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Analysis of the electric field behavior in the vicinity of a triple junction, using finite elements method computational simulations

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ABSTRACT

The authors studied the electric field behavior in the vicinity of a triple junction, composed by metal, vacuum and dielectric parts, using computational simulations. A bi-dimensional model was constructed using ANSYS MAXWELL to analyze the magnitude of the electric field as a function of the contact angles of the materials. The results showed that a field enhancement or reduction could occur in vacuum for certain contact angles. The influence of the dielectric permittivity was also investigated, and the conclusions showed that the maximum electric field enhancement is proportional to the dielectric permittivity.

Introduction

A triple junction is essentially a contact between three materials, i.e., vacuum dielectric and metal. This type of contact is occasionally formed in imperfect dielectric depositions on metallic surfaces, where a vacuum environment is maintained during the deposition process. High intensity electric fields have been observed at the vicinity of metal and vacuum contacts [10,19]. Research has shown that this field enhancement occurs due to the presence of dielectrics at the interface, creating a region of triple junctions [1,17,18]. In the cases where field enhancement was found, dielectric breakdown and unwanted electric emissions were detected [7], causing destructive effects in the area.

Theoretical explanations about the triple junction phenomena were proposed by researchers [12,16], using mathematical models to understand the behavior of electric field E and the role of the dielectrics in the unexpected field enhancement. Values of the field enhancement were then calculated in the vicinity of the triple junction [3,11]. The study of the triple junction became interesting to the cold cathode emitter researchers, once the field enhancement obtained from this phenomenon narrowing the potential of vacuum barrier, increasing the probability of electron tunneling [15], in turn enabling electric current emissions from a metal – vacuum interface.

During this work, a physical model of the triple junction is studied and simulated to evaluate the veracity of the mathematical models for a field emission application. ANSYS MAXWELL (2014) was used to simulate the structure by finite element method (FEM). The field enhancement near the triple junction is investigated as a function of the contact angle of the materials and the potential applied in the metal. The goal is to understand consistently the phenomena in the triple junction, looking for further applications in field emissions components. However, the results in this work can clarify the behavior of the electric field for any other applications which the triple junction can be formed.

Methodology

It is known that the dielectric part plays a very important role in the triple junction effect. To understand the behavior of the electric field at the triple junction, it is necessary to evaluate the influence of the dielectric in the triple phenomena. For this purpose, a comparison between the values of the electric field in the presence

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and absence of dielectric field would be revealing. Thereby, two different models were built in MAXWELL's simulation environment. First, a triple junction composed by metal, vacuum and dielectric was built to obtain the values of the electric fields as a function of the physical parameters of the dielectric. Second, a double junction composed by metal and vacuum was built only as a reference, where the electric field is simulated for the same physical and electrical conditions of the metal present in the triple junction model, but, without the influence of dielectric field. Through the values of the electric field in the absence of dielectric (E_0), and presence of dielectric (E_1), the field enhancement β can be calculated through the ratio of the triple junction electric field and the double junction electric field (E_1/E_0).

The models were made in cylindrical geometries, where the materials are set in the cross-section of a cylinder with height h and radius R. The junction point of both models is set in the z axis. By making the height h much larger then R ($h >> R$), the analysis reduces to a two-dimensional model, being the cross-section the main interest of study. The radius R was set in 1 μm. The two-dimensional models of the triple and double junctions are shown in Fig. 1a and b respectively.

To delimitate the different parts of the junctions, variables were created in MAXWELL 2014 to parameterize the contact angles. The metal and the vacuum parts of the junctions had their contact angles α and θ_1 defined by the variables "Alpha" and "Theta1" respectively. For the dielectric part in the triple junction, the contact angle θ_2 was defined by the variable "Theta2". Both models were designed inside a vacuum section, where the boundary conditions were stated to restrict the simulation area. In all boundary regions, the applied electrical potential was referenced to the zero potential in the infinity.

