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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MODEL OF NANOINDENTATION EXPERIMENT

As we already mentioned the C-Pd film is modelled as homogeneous isotropic elastic solid using the Hooke's law $\sigma = ae$, where σ is the stress, a is the elastic modulus of the material and e is the strain that occurs under the given stress (cf (2)). In our model the C-Pd film is deposited on a glass substrate and is indented by means of a diamond indenter as shown in Fig. 1.

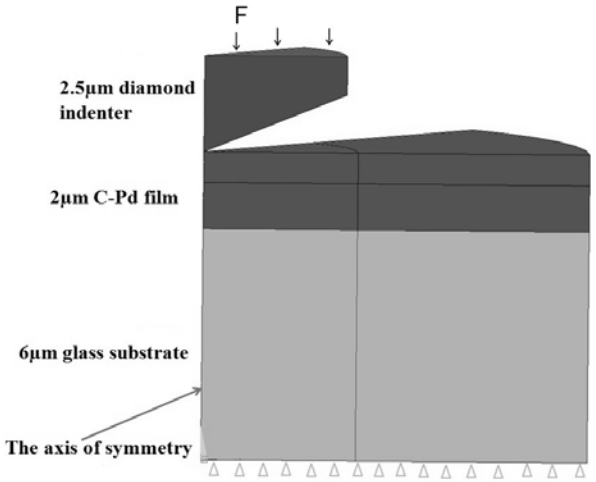

FIGURE 1. Axisymmetric model of the C-Pd film and indenter tip

The thickness for the C-Pd film is 2 μm and the glass substrate is 6 μm. In order to eliminate the influence of substrate effects on the results in the model the film of more thickness was used comparing to the actual size. In order to properly simulate the nanoindentation experiment a contact analysis was applied. For this purpose, contact elements were placed along the top surface of the film and target elements were used along the bottom surface of the tip. The contact is assumed to be frictionless. The indentation was simulated by applying the displacement boundary conditions in the y-direction to the nodes along the upper surface of the tip. The top surface of the tip was constrained in all directions. Since the problem possesses symmetry along the y-axis, only 1/8 of the geometry was modelled. Displacements along the symmetry planes were constrained. As a result of calculations we obtain a force-displacement curve. Force and penetration depth diagram provides information about e.g. the elastic and plastic deformation with increasing and decreasing load and permits to calculate nanohardness and reduced modulus depending on penetration depth.

HOMOGENIZATION

We briefly describe the mathematical model of isotropic, elastic solid used in the homogenization procedure. We treat the C-Pd film as a linear elastic body consisting of isotropic material, which occupies a region $\Omega \in \mathbb{R}^3$. The governing equation of linear elasticity for such material in an equilibrium can be written in the form

$$\frac{\partial \sigma_{ij}}{\partial x_j} + f_i = 0 \quad \text{in} \quad \Omega, \tag{1}$$

where $\sigma = (\sigma_{ij})$ is the stress tensor and $f = (f_i)$ is the external force field. The proper boundary conditions are assumed according to the previous section. We use the standard Hooke's law as the constitutive equation relating stresses and strains

$$\sigma_{ij}(u) = a_{ijkm} e_{km}(u), \tag{2}$$

where a_{ijkm} denotes the elasticity tensor end e_{km} is the strain tensor relating strains and displacements $u = (u_i)$ as follows

$$e_{km}(u) = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_m} + \frac{\partial u_m}{\partial x_k}\right). \tag{3}$$

In the considered case of the isotropic material the elasticity tensor can be written as follows

$$a_{ijkm} = \lambda \delta_{ij}\delta_{km} + \mu(\delta_{ik}\delta_{jm} + \delta_{im}\delta_{kj}), \tag{4}$$

where λ and μ are known as Lamé constants related to the Young's modulus E and Poisson's ratio ν by the formulas

$$\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}, \qquad \mu = \frac{E}{2(1+\nu)}. \tag{5}$$

Now we briefly describe the homogenization technique used to compute the mechanical parameters describing the C-Pd film as a homogeneous material. For detailed study of the homogenization theory we refer the reader to [7, 8, 9].

The C-Pd films are built of nanograins of palladium embedded in carbonaceous matrix, hence the two-dimensional plane cut of the material can be schematically seen as in Fig. 2 (we present the 2-d picture only for the simplicity of visualisation). In the ideal case such composite material can be treated as having the periodic structure (see Fig. 3 for 2-d schematic picture).

