Modelling of electron diffusion problem for nanocrystalline one-dimensional structures by homogenization method

W. Bielski [1)], A. Idzik [2)], and P. Kowalczyk [3)]

[1)] Institute of Geophysics, Pol. Acad. Sci., Warsaw, PL,
[2)] Institute of Mathematics, Jan Kochanowski University, Kielce, PL
[3)] Faculty of Mathematics, Informatics and Mechanics, University of Warsaw, Warsaw, PL
wbielski@igf.edu.pl; adidzik@ipipan.waw.pl; p.kowalczyk@mimuw.edu.pl

Summary: Analytical and numerical phenomena of the electron resistance in the electron flow in Pd nanocrystals embedded in a carbonaceous matrix are studied. For simplicity, only the one-dimensional case of the stationary diffusion equation is considered. A solution of the equation with a variable coefficient is presented. The asymptotic homogenization theory is applied to solve and analyse the problem. Effective resistivity coefficients and macroscopic diffusion equation are obtained by this method. Analytical and numerical solutions are presented for pallad and carbon data.

Keywords: diffusion equation, homogenization, pallad–carbon composite, conductivity, resistivity, macroscopic property.

Introduction

In applied physics and engineering, it is good to know the effective properties of composite or inhomogeneous materials. In heterogeneity spread over numerous regions a detailed analysis and numerical approach are very difficult and even impossible. The natural idea is to substitute the real *microscopic* problem by an averaged one, or *macroscopic problem*, with the property that the solution of a real problem differs slightly from the averaged one. A useful technique which allows obtaining accurate results is that of asymptotic homogenization, cf. [1], [3], [4].

A nanowire has a periodic microstructure composed of Pd nanocrystals embedded in a carbonaceous matrix. Our nanowire is a one-dimensional model and the electron flow is described by the one-dimensional diffusion equation. We assume that the nanowire consists of finite number of cells (containing Pd and C) of the length l periodically repeated on the interval [0,L], and the Pd nanocrystal has the length λl in each cell, $\lambda \in (0,1)$. The parameter λ can be estimated by method presented in [5].

We consider the stationary solutions in our model only. The diffusion equation therefore has the form

$$(1) \qquad \frac{d}{dx}\left(\sigma(x)\frac{dn}{dx}\right) = 0$$

where $\sigma:[0,L] \rightarrow \mathbf{R}$ is the electric conductivity, and $n:[0,L] \rightarrow R$ is the charge concentration in the nanowire. The equation is supplemented by the boundary conditions: $n(0) = n_0$, $n(L) = n_L$.

The nanowire has different areas of electric conductivity (for Pd and C60). So we consider the following form of the electric conductivity

$$(2) \qquad \sigma(x) = \sigma_{Pd}\chi_{Pd}(x) + \sigma_C\left(1 - \chi_{Pd}(x)\right),$$

where σ_{Pd} and σ_C denote the conductivities of Pd and C60, respectively, and χ_{Pd} is a characteristic function of the area occupied by the Pd nanocrystals.

Results

A characteristic feature of the homogenization applied to the one-dimensional equation in the divergent form is that an average coefficient is simply the harmonic mean, cf. [1,2].

Thus we obtain the homogenized or *macroscopic* equation and a constant effective coefficient σ^0 :

(3) $$\frac{d}{dx}(\sigma^0 \frac{dn^0}{dx}) = 0,$$

where σ^0 is given by the relation $\frac{1}{\sigma^0} = M(\frac{1}{\sigma(x)})$, and where M is the arithmetic mean, hence the homogenized coefficient σ^0 is a harmonic mean of the coefficient $\sigma(x)$.

In our model therefore the electric conductivity is constant and is equal σ^0. This assumption imply that solution of the equation (3) is of the form $n^0(x) = ax + b$. With the boundary conditions we obtain $n(0) = n_0 = b$. The coefficient *a* is determined by Fick's law

(4) $$J = -\sigma^0 \frac{dn^0}{dx},$$

and is equal: $a = -\frac{J}{\sigma}$.

Acknowledgement

This project is co-financed by the European Regional Development Fund within the Innovative Economy Operational Programme 2007-2013 (title of the project "Development of technology for a new generation of the hydrogen and hydrogen compounds sensor for applications in above normative conditions" No UDA-POIG.01.03.01-14-071/08-00)

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