

# Modelling of continuous steel coating by self-induced ion plating (SIIP)

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## Abstract

The present communication deals with the numerical simulation of a new physical vapour deposition process called self-induced ion plating (SIIP). SIIP can be defined as the evaporation of a metallic target thanks to ion bombardment of a magnetron sputtering system. The simulation of the SIIP process is based on three coupled models. The first one deals with magnetism and simulates a magnetron system, the second one defines the heat transfer phenomena (conduction, radiation) that occur in the SIIP process and the last one determines the coating thickness profile on the substrate using the theory of evaporation. The computed thickness profile is then compared to the measured one. We notice that the model results and measurements have the same order of magnitude but model results are under-estimated. We conclude that we have to improve our model by removing some assumptions.

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## 1. Introduction

Self-induced ion plating (SIIP) [1,2] is a new physical vapour deposition (PVD) process developed in order to produce continuous coating of flat steel products. This technique is based on two well-known PVD processes: vacuum evaporation and magnetron sputtering. SIIP presents the advantages of both techniques: the high deposition rate of the evaporation and the good adherence of the deposit layer generated by a magnetron sputtering process.

SIIP system (Fig. 1) is very similar to a classical magnetron sputtering system. An argon gas is ionized (under high vacuum  $\approx 0.03$  Pa) between a zinc target at a voltage of  $-770$  V (cathode) and a steel flat substrate at ground. The substrate has a displacement velocity of 1.3 m/min (for wide coating) at a few centimetres above the target. The argon ions  $\text{Ar}^+$  of the plasma are accelerated in the cathode sheath towards the target contained in a graphite crucible. Nevertheless, the ion bombardment in SIIP does not lead to

particles ejection as in sputtering but to the heating and evaporation of the zinc target. In fact, the SIIP target is not cooled but thermally insulated by an insulating layer located under the crucible. The argon plasma is confined near the target by the magnetic field due to neodymium magnets disposed under the insulating layer. Magnets are cooled by a water flow to keep good performance. The magnetic confinement induces a non-uniform ion bombardment heat flux distribution, with a maximum where the magnetic field lines are parallel to the cathode, and increases the efficiency of the process, in the well-known manner of a magnetron.

The aim of the present work is to develop a numerical simulation model of the SIIP process in order to predict the thickness profile of the coating deposited on the substrate. The simulations are carried out with the interactive environment MATLAB<sup>®</sup> and FEMLAB<sup>®</sup>, a tool for PDE-based multiphysics modelling in MATLAB<sup>®</sup>. The simulation of the SIIP process is based on three coupled models. The first one deals with magnetism. We evaluate the magnetic field generated by the magnetron in order to define the power distribution applied by the ion bombardment to the target surface. The second one deals with the heat transfer phenomena i.e. thermal conductivity and radiation that

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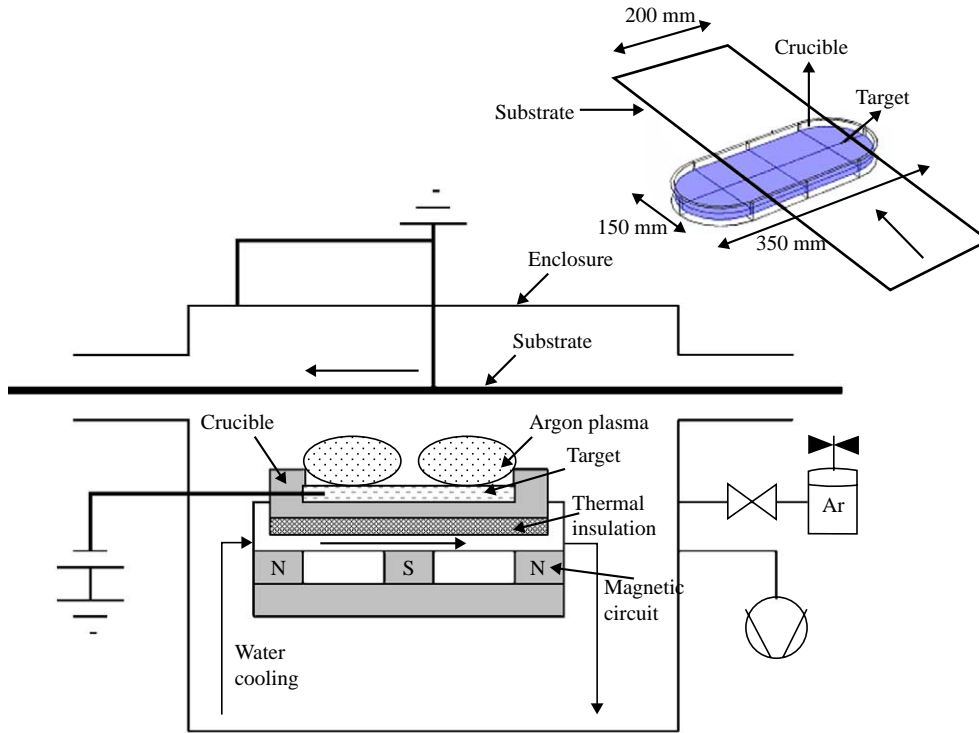