Despite the fact that the electric field will be simulated for all boundary regions, it is necessary to analyze the field intensities in a much smaller area, to avoid edge effects in the results. Thus, a semicircular probe with radius r << R was inserted in the models. For a good precision of the results, the probe radius r was set with r = 0.1 nm. This way, the analysis of the junctions will be made with the electric fields obtained nearby the semicircular probe, ensuring that the edge effects won't be present in the further analysis. The semicircular probes are shown in the Fig. 2a and b.

Seeking to a mesh refinement in the boundaries of the probe, a second area was introduced in the models to enable this operation. The refinement areas can be seen in Fig. 2a and b. To guarantee good mesh operations over the probe boundaries, the refinement areas were made in a semicircular geometry with a radius two times bigger than the probe radius (0.2 nm). The mesh refinement over the interest region allows a better resolution of the electric field, reducing the numerical calculation errors near the probe. The meshes were created over the role model and over the refinement areas for both models, and the mesh plots can be seen in Fig. 3a–d.

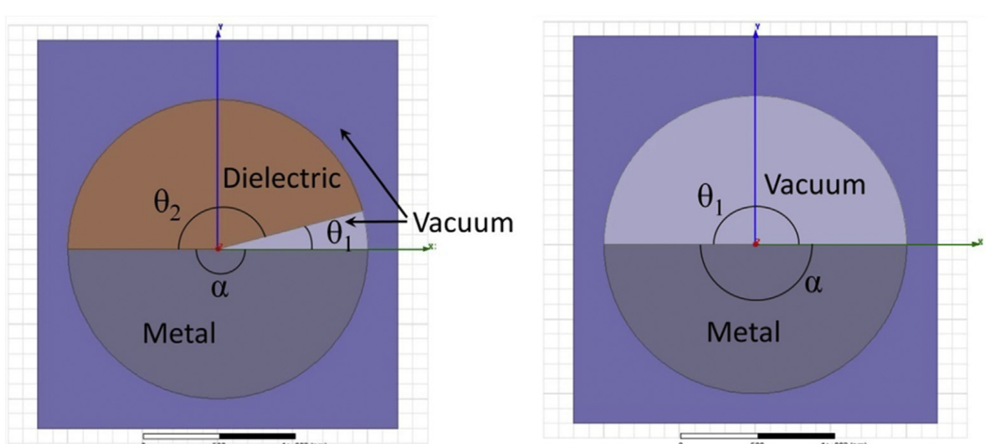
Smaller mesh elements were obtained next to the probe (Fig. 3c and d), which implies in more precise values of the electric field in the region, in the cost of more computational time for the resolution. However, in the regions far from the probe a crude mesh was obtained with bigger mesh elements (Fig. 3a and b), avoiding long computational time of resolution in a non interest region of analysis.

Geometric variations of the junctions were obtained by the parameterization of the variables of the models. In the triple junction model, three parameterizations were made: First, the variable containing the values of the dielectric contact angle was programmed to vary in the range of $5^\circ < Theta2 > 175^\circ$ in a 5° step. Second, the applied potential in the metal *Vmetal* was parameterized to vary between five different values (1, 2, 3, 4 and 5 V). At least, the dielectric permittivity ε_r was parameterized to obtain four different values (5,75; 9; 11 and 13). The idea of the parameterizations is to observe the variations of the electric field in the triple junction in function of dielectric contact angle θ_2, and it's field enhancement in function of the dielectric permittivity. For double junction, the same parameterizations of *Vmetal* were made, seeking the same geometrical and electrical configurations in both models. The metal contact angle *alpha* was maintained constant in the value of 180° for both models. The metal region of the junctions were set as a perfect electrical conductor (PEC), having its conductivity tending to infinity. The vacuum region of the junctions were set as a perfect vacuum, been a lack of material.

The convergence criteria was set as the error between iterations, validating the results when this criteria is less than or equal to 1%. The stoppage criteria was defined with 10 steps, avoiding system crash due to divergences issues between interactions. Both models were configured with the same convergence and stoppage criteria, allowing a constant simulation condition for all geometric configurations of the junctions.

Results and discussion

The result of the electric field in a double junction can be seen in Fig. 4, where the double junction model was simulated for five



(a) Triple junction (b) Double junction

Fig. 1. Two-dimensional models.