FEM application in studies of mechanical properties of C-Pd film

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INTRODUCTION

Topography, structure and contents of Pd in carbonaceous – palladium nanostructural C-Pd films (C-Pd) have a significant impact on their nanomechanical properties. Such 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. One of a new methods of investigations of nanomechanical properties is nanoindentation method. C-Pd films studied here by nanoindentation was obtained by Physical Vapour Deposition (PVD) method. The films are built of nanograins of palladium embedded in carbonaceous matrix. The shape and the size of Pd nanograins are important factors determining mechanical properties of C-Pd films. Similarly, structure of carbonaceous matrix also affects such properties. The influence of a number and a distribution of nanograins embedded in a carbonaceous matrix in the nanoindentation experiment was analyzed.

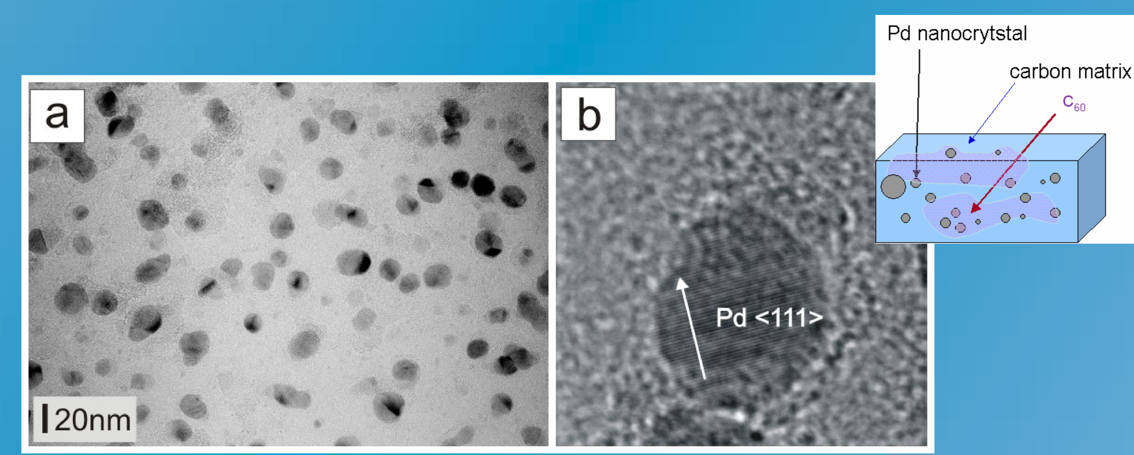
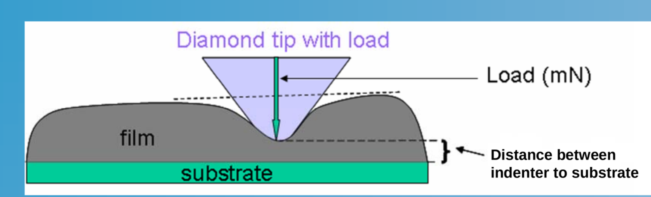


Fig. 1 TEM image of carbonaceous-palladium film (b) high resolution image from Pd crystallite

NANOINDENTATION METHOD



Nanoindentation is designed to measure the mechanical properties of materials such as nanohardness and reduced modulus of elasticity of ultra-thin layers.

The nanohardness of the sample (HN) is determined using the formula: $HN = \frac{F_{max}}{A_c(h_c)}$

where F_{max} is the maximum applied load and Ac is the cross-sectional area corresponding to the depth hc. The determination of the contact depth hc is given by:

$h_c = h_{max} - 0.75\frac{F_{max}}{S}$ where S is the contact stiffness $S = \frac{dF}{dh}$ with dF/dh being the slope of the unloading curve at the initial point of unloading.

