Simulation of the electron dynamics in a magnetron sputtering device with equipotential and non-equipotential cathode

P A Tsygankov, E A Orozco, V D Dugar-Zhabon, J E López, and P A Cárdenas

1 Universidad Industrial de Santander, Bucaramanga, Colombia

E-mail: jesus2198136@correo.uis.edu.co, eaorozco@uis.edu.co

Abstract. The magnetron sputtering of cathode material is one of the ways of producing a thin film deposition on solid surfaces and maintaining the cathode system under a certain potential. Recently, some experimental study of a magnetron sputtering system with the segmented cathode at different electric potential on each segment has been conducted. It allows the system productivity regarding the rate of deposition to be over the volt-ampere current limitations imposed on each segment. The physical processes associated with generating and sustaining it in this system are complex and have not been explained so far from a theoretical point of view. In this work, we present a computational study of the electron dynamics in the simple particle approximation which is found in a two-segments magnetron discharge under the influence of both the magnetic field and the segment electric potentials of 750 V and 500 V. The fields are calculated by using comsol multiphysics R⃝. The particle dynamics is studied through numerical solution of the Newton-Lorentz equation. The simulations show that the Hall current symmetry is determined by the electrode segments geometry. The obtained results are checked through the simulations fulfilled to maintain the cathode system at the same potential.

1. Introduction

The magnetron material sputtering method suggested by Penning [1] some years ago forms a basis for sputtering devices and presently is one of the most popular methods to produce thin films. In recent years there have been developed many magnetron systems with different geometries, magnetic field configurations and discharge voltage modes aimed to enhance the system productivity which depends on the current density and bombarding ions energy [2,3]. In 2010, a modification of the magnetron sputtering system which consists in dividing the cathode into segments insulated from each other, thus forming non-equipotential cathode (NEC), has been suggested [4,5].

A regular discharge initiated in a two-segment cathode magnetron system shows that the magnetized electrons form the Hall current [6,7]. This new configuration provides multiple advantages, such as an increasing productivity and a flexible regulation of the deposited film profile [8,9]. In this work, we present a numerical study of the electron dynamics in a single particle approximation in a magnetron sputtering device with NEC cathode, which aims at deriving in space both the electron distribution and current density profiles, in order to gain some insight into the mechanism of NEC functioning.
The electric and magnetic fields are calculated using comsol multiphysics®. The obtained Hall profiles are calculated, and the cases of equipotential cathode are compared with non-equipotential ones of the same magnetron geometry.

2. Physical scheme
The magnetron sputtering NEC device used consists of two magnets, the first one with a ring shape and the second one of a cylinder type. Their magnetizations are oppositely directed along the z-axis in such a manner as to confine the electrons in the discharge volume through maintaining \( \vec{E} \times \vec{B} \) drift motion. The configuration of the NEC magnetron is shown in Figure 1.

2.1. Magnets
The magnetic system in use is of two-sections: a cylinder which is axially enclosed by a ring. The geometry dimensions and axial magnetization values \( M_z \) are tabulated in Table 1.

| Magnet | \( M_z \times 10^5 \) (A/m) | Ri (cm) | Re (cm) | Height (cm) |
|--------|-----------------------------|---------|---------|-------------|
| Ring   | -3.75                       | 2.0     | 2.5     | 1.0         |
| Cylinder | 3.75                      | –       | 1.0     | 1.0         |

2.2. Anode and non-equipotential cathode
The elements of magnetron system are displayed in two projection in Figure 2. The segmented cathode is a thin disk of 2.5 cm in diameter sectored by a 0.1 cm space into two equal parts. One can choose the chamber walls for the anode; however, we have taken a solid thin disc as the anode whose parameters are identical to the cathodic ones. The anode is placed over the cathode at a distance of 2 cm.
Figure 2. Individual components of a magnetron sputtering device. A magnetic ring (a) and a magnetic cylinder (b) with axial and opposite magnetization produce the magnetic field. The segmented cathode (c) and anode (d) produce the electric field.

3. Numerical scheme

To obtain the electron dynamics we solve the relativistic Newton-Lorentz equation, which in dimensionless variables, Equation (1), takes the form:

$$\frac{d\vec{U}}{d\tau} = \vec{g}_0 + \frac{\vec{U}}{\gamma} \times \vec{b},$$

where $\vec{U} = \vec{p}/m_e c$ is the momentum of the electron, $\vec{g}_0 = -e\vec{E}/m_e c\omega$ is the electric field due by the cathode, $\vec{b} = -\vec{B}/B_0$ is the magnetic field at the electron position, $\tau = \omega t$ is the time and finally $\gamma = (1 + U^2)^{1/2}$ is the relativistic factor. The parameters $B_0$ and $\omega^{-1} = m_e/eB_0$ represent the characteristic values for the magnetic field and time respectively. In a finite differences scheme, the Equation(1) transform in Equation (2).

$$\frac{\vec{U}^{n+1/2} - \vec{U}^{n-1/2}}{\Delta \tau} = \vec{g}^n + \frac{\vec{U}^{n+1/2} + \vec{U}^{n-1/2}}{2\gamma^n} \times \vec{b}^n$$

Equation (2) is solved using the Boris-Bunneman algorithm in a leap-frog scheme [11, 12], where the new position in each simulation time step is calculated employing the Equation (3).

$$x^{n+1} = x^n + \frac{\vec{U}^{n+1/2} \Delta \tau}{\gamma^{n+1/2}}.$$

here $\gamma^{n+1/2} = [1 + (U^{n+1/2})^2]^{1/2}$. These positions are normalized with respect to $l_o = c/\omega$.

