Collision

$$\begin{aligned} K(1) &= 1.19 \times 10^{-21} V_p^6 - 1.71 \times 10^{-19} V_p^5 + 9.67 \times 10^{-18} V_p^4 - 2.68 \times 10^{-16} V_p^3 \\ &\quad + 3.54 \times 10^{-15} V_p^2 - 1.11 \times 10^{-14} V_p + 9.55 \times 10^{-15} \\ K(3) &= -8.11 \times 10^{-22} V_p^6 + 9.06 \times 10^{-20} V_p^5 - 3.30 \times 10^{-18} V_p^4 + 2.81 \times 10^{-17} V_p^3 \\ &\quad + 6.69 \times 10^{-16} V_p^2 - 6.67 \times 10^{-15} V_p + 1.26 \times 10^{-14} \end{aligned} \tag{C.1}$$

If $V_p < 14$ eV,

$$\begin{aligned} K(5) &= -4.46 \times 10^{-20} V_p^6 + 1.52 \times 10^{-18} V_p^5 - 1.64 \times 10^{-17} V_p^4 + 7.49 \times 10^{-17} V_p^3 \\ &\quad - 1.46 \times 10^{-16} V_p^2 + 9.51 \times 10^{-17} V_p - 4.04 \times 10^{-18} \\ K(10) &= -1.14 \times 10^{-20} V_p^6 + 9.05 \times 10^{-19} V_p^5 - 1.76 \times 10^{-17} V_p^4 + 1.50 \times 10^{-16} V_p^3 \\ &\quad - 5.99 \times 10^{-16} V_p^2 + 1.05 \times 10^{-15} V_p - 5.98 \times 10^{-16} \end{aligned} \tag{C.2}$$

If $V_p \geq 14$ eV,

$$\begin{aligned}
K(5) &= -1.43 \times 10^{-22} V_p^6 + 2.65 \times 10^{-20} V_p^5 - 2.08 \times 10^{-18} V_p^4 + 9.04 \times 10^{-17} V_p^3 \\
&\quad - 2.40 \times 10^{-15} V_p^2 + 4.12 \times 10^{-14} V_p - 2.58 \times 10^{-13} \\
K(10) &= -9.70 \times 10^{-23} V_p^6 + 1.92 \times 10^{-20} V_p^5 - 1.60 \times 10^{-18} V_p^4 + 7.39 \times 10^{-17} V_p^3 \\
&\quad - 2.09 \times 10^{-15} V_p^2 + 3.86 \times 10^{-14} V_p - 2.68 \times 10^{-13}
\end{aligned} \tag{C.3}$$

C.2 Total Collision

$$\begin{aligned}
K(1) &= 8.45 \times 10^{-20} V_p^6 - 1.20 \times 10^{-17} V_p^5 + 6.68 \times 10^{-16} V_p^4 - 1.79 \times 10^{-14} V_p^3 \\
&\quad + 2.21 \times 10^{-13} V_p^2 - 6.99 \times 10^{-13} V_p + 6.07 \times 10^{-13} \\
K(3) &= 1.20 \times 10^{-19} V_p^6 - 1.95 \times 10^{-17} V_p^5 + 1.28 \times 10^{-15} V_p^4 - 4.28 \times 10^{-14} V_p^3 \\
&\quad + 7.42 \times 10^{-13} V_p^2 - 5.85 \times 10^{-12} V_p + 1.68 \times 10^{-11} \\
K(5) &= 6.70 \times 10^{-20} V_p^6 - 1.27 \times 10^{-17} V_p^5 + 9.64 \times 10^{-16} V_p^4 - 3.68 \times 10^{-14} V_p^3 \\
&\quad + 7.27 \times 10^{-13} V_p^2 - 6.59 \times 10^{-12} V_p + 2.16 \times 10^{-11} \\
K(10) &= -1.47 \times 10^{-19} V_p^6 + 1.88 \times 10^{-17} V_p^5 - 8.71 \times 10^{-16} V_p^4 + 1.66 \times 10^{-14} V_p^3 \\
&\quad - 7.17 \times 10^{-14} V_p^2 - 9.33 \times 10^{-13} V_p + 6.70 \times 10^{-12}
\end{aligned} \tag{C.4}$$

C.3 Ionization

$$\begin{aligned}
K(1) &= 2.70 \times 10^{-22} V_p^6 - 4.04 \times 10^{-20} V_p^5 + 2.34 \times 10^{-18} V_p^4 - 6.35 \times 10^{-17} V_p^3 \\
&\quad + 6.26 \times 10^{-16} V_p^2 + 6.61 \times 10^{-15} V_p - 3.68 \times 10^{-14} \\
K(3) &= 1.02 \times 10^{-21} V_p^6 - 1.65 \times 10^{-19} V_p^5 + 1.09 \times 10^{-17} V_p^4 - 3.65 \times 10^{-16} V_p^3 \\
&\quad + 6.47 \times 10^{-15} V_p^2 - 5.08 \times 10^{-14} V_p + 1.44 \times 10^{-13} \\
K(5) &= 7.92 \times 10^{-22} V_p^6 - 1.39 \times 10^{-19} V_p^5 + 9.85 \times 10^{-18} V_p^4 - 3.60 \times 10^{-16} V_p^3 \\
&\quad + 6.98 \times 10^{-15} V_p^2 - 6.21 \times 10^{-14} V_p + 2.00 \times 10^{-13} \\
K(10) &= -5.48 \times 10^{-22} V_p^6 + 5.78 \times 10^{-20} V_p^5 - 1.54 \times 10^{-18} V_p^4 - 3.16 \times 10^{-17} V_p^3 \\
&\quad + 2.16 \times 10^{-15} V_p^2 - 2.98 \times 10^{-14} V_p + 1.23 \times 10^{-13}
\end{aligned} \tag{C.5}$$

C.4 Double Ionization

$$\begin{aligned}
K(1) &= 2.53 \times 10^{-22} V_p^6 - 3.34 \times 10^{-20} V_p^5 + 1.68 \times 10^{-18} V_p^4 - 3.85 \times 10^{-17} V_p^3 \\
&\quad + 2.90 \times 10^{-16} V_p^2 + 4.07 \times 10^{-15} V_p - 1.97 \times 10^{-14} \\
K(3) &= 3.14 \times 10^{-22} V_p^6 - 4.34 \times 10^{-20} V_p^5 + 2.36 \times 10^{-18} V_p^4 - 6.31 \times 10^{-17} V_p^3 \\
&\quad + 7.95 \times 10^{-16} V_p^2 - 1.29 \times 10^{-15} V_p - 1.4223 \times 10^{-14} \\
K(5) &= 3.00 \times 10^{-22} V_p^6 - 4.19 \times 10^{-20} V_p^5 + 2.31 \times 10^{-18} V_p^4 - 6.33 \times 10^{-17} V_p^3 \\
&\quad + 8.46 \times 10^{-16} V_p^2 - 2.35 \times 10^{-15} V_p - 1.26 \times 10^{-14} \\
K(10) &= 2.87 \times 10^{-22} V_p^6 - 4.04 \times 10^{-20} V_p^5 + 2.25 \times 10^{-18} V_p^4 - 6.27 \times 10^{-17} V_p^3 \\
&\quad + 8.74 \times 10^{-16} V_p^2 - 3.20 \times 10^{-15} V_p - 1.10 \times 10^{-14}
\end{aligned} \tag{C.6}$$

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