Simulation of Photonic Crystals Particle Filling by Electrospray.

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Abstract: Photonic crystals are widely used in optical applications as waveguides and band filters. Filling the periodic structural material of photonic crystals with other materials is very useful in order to change the optical properties of the devices. In this paper electrostatic COMSOL simulations describing an electrospray deposition of particles in macroporous structures are performed.

Keywords: Photonic crystals, Electrospray, nanoparticles.

1. Introduction

The periodic structure of a photonic crystal which is often made of macroporous silicon, is used, besides of optical application, as a mould to build other structures from a different material, in microfluidic circuits, as micro chemical reactors for example.

Filling photonic crystals with other materials is very useful in order to change the physical properties of the devices. There are different ways to fill the photonic crystals with metals, most of them use electroplating and microfluidic related processes [1].

Electrospray is a deposition procedure process employing electric field to disperse a liquid from a needle into a fine aerosol [2].

The aim of this project is to check the capability of electrospray as a technique to fill photonic crystals with gold nanospheres. This technique is cost effective, faster and generates fewer waste products than other commonly used techniques. Electrospray of metallic, organic and magnetic particles [3] is useful for many applications like micropatterning, sensing and mass spectrometry. The simulations results we are looking for are aimed to estimate the charged particle motion through the crystalline structure, the interactions due to the electrical field between the electrospray source, the silicon/alumina structure and the back-electrode.

Simulation is a very helpful tool to validate the deposition conditions before actually using real macroporous silicon samples which are expensive to produce in terms of time consuming. In order to check preliminarily the procedure we have also performed experiments with alumina samples.

2. Electrospray and macroporous silicon structure simulation

The first simulation includes a macroporous structure with dead end holes (fig. 1). Electrostatic force is studied to analyze the particle tracing. The positive charged particles will follow the electrostatic field lines. Hence, electric field and potential plots are identified in different sections of the simulated structure and for different topologies, as shown in the following subsections.

2.1 Rear contact

The main structure we have considered is a silicon block of $12x10^{-5}$ m $3,8x10^{-5}$ m $3,8x10^{-5}$ m with rectangular holes of $2x10^{-12}m^2$ and 1x10-4m depth filled with air. These holes cross a part of the depth of the photonic crystal. In the top part of the structure there is a ring that helps the spreading of the particles as shown in fig.1. A point simulating the tip of the needle used in the electrospray experiments is the top electrode, and the voltage is set to 7000 volts. The second contact is placed in the rear part of the photonic crystal with -7000 volts. With all this conditions a simple simulation showing the electrical field was done.

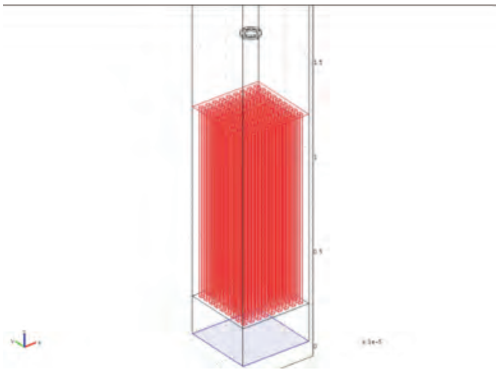

Figure 1. Structure of the photonic crystal with no trespassing holes and ring.

We realize that the ring helps to redirect the particles, homogenizing and focusing the beam, as shown in fig. 2.

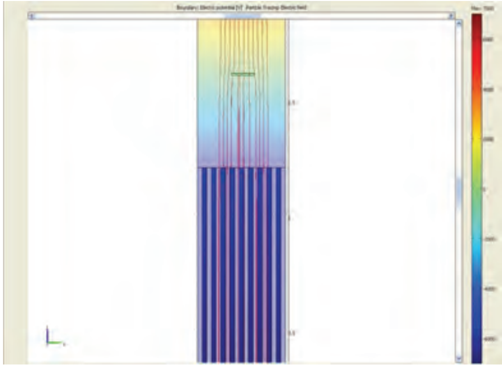

Figure 2. Structure of the photonic crystal with ring and particle tracking.

