FEM Modeling of Conductivity and Electrical Coupling in Polymeric Nanocomposite Material

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Abstract—**We propose an approach useful for the evaluation of electrical conductivity of nanocomposite materials. We consider the modeling of a polymeric matrix with gold nanoparticles by evaluating the electrical coupling of spherical gold nanoparticles embedded in chitosan polymer. The electrical coupling is generated by a voltage signal which provides a current distribution which is function of the gold nanonoparticles filling factor. We use a properly designed finite element method (FEM) tool.**

Keywords- FEM Modeling; Nanocomposite Materials; Polymers; Gold Nanoparticles.

I. INTRODUCTION

Polymers such as Su-8 [1]-[2], polydimethylsiloxane (PDMS), polyvinylidene fluoride (PVDF), polystyrene (PS), (PMMA), polyethylmethacrylate-comethylacrylate (PEMMA), topas, polyvinyl alcohol (PVA), polyanyline, polycarbonate (PC), and chitosan, are actually commonly used for sensor and actuators including MEMS technology. MEMS implementations are oriented on polymeric materials with metallic/organic micro and nano inclusions. Metallic/organic nanostructures added in polymeric materials generate nanocomposite materials (NMs). In particular, NMs strongly absorb the light becoming technologically interesting, since the light absorbed by the nanostructure can be locally released as heat. Therefore, researchers have utilized strongly absorbing metal nanostructures for a variety of applications, such as localized photothermal ablation treatment of cancer [1]-[3]. Conversely, the ability of the metallic nanocomposite to strongly scatter light is critical for optical sensing, tagging and imaging applications [4]-[5]. Applications involving light scattering are numerous, and include the use of metal nanostructures as contrast agents in cancer cell imaging [6]-[7], the use of composite metal nanostructures for optical labeling and tagging applications [8]-[11], and the use of metal nanostructures as optically active strain sensors [12]. All the above listed NMs applications can be implemented in robotic systems including RF/microwave and radiation applications [13]-[14]. One way to characterize NMs is to evaluate the conductivity. In particular we focus on the study of the conductivity of chitosan polymer with gold nanoparticles (see experimental atomic force microscopy image reported in Fig. (a)) by analyzing the electrical coupling of gold nanoparticles embedded in the polymeric matrix by means of a 3D finite element method tool (FEM) previously used for photonic crystal design [15].

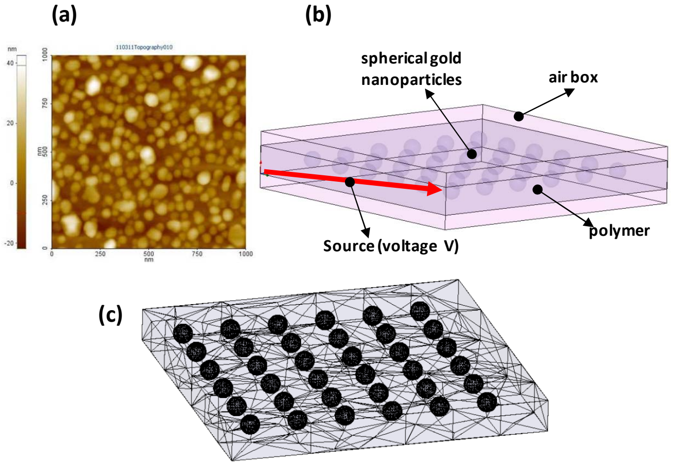

Fig. 1. (a) AFM image of chitosan polymeric material with gold nanoparticles. (b) 3D FEM Modeling. (c) 3D FEM mesh.

II. 3D FEM MODELING AND RESULTS

The FEM modeling [15] considers a chitosan 10 μm x 10 μm x 1 μm polymeric box (unit cell) with gold spherical nanoparticles embedded in the box. In order to define a gold particles filling factor, the radius of the gold nanoparticles changes according to the controlledtechnology. We assume the monodispersion hypothesis. As consequence of this hypothesis, the spherical metallic nanoparticles assume the same distance as in indicated in Fig. 1 (b). A voltage signal excites the unit cell from an input port as indicated in Fig. 1 (b), and the unit cell is embedded in an air box which isolates the NMs from external electromagnetic interactions. In Fig. 1 (b) are illustrated the FEM mesh used for the simulations. The voltage signal allows to transfers the current **J** inside the unit cell: the electric current flows helped by means of the electrical coupling of the gold nanoparticles. As observed in Fig. 2, the current distribution increases by increasing (gold particles filling factor). We observe that we can modify the filling factor by two ways: the first one is to increase the density of particles,and, the second one is the size increase of particles until the limit case of Fig. 2 (b). The case of Fig. 1 (a) proves that for low filling factors (small diameters of the gold nanoparticles) the unit cell can be non conductive, and, the limit case of Fig. 2 (b) indicates a maximum of the current J. This maximum is obtained by spherical particles tangent to each other (maximum filling factor) allowing to transfer the current as in quasi-continuous metallic layers. These results are useful in order to design NMs with electrical connections integrated in MEMS/NEMS systems including the case of gold nanoparticles semi-embedded in the polymeric matrix as shown in Fig. 3.

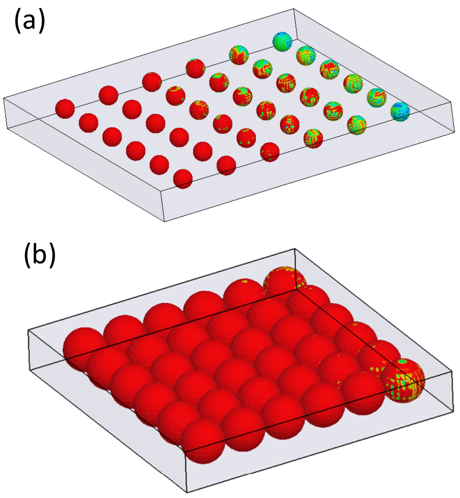

Fig. 2. (a) 3D FEM simulation of density of current **J** distribution calculated on the surface of gold nanoparticles. (a) low filling factor, and (b) high filling factor of spherical gold nanoparticles in a chitosan polymeric matrix.

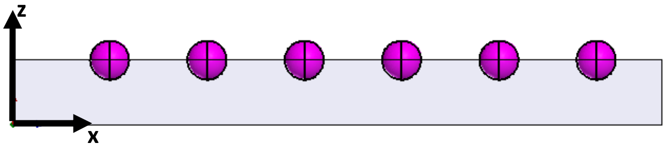

Fig. 3. Perspectives: modeling of spherical gold nanoparticles semi-embedded in a polymeric material.

III. CONCLUSIONS

The proposed FEM simulations proves that it is possible to obtain innovative conductive materials by using nanocomposite materials such as chitosan with gold nanoparticles. The FEM modeling can be used also to design complex circuits such as MEMS devices made by nanocomposite materials also when the monodispersion is not obtained and for gold nanoparticles arranged on the polymeric surface as happens by applying laser texturing techniques. The comparison of the FEM results with the experimental ones are under investigation and will presented in the extended version of the paper.

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