Modeling Spectral Emission Phenomena in Beryllium Plasma, Using Comsol Multiphysics

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Abstract: The purpose of this paper is to present a numerical modeling of plasma phenomena in beryllium emissions using COMSOL Multiphysics software which contains a number of methods for solving problems governed by partial differential equations by finite element method.
The Beryllium films were deposited on mirror polished fine grain graphite substrates using the Thermionic Vacuum Arc (TVA) technology available at NILPRP – Magurele, Romania. The TVA technique involves production of a high potential, between 300 and 2000 V - low current plasma between 0.1 and 2 A in the pure vapors of the metal to be deposited without using any buffer gas [1].
To study this type of plasma we using an experimental approximation based on spectral emission.

Keywords: Thermionic Vacuum Arc method, numerical simulation, Be deposition phenomena.

1. Introduction

Thermionic Vacuum Arc (TVA) is described as a new very suitable for deposition of high purity thin films with compact structure and extremely smooth, just convenient for nanostructure film realization. TVA can generate pure metal vapor plasma source inside of a vacuumed vessel (including H. V. conditions), ensuring energetic ions bombardment of the just depositing material own atoms of the condensing film [2]. The energy of the ions can be fully controlled and changed even during deposition.

2. Theory

The mathematical modeling of TVA method needs a multi-physics approach including fluid mechanics, thermal transfer and magneto-electrodynamics. The corresponding conservation equations are highly coupled, on the one hand implicitly, because all thermodynamic properties and transport coefficients depend strongly on the temperature [3], and on the other hand, explicitly, mainly because the flow depends on electromagnetic forces, temperature depends on Joule effects and electric field is linked to the shape and value of the temperature field. The model is based on the following main assumptions:

- The geometry device is axi-symmetric and then can be described in 2D cylindrical coordinates;
- The flow is laminar and in steady-state;
- The plasma is in Local Thermodynamic Equilibrium;
- Thermodynamic properties and transport coefficients depend only on temperature;
- The gravity effect, electrode erosion and electrode sheaths are not taken into account.

3. Experiment

The Beryllium films were deposited on mirror polished fine grain graphite substrates using the Thermionic Vacuum Arc (TVA) technology available at NILPRP – Magurele, Romania. The TVA technique involves the production of a high potential, between 300 and 2000 V - low current plasma between 0.1 and 2 A in the pure vapors of the metal to be deposited without using any buffer gas [4-5]. The TVA principle scheme is presented in Figure 1 where: “A” is the melted zone, “B” is the plasma created in pure metal vapour and “C” is the electron beam produced by an externally heated cathode (tungsten filament) [4-5]. The evaporation of the metal takes place in high vacuum conditions (about 10-5 Torr and less), figure 2. An externally heated cathode (W filament) produces a thermally emitted electron current of about 100 mA. These electrons are accelerated and focused by a Whenelt cylinder to the anode that is biased to high voltage (1 – 6 kV). The electron focusing is necessary in order to ensure an easy ignition of the electrical discharge.

Indeed, before the discharge ignition, the electrons are concentrated on a spot of the anode surface and being accelerated by the high positive voltage applied on the anode. This creates a strong local heating and consequently evaporation up to a local pressure of about 100 Pa, accompanied by a possibility to ionize this vapors and initiate the discharge.

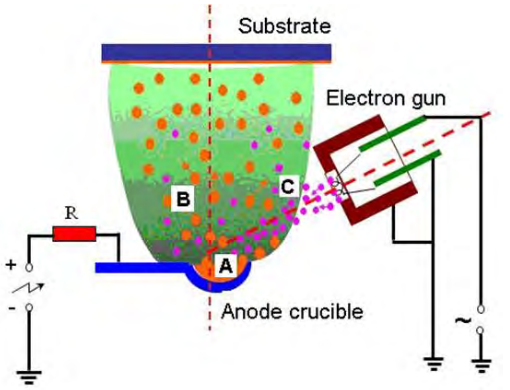

Figure 1. Schematic representation of the Thermionic Vacuum Arc deposition method

Figure 2. Photo of TVA plasma in metal vapors

After this, the plasma expands into the evacuated volume, contributing itself to the evaporation increase and to the discharge current build up. Using this technique, deposition rates in the range of 0.1-5 nm/s were obtained with the advantage that the high energy metal ion bombardment during deposition ensures high density layers with bulk-like structure and high adhesion to the substrate. The discharge conditions and, therefore, the deposition process was controlled by adjusting the filament heating current and anode voltage. During the deposition process the substrate was bombarded by neutral atoms and positive ions generated in metal vapor plasma.

4. Results and discussion

The mathematical model is implemented in the COMSOL software from the governing equations of the following models:

- Weakly Compressible Navier-Stokes (Heat Transfer Module);
- General Heat Transfer (Heat Transfer Module);
- Meridional Electric and Induction Currents, Potentials (AC/DC Module).

The specific thermodynamic properties (mass density, specific heat), transport coefficients (thermal and electrical conductivity, viscosity), and radiative losses are all temperature dependent and are previously calculated or taken from the literature [6-7].

As previously mentioned, these equations are highly coupled and a careful attention is necessary to initiate the calculation and to reach convergence. We build the geometry of the model, and then we fixed the boundary settings, and compute the final solution. Figure 3 show electric potential field of the plasma. These results are in good agreement with the experimental results of the literature and with those of previous calculations obtained with finite volumes method based software.

