

Monte Carlo simulation of ionization in a magnetron plasma

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A Monte Carlo simulation of electrons emitted from the cathode of a planar magnetron is tested against experiments that were reported by Wendt, Lieberman, and Meuth [J. Vac. Sci. Technol. A 6, 1827 (1988)] and by Gu and Lieberman [J. Vac. Sci. Technol. A 6, 2960 (1988)]. Comparing their measurements of the radial profile of current and the axial profile of optical emission to the ionization profiles predicted by the model, we find good agreement for a typical magnetic field strength of 456 G. We also find that at 456 G the product of the average number of ionizations $\langle N_i \rangle$ and the secondary electron emission coefficient γ is ~ 1 . This indicates that secondary emission contributes significantly to the ionization that sustains the discharge. At 171 G, however, $\langle N_i \rangle \gamma \ll 1$, revealing that cathode emission is inadequate to sustain a discharge at a low magnetic field.

I. INTRODUCTION

Magnetrons are glow discharge sputtering devices used for thin film deposition and etching.^{1,2} They employ electric and magnetic fields that are configured to trap electrons and enhance ionization near a cathode surface. Ions produced in the plasma are accelerated by the electric sheath toward the cathode. They strike the cathode surface, producing the desired sputtering as well as the emission of secondary electrons that help sustain the discharge.

The electrons in the plasma can be categorized according to their point of origin: (1) the cathode surface, (2) the sheath, and (3) the main plasma region. Electrons in the third category are called the bulk because they comprise the largest part of the electron population. The total electron loss rate, including all three categories, is balanced in equilibrium by the ion loss rate, as described by Sheridan, Goeckner, and Goree.³

The same authors described a model of the transport that is applicable only to the energetic electrons, i.e., to those electrons with enough energy to ionize neutral atoms.⁴ This includes all the electrons in the first two categories plus the tail of the bulk distribution. The model is useful for predicting where the ionization takes place. Electrons are assumed to interact only with prescribed static electric and magnetic fields and undergo collisions with neutrals. These collisions reduce an electron's energy and scatter its velocity vector, eventually leading to its escape from the trap region. While the electrons also undergo Coulomb collisions with ions, these are negligible in comparison to collisions with neutrals for the range of pressures and electron densities found in sputtering magnetron discharges.⁴ Ions are assumed to be accelerated by the electric field directly to the cathode from the ionization sites, their trajectories not influenced by the magnetic field.

In a fully self-consistent model, the electric fields would evolve in order to balance the loss rates of ions and electrons, exactly as they do in the actual plasma.³ For practicality, the electric field is prescribed in our model and does not evolve in time; therefore, an accurate expression for the electric field relies on the use of empirical data. In particular, the electric field model must be supplied with laboratory mea-

surements of the bulk electron temperature and density T_e and n_e . (We did not develop the model to predict T_e or n_e .)

This physical model for energetic electrons has been implemented numerically in a Monte Carlo code, which has been documented in Ref. 4. It takes into account ionization, excitation, and elastic collisions by making use of differential cross sections for argon. As an initial test of this code, the authors compared its prediction of the radial ionization profile to the etch track profile measured in a planar magnetron, and found good agreement. The device that was simulated was the Iowa magnetron,⁴ which has a cylindrically symmetric magnetic field formed by a set of permanent magnets. One magnet is on the axis and the other is a concentric outer ring of the opposite polarity. The code was used to simulate only the electrons emitted from the cathode, ignoring the electrons born in the sheath and in the main plasma region.

We report in this paper a test of the model that is more rigorous than the test that was described when the code was first reported.⁴ The experiments we evaluate were carried out at the University of California at Berkeley by Wendt, Lieberman, and Meuth⁵ and by Gu and Lieberman.⁶ Our presentation begins in Sec. II with a synopsis of the experimental and simulation methods. We then show results in Sec. III for the ionization efficiency predicted by the code and a comparison of the radial and axial profiles from experiment and simulation.

