Pressure dependence of ionization efficiency in sputtering magnetrons

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Using a Monte Carlo simulation, we show how electron confinement allows sputtering magnetrons to operate at lower neutral pressures than similar unmagnetized devices. We find that at both high and low pressures, the ionization efficiency in a magnetron is constant, and it varies by only 40% between the two regimes. In contrast, the efficiency of an unmagnetized discharge varies linearly with pressure, becoming very small at low pressures.

Sputtering magnetrons are plasma devices used for thin-film deposition and sputter etching. In these devices crossed electric and magnetic fields confine electrons in complicated obtains near a cathode target.[1,2] These trapped electrons create ions from the neutral background gas, which are accelerated to the cathode and cause the emission of secondary electrons. These secondary electrons replace electrons lost from the trap through scattering with neutral collisions,[2] helping to sustain the discharge. Since the principal virtue of the magnetron is its ability to sputter at low neutral pressures, it is worthwhile to study the pressure dependence of electron transport.

In this letter we use a Monte Carlo simulation[2,3] of the transport of electrons emitted from the cathode[4] to explore the neutral pressure dependence of the ionization efficiency. The device we simulate is our cylindrically symmetric planar magnetron.[5] The Monte Carlo code was described in detail in Ref. 2, where we simulated a 1 Pa argon discharge. This code has also been used to simulate[3] a magnetron which has an adjustable magnetic field.[1]

We now briefly review this code. Single electrons are started at rest from the cathode and are followed as they move about within a cylindrical simulation box which extends 4 cm above the cathode and to a radius of 4 cm from the symmetry axis. Orbits are computed using prescribed, time-independent magnetic and electric fields. An electron's orbit is terminated when its total energy becomes too small to ionize an argon atom, or when it moves out of the simulation boundaries. The next electron is then started at a radius chosen in a manner consistent with previous ionization events.

The magnetic field **B** was calculated based on the actual device,[5] which has a central plug magnet surrounded by a ring of bar magnets. The field is 245 G and purely tangential to the copper cathode surface at a radius of 1.7 cm, where the etch track is deepest. We denote this radius a and take it to be a typical length scale of the device. Even though we perform our simulation for only one magnetron size, our results are reported in terms of a dimensionless neutral pressure a/mfp so that they can be applied to larger or smaller devices. Here mfp $= k_B T/\sigma P$ is the mean free path, where σ is the cross section for momentum transfer, and T is room temperature.

We assume a one-dimensional electric field perpendicular to the cathode surface.[6] This field was composed of a 1.0 V/cm linear presheath and a cathode sheath modeled[7] using typical experimental parameters: a 4 eV electron temperature, a 0.1 mm Debye length, and -400 V dc cathode bias. The resulting sheath width is about 3 mm. The same electric field is used in the simulation here, regardless of the pressure or magnetic field.

Collisions with argon neutrals are accounted for by using the total cross sections to evaluate the probability of elastic, excitation, and ionizing collisions at each time step. If a collision has occurred, the differential cross sections are used to scatter the velocity direction. The electron's energy is decreased by each collision. For ionizing collisions, we use the energy loss data reported by Carman for M-shell ejection,[8] which is an improvement upon the fixed energy loss assumed in our earlier[2,3,6] simulations.

For this letter we have used the simulation to determine the ionization efficiency, which is defined as follows. First, we denote the number of ionizations that a single electron performs as N_i. The average of N_i over an ensemble of simulated electrons is denoted by $\langle N_i \rangle$. Here $\langle N_i \rangle$ is found directly from the simulation; in general it will increase with cathode bias and pressure. The maximum possible number of ionizations $N_{i\max}$ is defined as the number of ionizations performed by a well-confined electron in the absence of excitation and elastic collisions.[9] Finally, we define the ionization efficiency, η, for a given pressure and cathode bias as

$$\eta \equiv \langle N_i \rangle / N_{i\max}. \qquad (1)$$

This efficiency for ionization by cathode emission will always lie in the range $0 < \eta < 1$. If $\eta \simeq 1$, electrons are efficiently confined, while if $\eta \ll 1$, the confinement is ineffective and electrons escape easily from the device. In practice, η can never reach a value of 1 because many electrons lose energy in excitation collisions. As a result, the highest possible η is about 0.9.

We ran the simulation for a wide range of neutral pressures[10] from 0.2 to 100 Pa. Under these conditions the mean free path (for electron momentum transfer in argon) ranges from 7.5 to 0.015 cm, assuming a cross section[11] of 1×10^{-16} cm^2. Note that over this pressure range, the mean free path ranges over values significantly smaller than the system size ($a/\text{mfp} \gg 1$) to those greater than the system size ($a/\text{mfp} \ll 1$). For good statistics we used at least 300 electrons in each ensemble, and for good energy conservation we selected a time step between 5 and 20 ps.