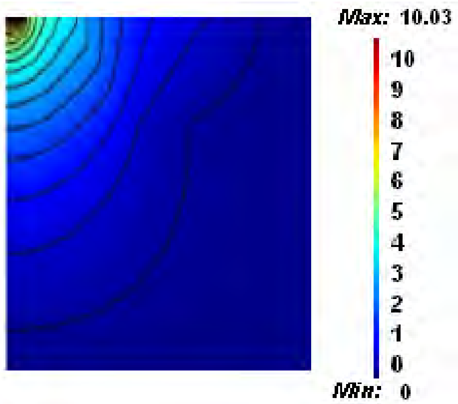

Figure 3. Electric potential field.

The calculated arc voltage concerns only the positive column voltage drop. To compare with arc voltage measurements, it is necessary to add the electrode voltage drops to the value we have obtained. This voltage drop is quite low due to the high temperature and then to the

high electric conductivity. The plasma is accelerated on the axis toward the anode and it is also constricted because of the electromagnetic forces. They take part in the stabilization of the plasma column. High temperatures on the axis also contribute the acceleration of the plasma whose maximum velocity is 256 m/s. The plasma temperature reaches 22200 K at the electrode tip because of the high current densities. In this case, the electric input power is more than 1 kW. The shape of the isotherms at the anode vicinity depends mainly to the boundary condition. A better simulation of the anode could be obtained considering the entire metallic electrode and performing heat transfer inside.
Figures 4 show the temperature field of the plasma.

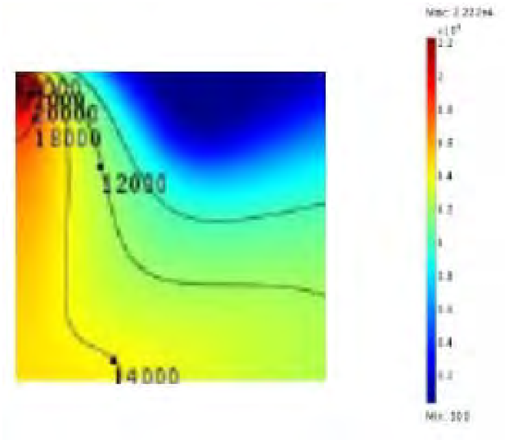

Figure 4. Temperature field

Figure 5 show electric potential field of the plasma.

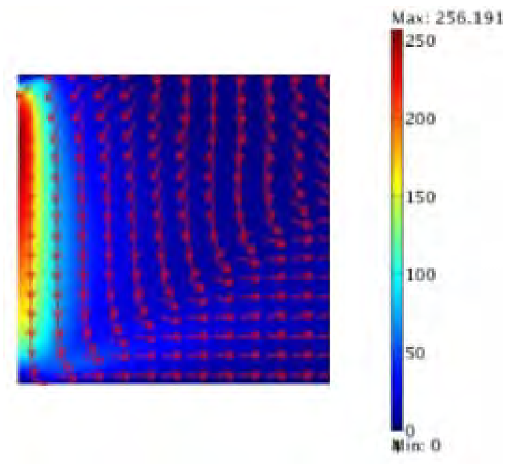

Figure 5. Velocity field and flow direction (arrows).

Figure 6 shows the optical emission spectrum acquired during the plasma process. Three main lines were observed: Be I 440.79nm, 2s2p - 2s4s, Be I 457.26nm, 2s2p - 2s3d and Be I 825.40 nm, 2s2p - 2s3s. The intensity of the observed spectral lines emitted by the plasma is proportional to the population of the upper level, to the transition probability and to the energy of the quantum [8].

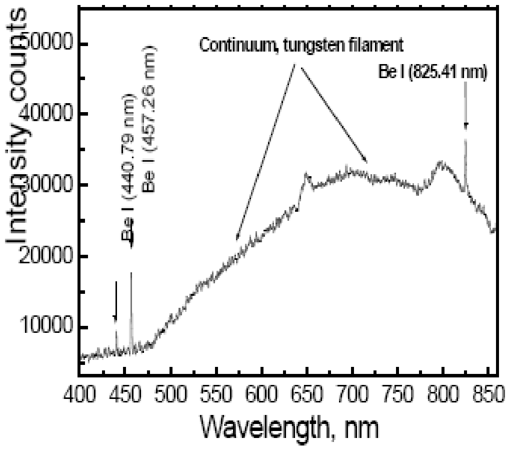

Figure 6. Optical emission spectrum of Be plasma

Image in Figure 7 show the structure of beryllium layers deposited by TVA technique; it is noticed that film obtained by TVA is quite smooth. X-ray diffraction studies have also proven highly ordered crystalline structure of TVA-produced films.

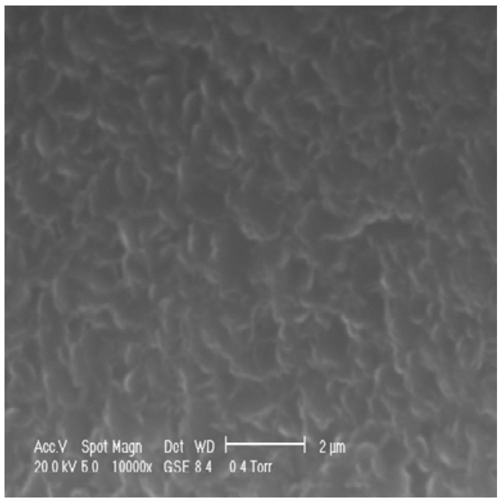

Figure 7. Be coating by TVA method on smooth stainless steel (10000x)

7. Conclusions

In this paper we have demonstrated the versatility of COMSOL Multiphysics regarding the numerical simulation of the phenomena in Be plasma. We can conclude that Thermoionic Vacuum Arc (TVA) can be used successfully for beryllium film deposition. The developed system for thin film deposition using thermionic vacuum arc (TVA) is a very promising one both to obtain high quality of the film and extreme purity. Because of large number of parameters directly controlling the film quality, TVA will be soon considered as one of the best systems to produce thin films for nanostructures.

8. References

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