Numerical Modelling of Mechanical Properties of C-Pd Film by Homogenization Technique and Finite Element Method

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Abstract. The nanomechanical properties of nanostructural carbonaceous-palladium films are studied. The nanoindentation experiments are numerically using the Finite Element Method. The homogenization theory is applied to compute the properties of the composite material used as the input data for nanoindentation calculations.

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INTRODUCTION

We study nanostructural carbonaceous-palladium films (C-Pd films) by means of a numerical simulation of the nanoindentation experiments. Nanoindentation method is designed to measure the mechanical properties of materials such as nanohardness and reduced modulus of elasticity of ultra thin layers.

C-Pd films studied here by nanoindentation were obtained by Physical Vapour Deposition method. These films are built of nanograins of palladium embedded in carbonaceous matrix (see [1]). Knowledge of the mechanical properties of a new type of material is very important because of practical applications of films. C-Pd films could be applied as active layer in many types of sensors due to their chemical, mechanical and physical properties connected to a presence of palladium nanograins and carbonaceous matrix structure. The experimental results of the nanoindentation obtained for several C-Pd films were presented in [2].

The material studied here is a two-phase inhomogeneous nanocomposite material, in which the volume of inhomogeneities is very small in comparison with the volume of the material. The numerical study of such materials presents a very difficult task. Hence to simplify the computations we propose to model this material as a homogeneous one having the same properties. To that end we apply the homogenization technique to compute numerically the estimates of the unknown parameters of C-Pd film: Young's modulus and Poisson's ratio, assuming that the material is isotropic.

The results obtained by the homogenization method are used as the initial conditions for calculation the nanomechanical properties of the C-Pd film. We use the Finite Element Method for the numerical simulation of the nanoindentation experiment. FEM gives many opportunities to study an influence of the form and composition of a material on its mechanical properties. It allows for wider investigations of materials from macro- to nanoscale. For the FEM modelling of nanoindentation experiment, we apply the standard Oliver-Pharr method [3] for the indenter. The preliminary FEM study demonstrated that this method can be applied to simulate the nanoindentation experiment and used to fit experimental load-displacement data obtained in the nanoindentation test.

The computations are performed using the ANSYS program (Ansys, Inc). The materials are modelled as isotropic, elastic solids. The program iteratively computes the best fit of the nanomechanical parameters of the C-Pd film starting from the initial data obtained by homogenization method.

For the detailed description of nanotechnology and nanoindentation we refer the reader to [4, 5, 6].

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