The magnetic and electric fields are calculated by solving the corresponding Laplace equations in finite elements form through comsol multiphysics® [10]. Figure 3(a) shows the electric field profile in the plane and Figure 3(b) represents the electric and magnetic vectoral fields. One can
determine the region where the electric and magnetic fields are perpendicular and, consequently, the electron confinement is effective due to the $\vec{E} \times \vec{B}$ drift motion in the anti-clockwise direction.

![Electrostatic Potential](image)

**Figure 3.** (a) Electric potential profile at plane $y = 0$ and (b) the magnetic and electric vectorial field obtained by comsol modules.

### 4. Results

In the simulations, three different scenarios are realized. We have started the study of the confining process with the segmented cathode maintained at a potential of -500 V. We have named this case equipotential. Initially, a uniform cylindrical electron cloud placed in the inter-electrode volume is taken cold with the velocities very close to zero. In the magnetron volume, the electrons begin to move due to the electric field and at the same moment some electrons initiate the $\vec{E} \times \vec{B}$ drift motion. Other types of drift motions caused by the magnetic field gradient and curvature of the magnetic force lines are insignificant. Figure 4(a) shows the 3D trajectory of a trapped electron during its azimuthal motion and Figure 4(b) presents its projection on the $xy$-plane. One can see that the trapped electron in the equipotential case executes periodic oscillations in the azimuthal direction.

![Electrostatic Potential](image)

**Figure 4.** Full trapped electron trajectory: (a) with equipotential cathode case and (b) its respective 2D projection in $xy$ plane.
The fact that the segmented cathode is equipotential implies that the electric field is axisymmetric together with the Hall current and the electron space distribution. Figure 5 demonstrates that the current density and electron concentration profiles are symmetric about the $z$-axis. Figure 5(a) shows the variation of the current density along the $x$-axis at $y = 0$ and $z = 0.5$ cm. In this case the current density component $J_y$ is dominant because in $y = 0$ plane the azimuthal component coincides with the $J_\phi$ component. Figures 5(b) and 5(c) evidence the symmetric distribution of the electron concentration and $z$-component of current density at $y = 0$ for different $z$-values.

![Figure 5](image_url)

**Figure 5.** Results for equipotential cathode: (a) Current density components profiles along $x$-axis at $y = 0$ and $z = 0.5$ cm. Behavior of (b) electronic concentration and (c) $J_y$ for different $z$-values at $y = 0$ plane.

One of the other two scenarios refers to the non-equipotential cathode system where the right-hand cathode segment shown in Figure 2(c) is under the potential of -750 V with reference to the anode while the other segment is related to d.c. source of -500 V. The right-hand segment is called a high voltage (HV) segment and the left-hand segment is named a low voltage (LV) segment. The second non-equipotential scenario is realized at the HV segment potential of -600 V with the LV segment potential remaining at -500 V. Hence, the electric fields in non-equipotential case don’t possess the axial symmetry. The simulations of electron motion are fulfilled at the same initial conditions as in the equipotential case. The calculation results are shown in Figure 6 for both HV potentials of -750 V and -600 V.

It should be noted that the azimuthal current density is dominant due to $\vec{E} \times \vec{B}$ drift motion as in the case of equipotential cathode but the concentration is out of symmetry (see Figure 6(a), Figure 6(d) and the major concentrations over the LH segment are observed for $z = 0.25$ cm and 0.5 cm while for HV segment the major concentration is detected at $z = 0.75$ cm and at $z = 1.0$ cm. The behaviour of electrons in non-equipotential field is clearly distinct from the case of equipotential field as can be seen in Figure 6(b), Figure 6(c), Figure 6(e), Figure 6(f). This is easy to explain: the electrostatic repulsion is higher in the HV side and the confinement is more effective in the higher $z$-plane. The electron concentration is found smaller than in the LV side. The symmetry of the electron distribution in the case of equipotential cathode and low confinement efficiency in the HV side are demonstrated in Figure 7 where 3D electron distribution is plotted. The distinction in the electron distributions between the HV and LV sides is noted but it is important to mention that the current density amplitudes in both sides are similar which occurs due to the higher velocity values in the HV side.
Figure 6. Results for non-equipotential cathode: Current density components profile along x-axis at y=0 and z = 0.5 cm and behavior of electronic concentration and $J_y$ for different $z$-values at $y=0$ plane: (a), (b) and (c) for HV = -600V and (d), (e) and (f) for HV = -750 V.

Figure 7. Final distribution of trapped electrons in a magnetron sputtering with (a) equipotential cathode (-500 V) and (b) non-equipotential cathode (LV = -500 V, HV = -750 V).
5. Conclusions
The dynamics of electrons in a magnetron sputtering device volume is studied numerically. It is shown that the Hall current is generated in both cathode cases: equipotential and non-equipotential. We can emphasize that the electron concentration is varied in $z$-direction at low concentration values in HV side in comparison with the LV one which permits to control the deposition rate in the non-equipotential sputtering systems.

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