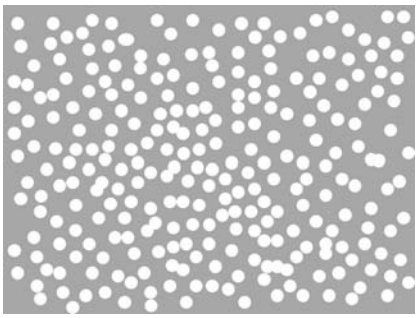

FIGURE 2. Schematic 2-d representation of the nanocomposite material (grey colour - carbonaceous matrix, white colour - Pd nanograins)

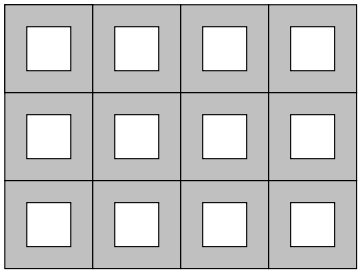

FIGURE 3. Periodic structure modelling the material (grey colour - carbonaceous matrix, white colour - Pd nanograins)

In order to apply the homogenization method we assume the C-Pd film is characterized by such periodic microstructure. It means that the large body with a characteristic dimension L consists of a finite number of periodic cubic cells with characteristic dimension l, where $l \ll L$; we introduce a small parameter $\varepsilon = l/L$. Moreover we assume that the periodic cell contains palladium nanocrystal in the form of a smaller cube surrounded by carbon.

The structure of C-Pd film imposes the following formula for the elasticity tensor

$$a_{ijkm}(x) = a^{Pd}_{ijkm}\chi_{Pd}(x) + a^{C}_{ijkm}(1-\chi_{Pd}(x)) \quad x \in \Omega, \tag{6}$$

where a^{Pd}_{ijkm} and a^{C}_{ijkm} denote the elasticity tensor of palladium and carbonaceous matrix respectively (both defined by (4) with respective values of Lamé constants) and χ_{Pd} is a characteristic function of the region occupied by the palladium.

In a periodic setting we introduce the microscopic variable $y = x/\varepsilon$ (while x is referred to as macroscopic variable) and assume that $a^{\varepsilon}_{ijkm}(x) = a_{ijkm}(x/\varepsilon) = a_{ijkm}(y)$ is Y-periodic, i.e. periodic with respect to the y-variable with a period being a unit cell $Y = [0,1]^3$.

Thus we now study the problem (cf (1) and (2) combined)

$$\frac{\partial\left(a^{\varepsilon}_{ijkm}e_{km}(u)\right)}{\partial x_j}+f_i=0 \quad \text{in} \quad \Omega. \tag{7}$$

The essential point of the homogenization method is to eliminate the microscopic variable by passing to zero with the small parameter ε (cf [8]). Applying the homogenization procedure we obtain the macroscopic version of the equations (7) for the homogenized material

$$a^{hom}_{ijkm}\frac{\partial e_{km}(u)}{\partial x_j}+f_i=0 \quad \text{in} \quad \Omega, \tag{8}$$

where

$$a^{hom}_{ijkm}=\int_Y a_{ijkm}(y)-a_{ijrs}(y)e_{ijrs}(\omega^{rs})\,dy \tag{9}$$

is the effective (homogenized) elastic tensor, which is computed using high order numerical quadrature. The unknown Y-periodic vector functions ω^{rs} are determined solving numerically by FEM the following local problem with Y-periodic boundary conditions

$$\frac{\partial\left(a_{ijkm}(y)e_{km}(\omega^{rs})\right)}{\partial y_j}=-\frac{\partial a_{ijrs}(y)}{\partial y_j} \quad y\in Y. \tag{10}$$

Now assuming that the homogenized material is isotropic the estimates of Young's modulus and Poisson's ratio of the C-Pd film are computed from the homogenized elastic tensor a^{hom}_{ijkm} (cf (4) and (5)).

CONCLUSIONS

In this work we propose the numerical simulation method for the nanoindentation experiment. The necessary input data for simulations is obtained by the homogenization method. We use FEM to compute the effective (homogenized) parameters of C-Pd films and to simulate the nanoindentation process. The preliminary numerical results are in satisfactory agreement with the experimental ones. This shows the usefulness of the averaging procedure we propose for the considered problem and justifies the method used for the numerical simulations.

ACKNOWLEDGMENTS

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