Fig. 1. SIIP process.

occur between all the components of the SIIP process. The last model determines the thickness profile of the coating on the substrate using the temperature field obtained in the previous step and the theory of evaporation.

## 2. Magnetic model

The first step in the simulation of the SIIP process is the evaluation of the magnetic field created by the magnetron and surrounding the target. In fact, we will use this information to define the power distribution imposed on the target surface.

In a current free region  $\vec{\nabla} \times \vec{H} = 0$ , we can define the scalar magnetic potential  $V_m$  as  $\vec{H} = -\vec{\nabla}V_m$ . The relationship between the magnetic flux density  $\vec{B}$  and the magnetic field  $\vec{H}$  is given by

$$\vec{B} = \mu_0(\vec{H} + \vec{M}) \quad (1)$$

where  $\vec{M}$  ( $A\ m^{-1}$ ) is the magnetization and  $\mu_0$  ( $4\ \pi\ 10^{-7}\ H\ m^{-1}$ ) is the vacuum permeability.

Using a linear expression for the magnetization,

$$\vec{M} = \vec{M}_0 + (\mu_r - 1)\vec{H} \quad (2)$$

where  $\vec{M}_0$  ( $8,9.10^8\ Am^{-1}$ ) is the pre-magnetization and  $\mu_r$  ( $\approx 1$ ), the relative permeability of the neodymium magnets.

We obtain the relation

$$\vec{B} = \mu_0\mu_r\vec{H} + \mu_0\vec{M}_0 \quad (3)$$

Considering also  $\vec{\nabla}\vec{B} = 0$ , we can determine  $V_m$  with the following equation:

$$-\vec{\nabla}(\mu_0\mu_r\vec{\nabla}V_m - \mu_0\vec{M}_0) = 0 \quad (4)$$

The differential Eq. (4) is solved with FEMLAB<sup>®</sup>. In Fig. 2, we can compare computed absolute value of the vertical component of magnetic induction ( $B_z$ , Gauss) at the target level with measurements (for a quarter of the SIIP geometry). We notice an excellent agreement between the measurements and the results of the FEMLAB<sup>®</sup> model.

To model heat transfer in the SIIP, we need to know the distribution of ion bombardment heat flux. Given the similarity between SIIP and sputtering process, we assume that the distribution of heat flux in SIIP can be computed as erosion profile in sputtering. Because of a lack of accurate model availability to predict erosion profile due to sputtering magnetron, we use a law presented on the Plasma Surface Engineering Corporation [3] website. It claims that the depth of erosion in the sputtering process could be defined, using horizontal ( $B_{xy}$ ) and vertical ( $B_z$ ) components of magnetic induction at the target level, as

$$\left(\frac{B_{xy}}{\sqrt{B_{xy}^2 + B_z^2}}\right)^3 \quad (5)$$

Thus, we assume that ion bombardment distribution is proportional to law (5). We multiply it by a constant value in