II. PROCEDURE

A. Berkeley experiments

Wendt *et al.*⁵ and Gu and Lieberman⁶ performed their experiments with a cylindrically symmetric planar magnetron that has a variable strength magnetic field produced by an electromagnet. The coil windings are encircled with an iron core that has a circular slit to form the magnetron's magnetic field. This magnetron differs significantly from the Iowa magnetron in its magnetic field geometry, yet the experiments that have been reported for these two devices are readily compared because they had in common the use of argon gas and a copper cathode.

Wendt *et al.*⁵ reported measurements of radial ion current

profiles, which were made using probes embedded in the cathode. Since this current is produced by ions that fall directly to the cathode from the site of an ionization event, it can be compared to the radial profile of ionization predicted by our Monte Carlo simulation. This test of the model has an advantage over the previously reported comparison to the etch track profile;⁴ the radial current profile is a better measurement because it is recorded in real time for a single set of discharge parameters.

Gu and Lieberman⁶ reported measurements of the axial profile of broadband optical emission. The emission is produced principally by electron-impact excitation of neutral atoms to a highly excited state. As a proxy for these excitation events, we use the ionization collisions for argon. This is an appropriate approximation since ionizing collisions and most excitation transitions have cross sections with nearly the same dependence on electron energy.^{7,8}

The locations of ionizations coincides with the glow emitted by neutral argon atoms. However, the sputtered metal atoms also emit light after they pass through the discharge, and this can overwhelm the argon neutral emission, especially at high discharge currents.⁹ For sputtered copper atoms, the brightest spectral line is at 511 nm, resulting from the metastable state $^2D_{5/2}$, which has a lifetime of $\sim 1 \mu\text{s}$.^{10,11} We have visually observed this green glow in the Iowa magnetron everywhere downstream from the discharge. Consequently, copper emission is not appropriate for comparison to the simulation of the locations of ionizing collisions. Gu and Lieberman did not filter out the copper glow. Therefore, we must explain from the outset that while their axial profile data is the best available, it is not as well suited for comparison to our simulation as the radial profiles of Wendt *et al.*

B. Simulation

Using the Monte Carlo code, we simulated the electrons emitted from the cathode of the Berkeley magnetron and produced spatial profiles of the ionization. We used a one-dimensional electric potential; it is composed of a linear pre-sheath that is connected to a sheath potential predicted by a numerical solution of Poisson's equation.¹² The electron orbits and collisions were handled the same way as in Ref. 4, including the approximations that all excitation collisions result in an energy loss of 11.6 eV, that two-step ionization processes^{13,14} can be ignored, and that the kinetic energy of the electron ejected in an ionization event is negligible. When the incident electron energy is several hundred eV, the kinetic energy of the ejected electron is typically between 0 and 10 eV,^{15,16} and by neglecting this we underestimate the energy loss in an ionizing collision ΔK_i by about 30%.

The magnetic field for the Berkeley magnetron, as shown in Fig. 1, was computed by Wendt using the POISSON finite-element code.⁵ By varying the current in the electromagnet coil, the Berkeley researchers were able to adjust the magnetic field strength up or down while maintaining its shape. We performed simulations for two field strengths: $|B|_{\text{max}} = 456 \text{ G}$, which is comparable to the field in the Iowa magnetron, and $|B|_{\text{max}} = 171 \text{ G}$, which is rather weak.¹⁷

