Numerical Modelling of Electric Current Flow in Nanocrystalline 2D Carbon-Palladium Structures via Homogenization Method

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Abstract. We present a model of electric current flow through a two-dimensional palladium-carbon nanocomposite material and study the electrical conductivity of such material. The asymptotic homogenization theory and the finite element method are applied to analyse and solve the problem. The results of numerical computations are compared with the experimental data.

Keywords: carbon, palladium, nanocomposite, homogenization, FEM
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INTRODUCTION

The problem of finding effective physical properties for composites or non-homogeneous materials is one of the essential problems in many physical and material sciences. Small regions of non-homogeneity of the material covering all of its volume, with diameters of these non-homogeneities much smaller than this volume, are the cause of serious difficulties in analytical and numerical study of the problem. In such cases, one can replace such non-homogeneous material with a homogeneous one which has identical macroscopic properties.

In this paper we study nanocomposites, which are examples of such non-homogeneous materials, built of nanograins of palladium embedded in a carbonaceous matrix. The properties of nanocomposite materials are different from the properties of their components having characteristics similar to their macroscopic counterparts. In particular, a large number of regions with sizes of the order of a few nanometres has a strong influence on the effective properties of the whole material and their dissimilarity to the characteristics of the material in a macroscopic form.

For the phenomenon of the transfer of electric charges in nanocomposite materials, there are various models used which are connected with the classical approach (cf [1, 2]). In [3, 4] the authors present the model of the one-dimensional nanocomposite material and study the macroscopic parameters of nanocomposite. In this paper we present the model of the electric charges transfer in the two-dimensional nanocomposite material based on a diffusion equation with the homogenization theory applied to obtain the macroscopic properties of the nanocomposite material. We assume that the considered material is isotropic in all respects. This assumption allows us to consider only the two-dimensional problem. The cross-section of such material is shown in Figure 1. In Figure 2 we present a two-dimensional simplified model, considered for homogenization computations, in which the nanocomposite consists of two materials: palladium (white squares) in the form of nanocrystallites and carbon (grey region) forming a matrix in which the nanograins of palladium are embedded.

MATHEMATICAL MODEL

In the proposed two-dimensional model, the C-Pd nanocomposite has a periodic microstructure consisting of palladium nanograins embedded in a carbonaceous matrix (cf Figure 2). We assume that the body occupying the region $\Omega := [0,L]^2$ consists of a finite number of identical periodic square cells with dimension l, where $l \ll L$. We introduce a

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