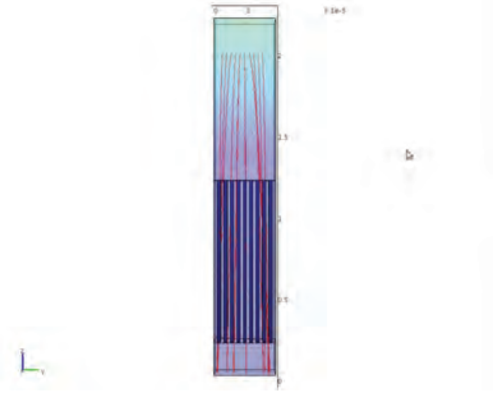

Figure 3. Structure of the photonic crystal without ring and particle tracking.

As seen on fig.3, where particle tracing is shown, some of the particles go to the holes and few of them go directly to the crystal, but near to the holes.

To analyze the electric field, one cross section at few nanometers from the beginning of the photonic crystal (from the top) is done. With this plot, is possible to check the electric field around and inside the holes, as shown in fig.4.

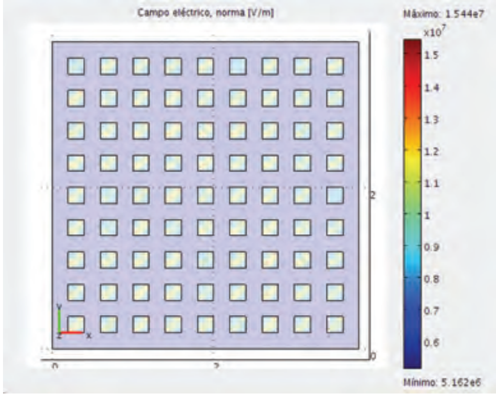

Figure 4. Electric field inside and around the holes.

Tracing a line that crosses diagonally the holes in the same plane, it's possible to simulate the electric field that shows large spikes attracting the particles, as shown in fig.5.

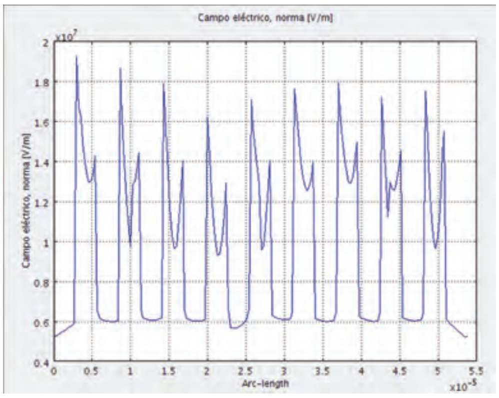

Figure 5. Electric field in a line that crosses the holes of the photonic crystal.

Some particles are attracted to the top silicon parts. This was experimentally observed in some electrospray depositions on uneven surfaces, as shown in fig.6.

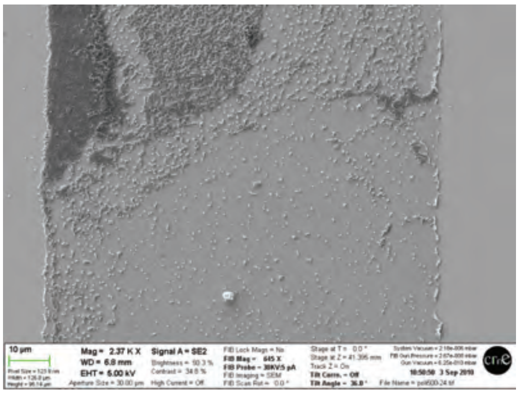

Figure 6. Polystyrene particles preferentially attracted to aluminum spikes over a silicon substrate.

2.2 Bottom contact

To study the possibility of "guiding" the particles inside the holes, the next situation was a photonic crystal with an electrical potential in the bottom inside the holes. The main structure is a silicon block with rectangular holes filled with air. These holes were crossing a ¾ of the photonic crystal.