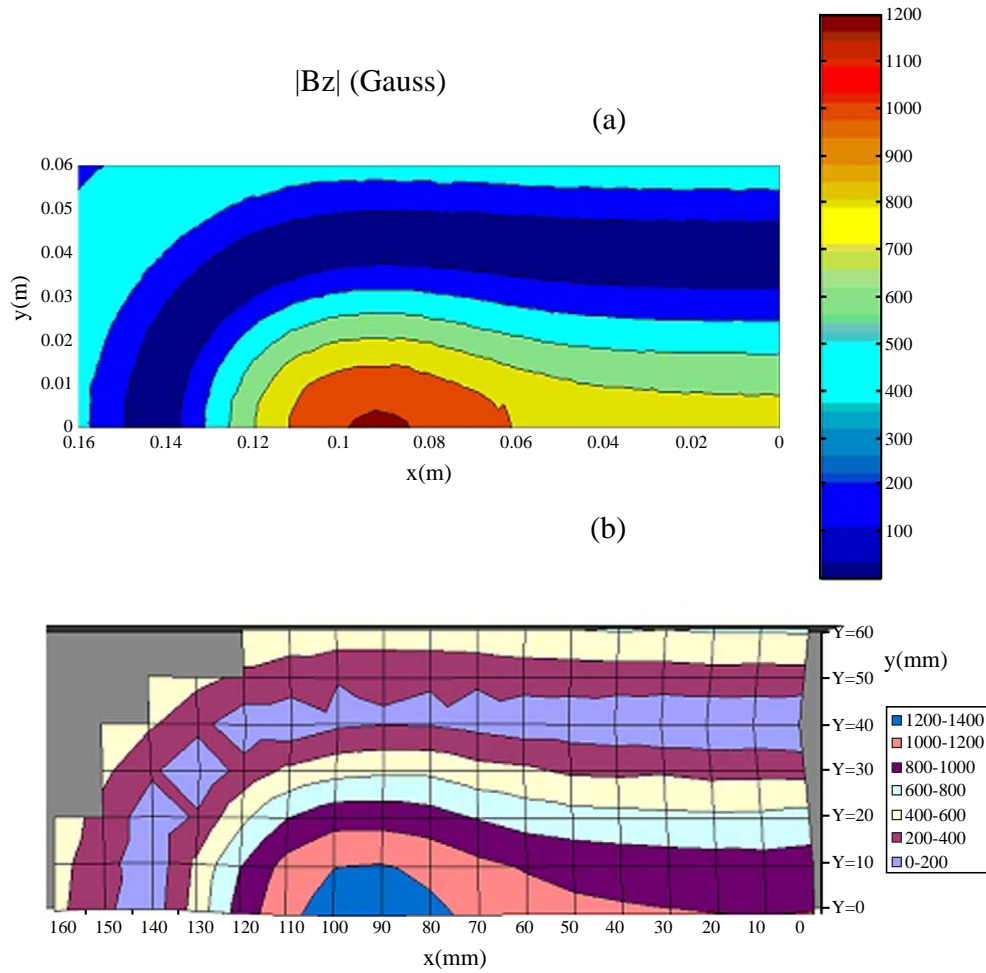


Fig. 2. Simulated (a) and measured (b) vertical component of magnetic induction (absolute value).

order to apply the total power of 2.5 kW on all the target surface.

### 3. Heat transfer model

Steady state heat transfer problems are governed by the energy conservation equation

$$\vec{\nabla}(k \vec{\nabla} T) = 0 \tag{6}$$

where  $k$  ( $\text{W m}^{-1} \text{K}^{-1}$ ) is the thermal conductivity and  $T$  (K) the temperature.

The computational domain (Fig. 4) is divided into two main parts that are the crucible and the metallic target. The boundary conditions applied on the different faces of the model are defined on Fig. 3:

1.  $q_1$  is the heat loss by conduction through the insulating layer and by forced convection with the cooling water flow. It is given by

$$q_1 = h(T - T_1) \tag{7}$$

where  $h$  ( $\text{W m}^{-2} \text{K}^{-1}$ ) is a global heat loss coefficient and  $T_1$ , the temperature of the cooling water ( $\approx 300$  K).

2.  $q_{in}$  is the heat flux applied on the target surface and resulting from the ion bombardment.  $q_{in}$  is defined using relation (5) as presented in the magnetic model.

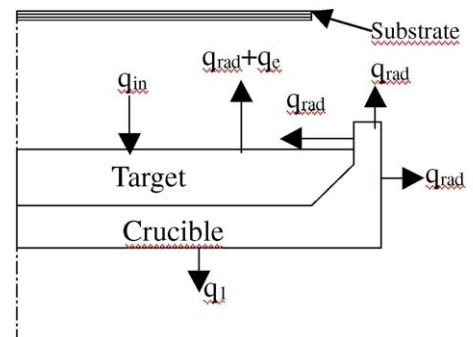


Fig. 3. Boundary conditions.