We have chosen the parameters of the simulation to con-

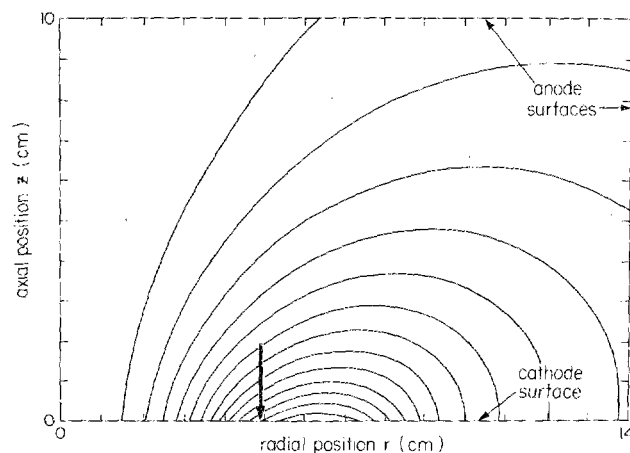


FIG. 1. Magnetic field of the Berkeley planar magnetron, computed by Wendt (Ref. 5). The coordinates used in this paper, r and z , are shown in the axes. The cathode surface is located at $z = 0$ and $0 < r < 11.4 \text{ cm}$. The heavy arrow indicates the point on the cathode surface where $|B|$ is maximum; values for $|B|_{\text{max}}$ are cited for this point (Ref. 17).

form as closely as possible to those of the experiments, as listed in Table I. Argon at a pressure of 0.67 Pa was used. The electric field model in the code must be supplied with values of the discharge voltage V_{dis} , the electron temperature T_e , and the Debye length λ_D . The Berkeley experimenters reported values for V_{dis} and the sheath thickness d for each of their runs, but they did not indicate T_e or λ_D . We have chosen $T_e = 5 \text{ eV}$, based on the measurements of Rossnagel and Kaufman,¹⁸ and we computed λ_D by using d in Child's Law.¹² These estimates for T_e and λ_D are not used for any purpose other than the electric field model. Given the

TABLE I. Parameters for planar magnetron experiments and simulations. The magnetic fields are listed for two points on the cathode: where $|B|$ is maximum (Ref. 17) and where B is tangential to the cathode. The results from Ref. 4 for the Iowa magnetron are listed in the last column for comparison. The average number of ionizations $\langle N_i \rangle$, is only for electrons emitted by the cathode (Ref. 19). The secondary emission coefficient in the last line is assumed to be $\gamma = 0.09$.

	Berkeley ^a high $ B _{\text{max}}$	Berkeley ^a low $ B _{\text{max}}$	Iowa ^b
Parameters reported for experiment			
$ B _{\text{max}}$ (G)	456	171	...
$ B _{\text{tan}}$ (G)	277	104	245
P_{Ar} (Pa)	0.67	0.67	1.0
V_{dis} (V)	362	520	400
I_{dis} (A)	0.5	0.5	0.15
Parameters assumed for simulation			
T_e (eV)	5	5	4
λ_D (mm)	0.0525	0.0802	0.1
Δ_i (ps)	5	5	50
No. of electrons	75	600	600
Simulation results			
$\langle N_i \rangle$	17.53 ± 0.62	3.72 ± 0.17	14.26 ± 0.44
$\langle N_i \rangle / N_{\text{max}}$	0.80	0.12	0.56
$\langle N_i \rangle \gamma$	1.6	0.3	1.3

^a References 5 and 6.

^b Reference 4.

assumptions that the discharge is radially uniform and that Child's Law is applicable, these estimates are probably accurate to within 50%. We determined that this accuracy is satisfactory by testing several values of λ_D within this range in the simulations described below and finding no statistically significant differences in the results.

The equation of motion was integrated in three dimensions using a fourth-order Runge-Kutta routine. A fixed time step Δt was selected to be small enough to provide for good energy conservation and to be small compared to the mean collision time and the gyroperiod. By examining a few representative electron orbits, we found that many of the electrons emitted from the cathode are trapped in a ring-shaped region a few millimeters above the cathode. This was also observed in the simulation reported previously for the Iowa magnetron.⁴ The orbits in the two magnetrons differ, however, in the way that electrons escape from the trap region. In the Berkeley device, we found that they escape toward the sides of the cylindrical vessel, not toward the anode plate at the end of the vessel opposite the cathode as they do in the Iowa magnetron.