The top positive electrode is the same than before but the other contacts are placed in the bottom of the holes of the photonic crystal with -7000 volts. These contacts in the bottom of the holes are not physically made. With all this conditions a simple simulation showing the electrical field is done.

A cross section at few nanometers from the beginning of the photonic crystal (from the top) was done. Our conclusion is that there are not large differences between the two arrangements for the contacts.

Tracing a line that crosses perpendicularly the holes in the same plane, it's possible to check the big spikes in the electric filed that attract the particles, as shown in fig.7.

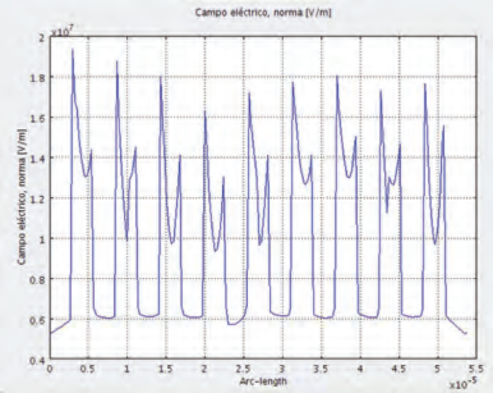

Figure 7. Electric field in a line that crosses the holes of the photonic crystal.

3. Alumina experiments

In order to do a first approach to experimental measurements a porous alumina sample was used. First of all, a simulation with a simple model of alumina is done. The basic model is a cubic part of alumina with holes crossing the whole block, as shown in fig. 8.

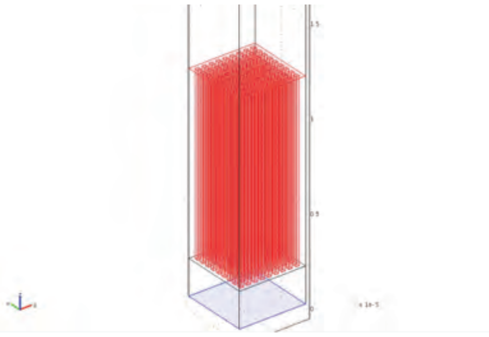

Figure 8. Structure of porous alumina.

The voltages are applied in the top section of the structure 7000 volts and -7000 volts in the bottom of the structure.

A cross section at few nanometers from the beginning of the photonic crystal (from the top) is done, as shown in fig. 9. However the results shown in Figure 9 may look similar to the ones shown in Figure 4, the truth is that the scale is different and hence the field distribution in Figure 9 is more intense than the one shown in Figure 4

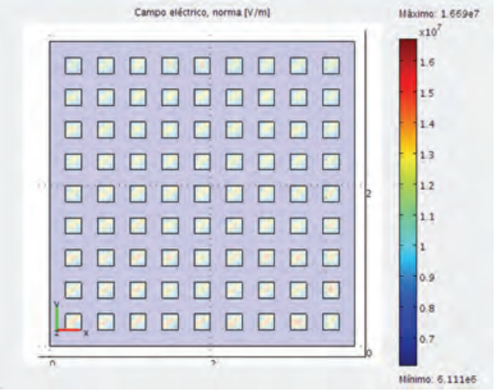

Figure 9. Electric field inside and around the holes.

Tracing a line that crosses perpendicularly the holes in the same plane, it's possible to check the spikes in the electric field that attract the particles, as shown in fig.10.

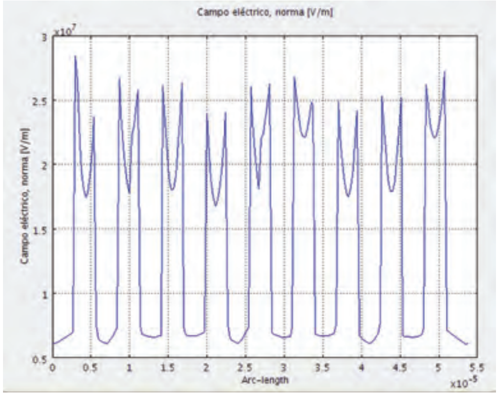

Figure 10. Electric field in a line that crosses the holes of the photonic crystal.