The principal results of this letter are shown in Fig. 1(a), where we plot the ionization efficiency η against the neutral pressure P. The efficiencies in unmagnetized and

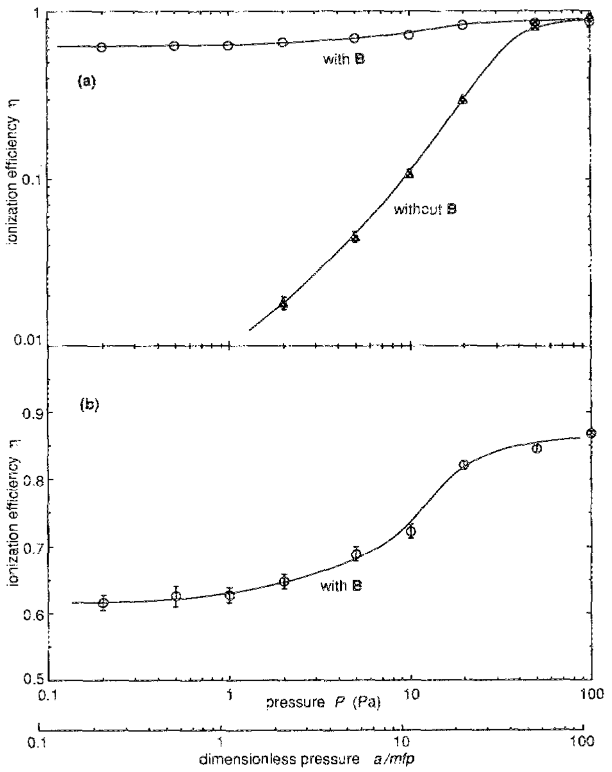

FIG. 1. (a) Pressure dependence of ionization efficiency $\eta = \langle N_i \rangle / N_{i\max}$. Without the magnetic field **B**, η varies almost linearly with pressure P. With **B**, η is nearly independent of pressure, allowing the magnetron to operate at lower pressures than unmagnetized devices. (b) The magnetized case is replotted on a linear scale with a suppressed zero, revealing that η is constant at both high and low pressures. The dimensionless pressure in the bottom scale is the ratio of the magnetron size a to the mean free path mfp.

magnetron discharges differ significantly at low pressures and merge for $P > 50$ Pa. Without the magnetic field, we find that η increases nearly linearly with P until it saturates at $P \approx 50$ Pa. On the other hand, with **B**, the ionization efficiency is almost independent of P. The weak dependence of η on P demonstrates the effectiveness of the magnetron configuration in trapping electrons. This effectiveness is the reason magnetrons can be used for sputtering at low neutral pressures.

In Fig. 1(b) we examine in greater detail the pressure dependence of η for the magnetized case. Note that the average number of ionizations per electron varies by only 40% as the neutral pressure is scanned over three decades from 0.2 to 100 Pa. Two limiting regimes, at low and high pressures, are evident in Fig. 1(b). At low pressures ($P < 1$ Pa), η is constant because the mean free path is much longer than the system size ($a/\mathrm{mfp} \ll 1$). At high pressures ($P > 50$ Pa), η saturates since the mean free path is much shorter than the system size. In this regime, collisions are frequent and electron transport becomes diffusive, leaving no chance that an electron will escape while it still has enough energy to ionize a neutral atom.

Even though the simulation predicts that η becomes constant at low pressures, real magnetron discharges extinguish at very low pressures. This paradox is resolved by noting that our prescribed electric field omits self-consistent effects,[12] which play a particularly significant role at low pressures. The electric field in a discharge self-consistently adjusts so that electrons and ions are expelled at the same rate. At low pressures, energetic electrons require more time to perform a given number of ionizations. The ion-transit time, however, is relatively constant in a magnetron, meaning that at a sufficiently low pressure, the electrons will be forced out of their confined orbits too quickly, and the discharge will go out.

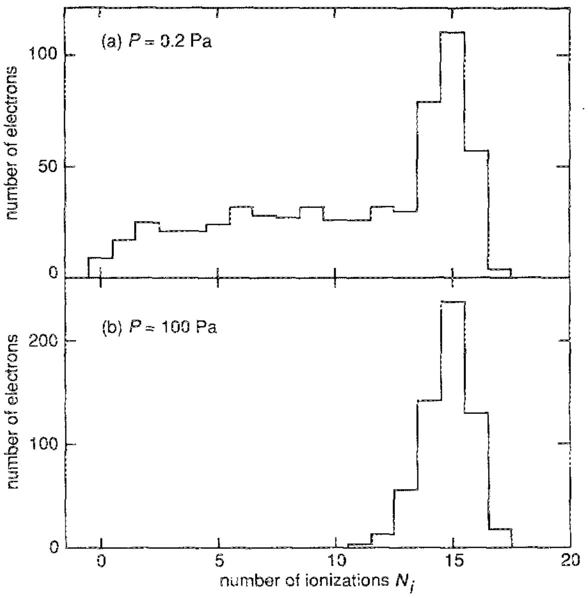

FIG. 2. Histogram of ionizing collisions: (a) At 0.2 Pa the distribution is peaked at 15 ionizations, but has a tail extending down to zero, showing that some electrons escaped while they still had the energy to create ions. (b) At 100 Pa the distribution has no tail, due to the short mean free path ($a/\mathrm{mfp} \gg 1$). These results were obtained with the magnetic field **B**.

We further explore electron loss in the low- and high-pressure regimes in Fig. 2, where we show histograms for the number of ionizations N_i performed by each electron for a magnetron at $P = 0.2$ Pa and $P = 100$ Pa. Both histograms have a peak at 15 ionizations, representing electrons that do not escape from the simulation before expending most of their energy. This peak has a finite width, due to energy lost in excitation collisions, which account for about one quarter of all inelastic collisions. The histogram for the low pressure displays a flat tail that extends down to zero ionizations. This tail reveals that some electrons escape carrying energy that could have created additional ions. It does not appear in the histogram for 100 Pa, where the ionization efficiency is saturated.

In summary, we have used a Monte Carlo simulation of our magnetron device to determine the average number of ionizations per electron. We find that the ionization efficiency varies by only 40% as the neutral pressure is scanned from 0.2 to 100 Pa. This weak dependence is due to the electron confinement; even at low pressures only a few electrons are lost before using up their energy ionizing neutral atoms. Without the magnetic field, the ionization efficiency has a strong linear dependence on pressure.

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