3.  $q_e$  is the heat flux due to the zinc evaporation. This boundary condition is defined by

$$q_e = J_e * L_v \tag{8}$$

where  $J_e$  ( $\text{kg s}^{-1}\text{m}^{-2}$ ) is the mass flux of evaporated material and  $L_v$  ( $\text{J kg}^{-1}$ ), the latent heat of evaporation.  $J_e$  is defined by the Hertz-Knudsen theory [4] as

$$J_e (\text{kg m}^{-2}\text{s}^{-1}) = 5834 \cdot 10^{-1} \sqrt{\frac{M_t}{T_e}} p_v \tag{9}$$

with  $M_t$ , the zinc atomic weight,  $T_e$  (K), the temperature of evaporation,  $p_v$  (Torr), the zinc saturation vapour pressure.

4.  $q_{\text{rad}}$  (Eq. (10)) is the radiative heat flux resulting from the temperature differences between the bodies involved in the SIIP process. To correctly define the radiative heat transfer condition, a radiation model using the zone method [5] has been programmed and coupled with the FEMLAB<sup>®</sup> model. The zone method involves subdivision of the radiating enclosure into isothermal surface zones. A total energy balance is written over each zone in terms of radiation arriving at it from all others zones in the enclosure. To compute total exchange areas ( $S_i S_j$ ), we use the relation of Noble [6].

$$q_{\text{irad,net}} = \frac{1}{S_i} \sum_j \bar{S}_j S_i \sigma (T_j^4 - T_i^4) \tag{10}$$

with  $S_i$  ( $\text{m}^2$ ), zone  $i$  surface;  $\sigma$  ( $5.67 \cdot 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$ ), Stephan–Boltzmann’s constant;  $S_i S_j$  ( $\text{m}^2$ ), total exchange area,  $T_i$  and  $T_j$  (K), zone  $i$  and zone  $j$  temperatures.

The temperature field (in Kelvin) obtained using FEMLAB<sup>®</sup> model coupled with the radiative model (under MATLAB<sup>®</sup>) is presented on Fig. 4. Fig. 4 shows a track of higher zinc temperature at the target surface. We can emphasize that the zinc target sublimates. In fact, the maximum value of the target surface temperature (687 K) is lower than the zinc melting point (692 K). Those results seem to be in good agreement with experimental observations.

#### 4. Evaporation model

Knowing the temperature distribution on the target surface, the profile of the coating on the substrate can be determined. To evaluate the coating thickness, we use the theory of evaporation [7].

We assume (Fig. 5) to have a point source ( $dS_e$ ), no collisions between atoms in the space between the target and the substrate and a substrate parallel to the source and located at a distance  $d$ .

In this case, the mass flow  $dq_{\text{md}}$  ( $\text{kg s}^{-1}$ ) deposited on the surface element  $dS$  around point  $M$  is equal to the mass flow evaporated  $dq_{\text{me}}$  ( $\text{kg s}^{-1}$ ) in the solid angle  $d\Omega$ .

$$dq_{\text{md}} = dq_{\text{me}} \tag{11}$$

$$dq_{\text{md}} = \frac{J_e}{\pi} dS_e \cos\theta \Omega \tag{12}$$

with  $J_e$  ( $\text{kg m}^{-2} \text{ s}^{-1}$ ) given by the Hertz-Knudsen theory (Eq. (9)).

