Modeling Photonic Properties of Quasi-random Nanoporous Anodic Alumina for Application in Organic Devices

Josep Ferré-Borrull, Mohammad Mahbubur Rahman, Pedro Granero, Lluis F. Marsal, Pilar Formentín, Josep Pallarès
Nano-electronic and Photonic Systems, NePhoS
Universitat Rovira i Virgili
Tarragona, Spain
josep.ferre@urv.cat

***Abstract*—We report the progress on the numerical modeling of the photonic properties of nanostructures based on the nanoporous anodic alumina. With the use of FDTD we show that the quasi-random structure of the material possesses a photonic stop band. We also show the light trapping effect caused by the nanostructuring of organic solar cells using nanoporous anodic alumina as template.**

Nanoporous Anodic Alumina, Modeling,Photonic Stop Band, Organic Photovoltaics

I. Introduction

Nanoporous anodic alumina (NAA) is a material obtained by the electrochemical etching of aluminum in acid electrolytes with greatly increasing interest in nanotechnology [1,2]. When produced in the adequate conditions NAA shows a porous nanostructure with a self assembly of the pore distribution. The size of the pores and the average interpore distances in such structures can be modulated from a few nanometers to some hundreds of nanometers by combining different anodization conditions, acid electrolytes. Pores in the structures grow perfectly parallel with lengths from shallow pores to several hundreds of microns. Given these possibilities in shaping this nanostructure, NAA has found a great wealth of applications.

Furthermore, the self-assembled nature of NAA is close to that of a Photonic Crystal: it consists of a 2-D triangular lattice of cylindrical parallel pores in an aluminum oxide matrix. However, although the periodicity can be made artificially perfect by using nanoindenting procedures, usually, NAA shows symmetry breaking points that produce domains of random size and orientation. In this sense, we have called such a structure *quasi-random*[3]. In this communication we review the progress achieved in the group NePhoS in the numerical modeling of the photonic properties of NAA. In particular, we use the finite-differences time-domain (FDTD) method to predict the existence of photonic stop bands in the structure in much the same way they are formed in photonic quasicrystals. Then, we use the finite-element method to study the light absorption properties in nanostructured organic solar cells that model those that can be obtained using the NAA as a template.

II. Results

A. Photonic Stop Bands in Nanoporous Anodic Alumina

Fig. 1 shows a typical example of the quasi-random distribution of the pores on NAA. It can be seen that this structure is similar to that of a 2D quasicrystals, which exhibit photonic stop bands even with smaller refractive index contrast that its periodic counterparts because of its higher rotational symmetry.

In order to investigate the existence of a photonic stop band we have applied FDTD to simulate the propagation of a wide-band pulse through a given length L of NAA in a direction perpendicular to the pores. The data for the pore distribution was obtained from SEM images of real samples such that in Fig. 1. The simulations permitted to obtain the transmittance spectra but given the random nature of the pore distribution, it was necessary to calculate the ensemble average of the transmittance for a great number of realizations of the nanostructure.

Fig. 2 shows the transmittance spectra for TE polarized light for different pulse path L, expressed in terms of the average interpore distance a. The vertical lines indicate the wavelength range of the photonic band gap of a periodic photonic crystal with a triangular lattice with the same refractive indices and lattice constant a. It can be seen that transmittance through the NAA shows a clear stop band at the same wavelength range.

B. Light Ttrapping and Absorption in Organic Solar Cells Nanostructured by NAA

One of the applications of NAA is as a template to shape at the nanometric scale organic photonic devices such as solar cells. Light interaction with such nanostructures cannot be modeled by the usual methods of the transfer matrix for stratified media given the non-planar geometry and the subwavelength dimensions. We have used the finite-element method to obtain the absorption map on a 2D model of a nanostructured organic solar cell.

The cell model consisted of an interdigitated structure of two organic semiconductors, P3HT and PCBM. We studied the absorption at P3HT, where excitons are generated that subsequently diffuse to the interface where charge separation occurs. Fig. 3 shows the absorption map on the structure for a wavelength of 450 nm for an inter-digit spacing of 250 nm, 400 nm and 500 nm. It can be seen that for these sizes, which can be obtained with NAA template-assisted nanostructuring, spacing is of the order of wavelength and light forms standing waves in the structure that result in an increase of absorption.

The results for the complete spectrum are shown in Fig. 4, where the total absorption as compared with the absorption of a two-layer planar cell with the same quantity of P3HT is presented. Although for some wavelengths absorption is smaller, for others it is increased because of the light trapping effect observed in Fig. 3.