An orbit was terminated when the electron escaped from the work space (5.22 cm axial by 14 cm radial), or its total energy fell below the ionization potential $qV_i = 15.8$ eV of argon, or a time limit of 10 μ s elapsed, whichever came first. A new orbit was then begun on the cathode surface at a random location chosen in a manner consistent with the history of previous ionizations.⁴ This procedure was repeated for an ensemble of 75 or more electrons.

We used the simulation results to compute the average number of ionizations per electron emitted by the cathode $\langle N_i \rangle$. This value can be compared to the maximum possible number of ionizations

$$N_{\max} \equiv \text{Int}(-qV_{\text{dis}}/\Delta K_i), \quad (1)$$

where the Int operator indicates truncation to an integer, and ΔK_i represents the average energy lost in an ionizing collision. The ratio $\langle N_i \rangle/N_{\max}$ thus serves as a figure of merit for a magnetron at a given gas pressure.¹⁹

We will show in Sec. III that when a magnetron device has extremely effective electron confinement, $\langle N_i \rangle/N_{\max}$ will be as high as 0.8 for $P_{\text{Ar}} \approx 1$ Pa, while a device that provides virtually no confinement at all will have $\langle N_i \rangle/N_{\max}$ on the order of 0.1. The figure of merit can never reach a value of 1.0 due to the energy lost in excitation collisions.

The simulation also predicted the density of ionizations $\rho_i(r, z)$ on the r - z plane, where r is the radial coordinate and z is the axial coordinate measured from the cathode surface. Using $\rho_i(r, z)$, we computed the radial ionization profile

$$n_r(r) = \frac{1}{2\pi r} \int \rho_i(r, z) dz, \quad (2)$$

and the axial ionization profile

$$n_z(z) = \int \rho_i(r, z) dr. \quad (3)$$

Gu and Lieberman's optical collimator viewed the discharge tangentially to the cathode, thereby integrating the emission over a pencil-shaped volume of diameter 0.28 mm.⁶

Our definition of $n_z(z)$ in Eq. (3) is also a volume integral. While we could calculate the integral for the same small volume, we choose instead to improve our statistics by counting the number of ionizations inside the entire slab parallel to the cathode between $z - \Delta z/2$ and $z + \Delta z/2$, where the spatial resolution is defined to be $\Delta z = 0.5$ mm. This discrepancy in the shapes of the volumes in the experiment and simulation is equivalent to a different radial weighting in the integral, and it is probably insignificant due to the large radius of the plasma ring.

III. RESULTS

A. Ionization efficiency

We found that the average number of ionizations per fast electron $\langle N_i \rangle$ was 17.53 for the Berkeley magnetron with a 456-G field and $V_{\text{dis}} = 362$ V. This yields a figure of merit $\langle N_i \rangle/N_{\max} = 0.80$, indicating that the confinement of fast electrons is very effective.

For the discharge with the 171-G field and $V_{\text{dis}} = 520$ V, we found that $\langle N_i \rangle$ is only 3.72, which yields a figure of merit of 0.12. This reveals that the fast electrons are ineffectively confined when the field is weak. For comparison, $\langle N_i \rangle$ was reported to be 14.26 for $V_{\text{dis}} = 400$ V in the Iowa magnetron,⁴ corresponding to a figure of merit of 0.56.

Since the simulation took into account only the electrons born on the cathode surface, one can determine whether secondary emission is adequate to sustain the discharge by considering the product $\langle N_i \rangle \gamma$, where γ is the secondary electron emission coefficient. Recalling that for each ion that strikes the cathode, the average number of secondary electrons emitted is γ , and assuming that all the ions are collected by the cathode, we see that a discharge can be sustained by cathode emission if $\langle N_i \rangle \gamma$ is comparable to unity. Because our simulation overestimates $\langle N_i \rangle$ by about 30%,¹⁹ the computed value of $\langle N_i \rangle \gamma$ must actually be somewhat larger than one in order for cathode emission to sustain the discharge. For 400-eV argon on copper, the secondary emission coefficient²⁰ is $\gamma \approx 0.09$. For the low magnetic field (171-G) discharge, $\langle N_i \rangle \gamma \ll 1$, indicating that the electrons we have simulated cannot account for the ionization needed to sustain the plasma.