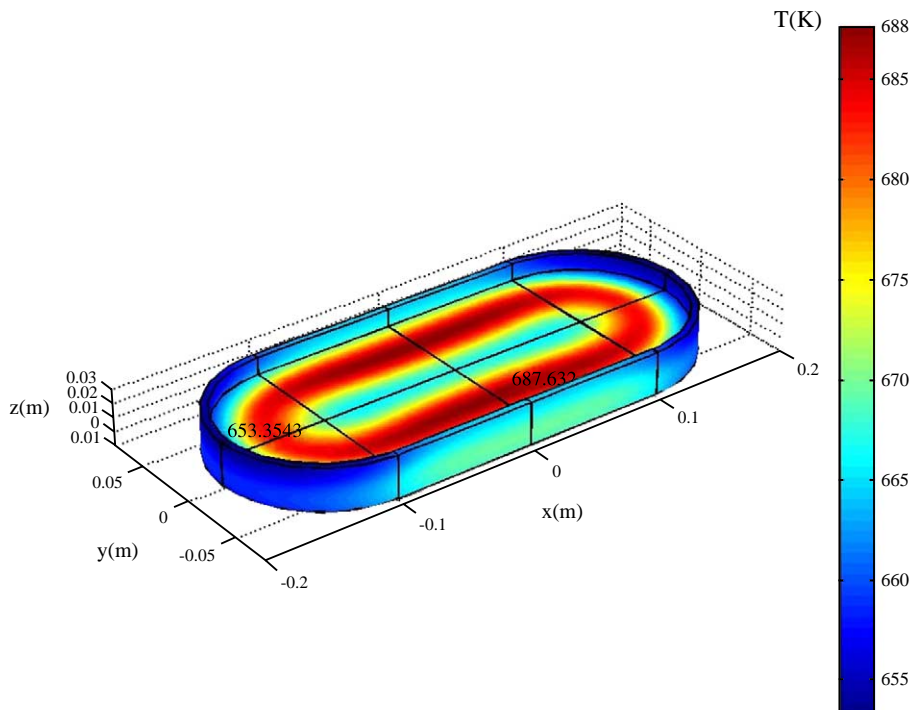


Fig. 4. Results of the heat transfer simulation.

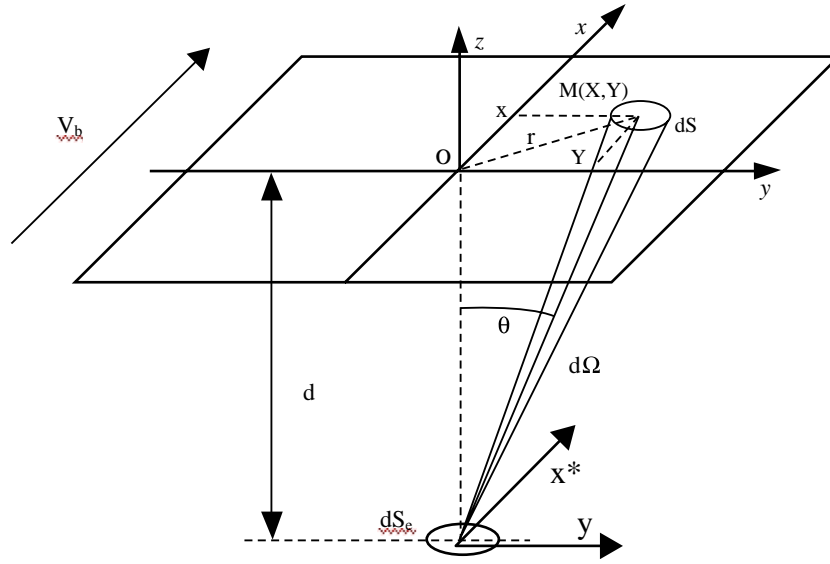


Fig. 5. Evaporation model.

We deduce from Fig. 5 that

$$d\Omega = \frac{dS \cos\theta}{(r^2 + d^2)} \tag{13}$$

$$\cos\theta = \frac{d}{\sqrt{r^2 + d^2}} \tag{14}$$

$r$  (m) is the distance between point  $M$  and the projection of the point source on the deposition surface and  $d$  (m) is the distance between the target and the substrate.

So we can write

$$\frac{dq_{md}}{dS} = dJ_d = \frac{J_e}{\pi} \frac{d^2}{(r^2 + d^2)^2} dS_e \tag{15}$$

with  $dJ_d$  ( $\text{kg m}^{-2} \text{s}^{-1}$ ), the mass flux of deposited material coming from the point source  $dS_e$ .

The total mass flux of deposited material  $J_d$ , coming from the sources  $dS_e$  of an evaporating surface  $S_e$  is then given by

$$J_d = \int_{S_e} \frac{J_e}{\pi} \frac{d^2}{(r^2 + d^2)^2} dS_e \tag{16}$$

If we consider that  $dS$  moves (Fig. 5) with a velocity  $v_b$  ( $\text{m s}^{-1}$ ), the total coating thickness on point  $M(X,Y)$  is

$$e_d(X,Y) = \int_0^\infty \frac{J_d(x^*,y)}{\rho_e} dt \quad x^* = v_b \tau \tag{17}$$

where  $x^*y$  is a global axis system that is initially identical to the local axis system  $xy$ .

Discretizing the displacement of the surface in the  $x^*$  direction with  $x^*_{i+1} = x^*_i + v_b \Delta t$ , we can write

$$e_d(X,Y) = \sum_{i=0}^{n-1} \frac{J_d(x^*_i,Y)}{\rho_e} \Delta t \tag{18}$$

$e_d$  (m) is the deposit thickness,  $\rho_e$  ( $\text{kg m}^{-3}$ ), the density of the evaporated material and  $\Delta t$ , an elementary interval of time.