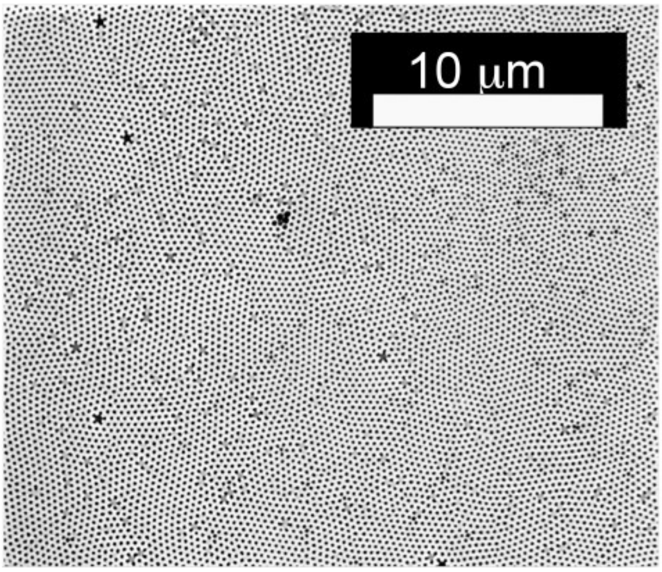

Figure 1. Example of a typical quasi-random nanoporous anodic alumina structure

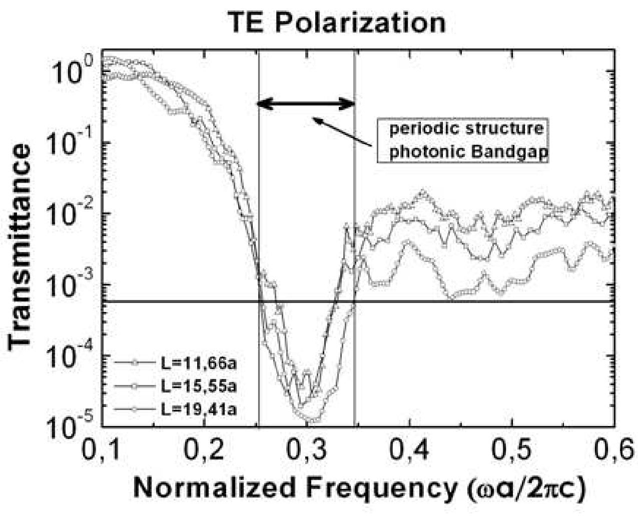

Figure 2. Transmittance in direction normal to the pores of a nanoporous anodic alumina. The minimum in transmittance appears at the same wavelength range than the photonic bandgap in a periodic structure with lattice constant equal to the average interpore distance *a*.

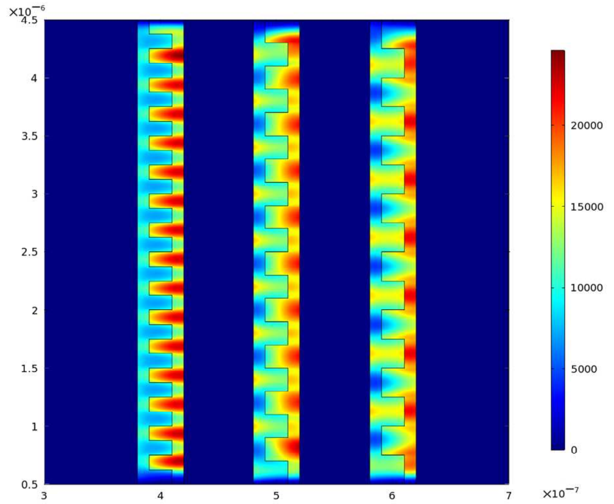

Figure 3. Absorption maps of 2D interdigitated organic solar cells for a wavelength of 450 nm. The inter-digital distances are 250 nm (left), 400 nm (center) and 500 nm (right). The units of the axes are microns.

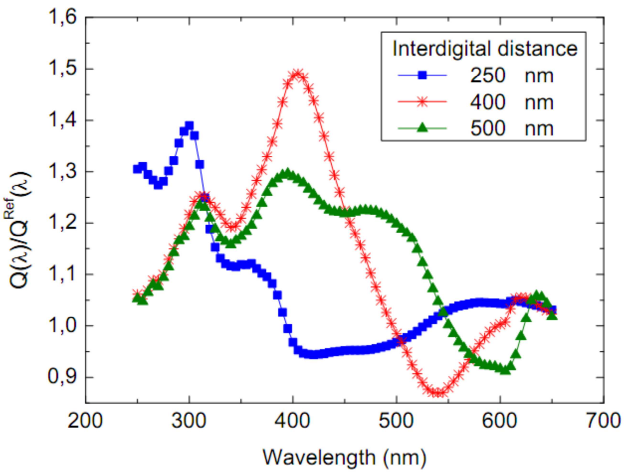

Figure 4. Spectrum of total absorbed energy of the interdigitated organic solar cells with respect to the total absorbed energy by a planar bilayer cell with the same amount of material.

ACKNOWLEDGMENT

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