Considering that the experimenters were able to maintain a discharge at $|\mathbf{B}|_{\max} = 171$ G, we conclude that there is some physics missing from our model that is important at low magnetic fields. Most likely, this indicates that the electrons born in the sheath and in the plasma, which we have not included in the simulation, dominate the ionization for discharges with weak magnetic fields. We would expect some of the electrons born in the sheath to have trapped orbits that periodically reenter the sheath, resulting in a sheath avalanche; however, we have not performed any simulations to determine the effectiveness of this avalanche. In any case, such a weak magnetic field would not likely be used in a practical sputter deposition process.

On the other hand, in the higher field (456 G) and also in the Iowa magnetron, we find that $\langle N_i \rangle \gamma \gg 1$, revealing that cathode emission contributes significantly to the ionization

and may indeed be able to sustain the discharge without assistance from electrons born in the sheath or in the main plasma.

The energy cost of creating an ion–electron pair can be estimated from the results above. This cost is $C_E = qV_{\text{dis}} / \langle N_i \rangle \gamma$, the ratio of the energy required to accelerate one ion across the cathode sheath to the number of ionizations resulting from the impact of one ion on the cathode. This cost depends on the secondary emission coefficient γ of the material used in the cathode target. For the Berkeley magnetron at 456 G and assuming $\gamma = 0.09$, we find that $C_E = 362 \text{ eV} / 1.6 = 226 \text{ eV}$. The sputtering magnetron can be readily compared to other types of plasma sources based on the value of C_E . While the ionization efficiency $\langle N_i \rangle / N_{\text{max}}$ is quite high for a magnetron, the energy cost is considerable. The principal energy loss is the deposition of ion kinetic energy into the cathode target.

B. Radial and axial profiles

As explained in Sec. II A, the results reported by Wendt *et al.*⁵ are the best experimental data available for comparing to our simulation. Their radial ion current profile for $|B|_{\text{max}} = 456 \text{ G}$ is reproduced in Fig. 2, where it is overlaid on the radial ionization profile $n_r(r)$ from our simulation. The experiment and the simulation show excellent agreement: the radial profiles are peaked at the same location, and the widths of the peak are nearly the same.

The axial optical emission profile measured by Gu and Lieberman⁶ for $|B|_{\text{max}} = 456 \text{ G}$ are compared to $n_z(z)$ from our simulation in Fig. 3. Both the experiment and the simulation exhibit a dark space adjacent at the cathode surface and a peak in the electron trap region. The simulation shows good agreement with the experiment for the first few millimeters.

However, farther from the cathode the glow observed in the experiment exceeds the simulation prediction. We have determined from visual and spectroscopic observations of the Iowa magnetron that in this region the copper glow

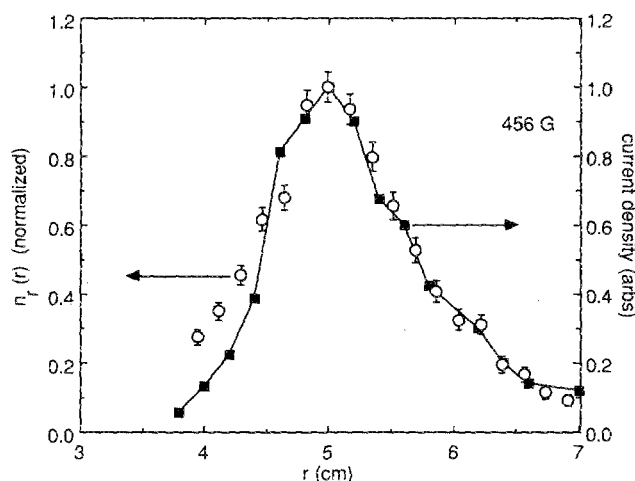


FIG. 2. Radial profiles for $|B|_{\text{max}} = 456 \text{ G}$. The experimental data (■) of Wendt *et al.* shown here is the ion current collected by probes imbedded in the cathode (Ref. 5). The error bars for the simulation results (○) are based on the counting statistics for the number of ionizations in each radial bin.