As can be seen the spikes are smaller and this situation helps the redirection of the particles to the hole. The next step is particle tracking considering the electric field as governing force, as shown in fig.11.

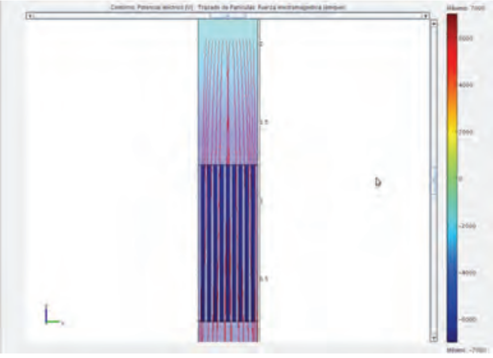

Figure 11. Particle tracking of some particles with electric field as main force.

As seen in the fig.12, the particles tend to fall into the holes. First they go directly to the corner between the holes and the photonic crystal, and it's possible that some of them finally fall into the hole

In a real experiment some polystyrene particles were pushed through a porous alumina with non uniform 250nm holes, as shown in fig.12.

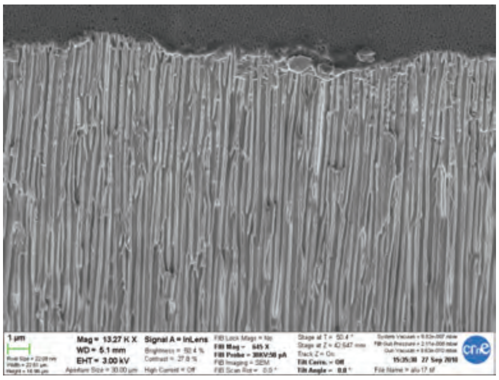

Figure 12. Vertical cross section of the porous alumina with non uniform holes.

Some particles fall into the holes of the alumina, as shown in fig.13 and fig.14.

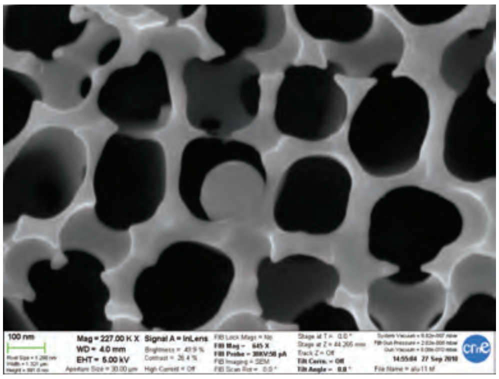

Figure 13. Polystyrene particle inside an alumina hole.

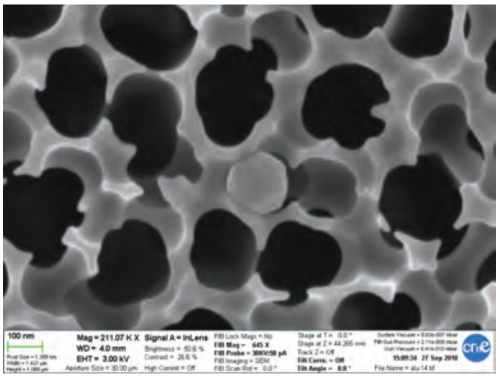

Figure 14. Another polystyrene particle inside an alumina hole.

7. Conclusions

The main conclusion is that it’s plausible to fill the holes of photonic crystals with electrospray, although not all the particles will fall into the holes directly. The fact that the photonic crystal is an isolator or a conductive material is not so important. Simulations also show that the particles tend to go directly to the corners, so it’s possible that some of them fall into the holes although some of them get stacked in them.

8. References

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9. Acknowledgements

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