Modelling of a Time Dependent Electron Diffusion Problem for Nanocrystalline One-dimensional Carbon-Palladium Structures *via* Homogenization

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Abstract. Analytical and numerical phenomena of the electron resistance in the time dependent electron flow in Pd nanocrystals embedded in a carbonaceous matrix are studied. The asymptotic homogenization theory and Finite Element Method are applied to analyse and solve the problem.

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INTRODUCTION

In many physical science problems it is very important to know the effective properties of composites and/or inhomogeneous materials. When small areas of inhomogeneity are covering all of the material and their volume is very small in comparison with the volume of the material it is very difficult to solve analytical problem. In such situation it is proposed to change such inhomogeneous material with a homogeneous one representing the same properties in a macro scale.

We are studying a case of nanocomposite material built of nanograins of palladium placed in a carbonaceous matrix. In two dimensions a schematic representation of such nanocomposite is presented in Fig. 1 and real TEM image of a fragment of such material is presented in Fig. 2.

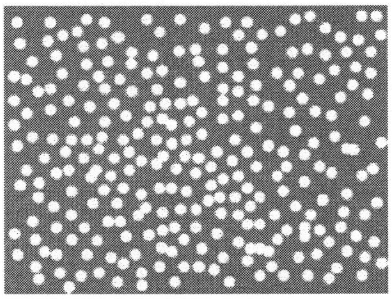

FIGURE 1. A schematic representation of nanocomposite material (grey colour - carbonaceous matrix, white colour - Pd nanograins)

In ideal case such composite material could be seen as periodic structure (see Fig. 3).

Such material is called a two-phase composite material. The problem of conductivity through this material can be explained in many ways. For example some authors [1, 2] suggest that the electrical conductance for the agglomerated metallic particles or the deposited nano-sized thin films depends on the filling factor of the connected and empty spaces. At low filling factor, the particles may be separated individually. The mechanism of conductivity on the thin film can be extensively addressed by a simple tunnelling between localized insulating states that imply a high resistivity

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