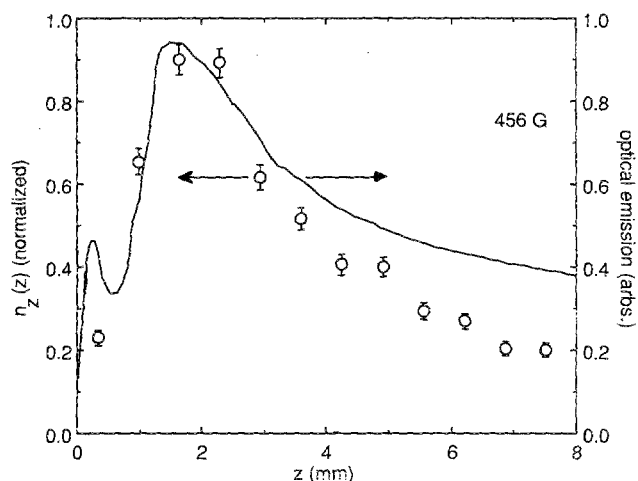


FIG. 3. Axial profiles for $|B|_{\text{max}} = 456 \text{ G}$. The experimental curves of Gu and Lieberman shown here represent the combined optical emission of argon and copper; the small peak near the cathode surface is an artifact of their measurement technique (Ref. 6). Only the first few millimeters are suitable for comparing experiment (—) to simulation (○) because of the copper glow. The parameters entering the simulation are the same as those for Fig. 2; they are listed in Table I.

dominates the optical emission. Accordingly, we dismiss the discrepancy between experiment and simulation found at $z > 4 \text{ mm}$. Because the experimental axial profile measurements were made with a broadband optical detector, one cannot expect agreement as good as exhibited by the radial profiles described above.

IV. SUMMARY

We have tested a Monte Carlo simulation of electrons emitted from the cathode of a planar magnetron. To make a more rigorous test of this code than previously reported,⁴ we compared its predictions to the experimental results reported by Wendt, Lieberman, and Meuth⁵ and by Gu and Lieberman⁶ for two different strengths of the magnetic field.

We found that the level of ionization due to secondary emission predicted by the code is adequate to sustain the discharge for the case with the typical field strength $|B|_{\text{max}} = 456 \text{ G}$, but not for the weak field of 171 G. This suggests that the electrons born in the plasma are important for maintaining the ionization at low magnetic fields. We also found that the energy cost of producing an ion–electron pair in a sputtering magnetron is on the order of 200 eV, depending on $|B|_{\text{max}}$ and γ .

The *radial* ionization profile predicted by the simulation shows excellent agreement with experiment for the 456-G field. This confirms the earlier finding⁴ that the simulation is useful for predicting the profile of the ion flux to the cathode. The *axial* profiles also show agreement as well as can be expected given the experimenters' use of a broadband optical detector.

ACKNOWLEDGMENTS

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- ⁷It would be desirable to compare the simulated ionization density to the optical emission of a specific spectral line, preferably one that results from electron-impact excitation that has a cross section with an energy dependence that nearly matches that of ionizing collisions. Most spectral lines of neutral argon have such an energy dependence, but not all of them (cf. Ref. 8). Because the experimenters of Ref. 6 employed a broadband optical detector that did not isolate a specific spectral line, this limits the accuracy of comparing their experiment to our simulation, although the copper atom emission discussed in the text is probably a more severe problem.
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- ²⁰S. C. Brown, *Basic Data of Plasma Physics*, 2nd ed. revised (MIT, Cambridge, MA, 1966), p. 225. The value we cite for γ is probably accurate to within 50%.