A program has been developed to simulate evaporation (Eq. (16)) and to compute the deposit thickness (Eq. (18)) using the temperature field obtained on the target surface. Fig. 6 compares the measured and computed thickness profiles across the steel band. Fig. 6 shows that our results are lower than the measured thickness profile. We can also notice that the model results and measurements have the same order of magnitude. Nevertheless, we can see that the measurements do not seem to be accurate because the thickness profile is not symmetrical. That shows that new experiments are required to validate our simulated results. In addition to those possible measurement errors, we know that several assumptions made to simplify the problem have to be confirmed, in particular the law (5) used to define ion bombardment heat flux. Moreover, to introduce the evaporation theory, we have supposed that there were no collisions between atoms during their displacement towards the substrate. This assumption is correct when the mean-free path of the particle is larger than the distance between the target and the substrate. In the current studied setup, it is not the case. So to take the collisions into account, we should introduce in the theory of evaporation an empirical coefficient  $n$  such as Eq. (16) becomes

$$J_d = \int_{S_e} \frac{(n+1)J_e}{2\pi} \frac{d^{(n+1)}}{(r^2 + d^2)^{\frac{(n+3)}{2}}} dS_e \tag{19}$$

The simulated thickness profile for  $n=1.5$  is presented on Fig. 6. We obtain the same profile shape that for  $n=1$  but

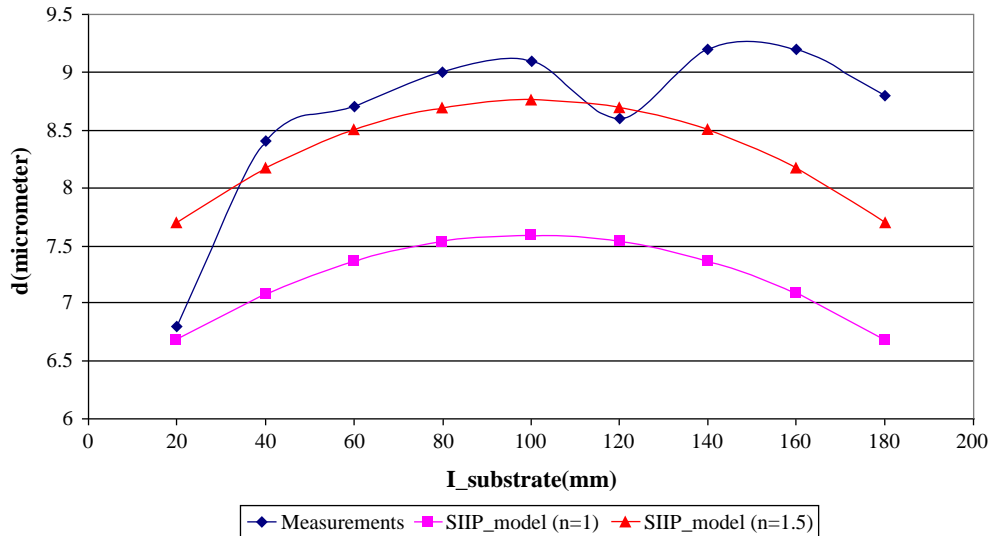


Fig. 6. Coating thickness profile ( $\mu\text{m}$ ) across the substrate.

the values of thickness are closer to measurements compared to the results computed with  $n=1$ .

## 5. Conclusions

In this paper, we have presented a model of a new vapour deposition technique that we refer to as self-induced ion plating. SIIP could be defined as the evaporation of a metallic target thanks to ion bombardment of a magnetron sputtering system. The SIIP model consists of three sub models: a magnetic model, a heat transfer model and an evaporation model. The first one is required in order to simulate the magnetic field generated by the magnetron and to define the profile of the ions bombardment heat flux on the target surface. The heat transfer model defines the heat exchange (conduction, radiation) between all parts of the SIIP. The solution of this second model gives the temperature field on the target surface. The third model evaluates the coating thickness profile from the temperature field obtained with the previous model combined with the theory of evaporation. The computational results achieved are compared with measure-

ments. The comparison shows that our results are lower than measurements with a maximal error of 30%. The reasons could lie in some inadequate assumptions but also in the experimental results that do not seem to be very accurate. In future developments, we have to check, using a Monte-Carlo method, the accuracy of the ion bombardment heat flux distribution and new experiments are planned to have more precise measurements.

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