The reduced modulus Er is a measure of the elastic properties of the tip-sample system and can be calculated from the load-depth curves according to the formula: $E_r = \frac{1}{2}\sqrt{\frac{\pi}{A_c(h_c)}}\frac{dF}{dh}$

Nanoindentation experiments were performed using the electrostatic transducer of the Hysitron Troboscope attached to a scanning force microscope the Nanoscope IV. The tip used in measurment is made of diamond and has the shape of a cube corner (three-sided pyramid). In this case the cross-section area (plane AED in fig.2) is given by: $A_p = \frac{3\sqrt{3}}{2}h^2 = 2{,}598 \cdot h^2$

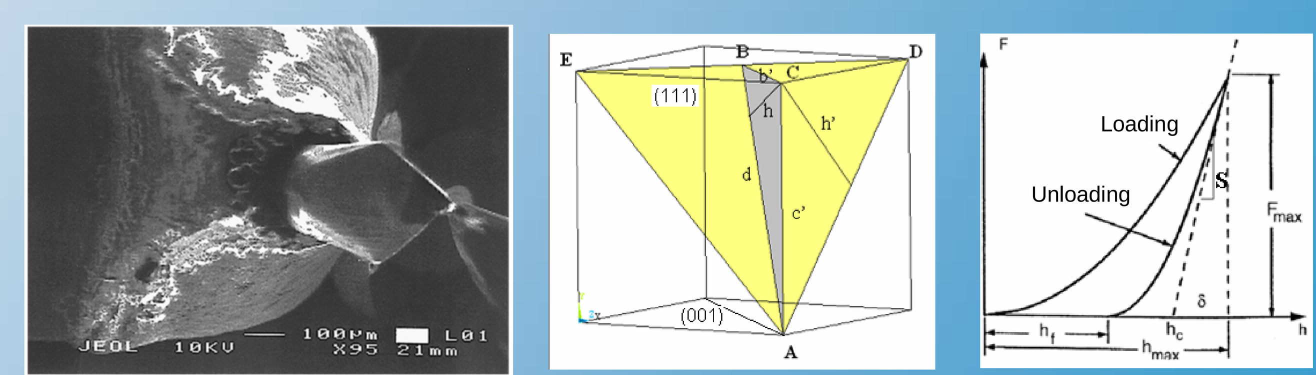
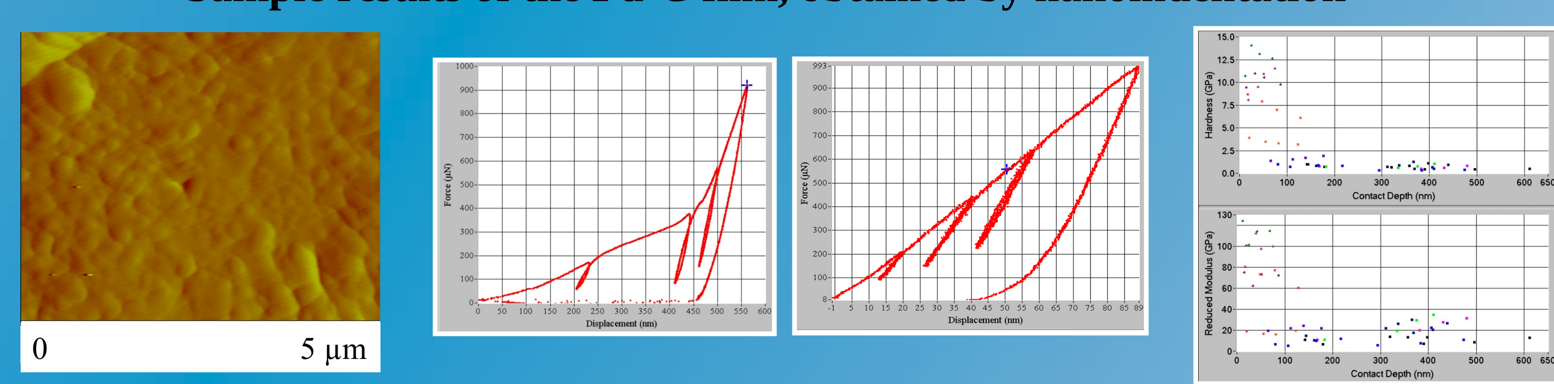


Fig.2 Geometry of the indentation tip; a) scanning electron micros-copy image; b) schematic crystal geometry the angle between (001) and (111) planes is 54° 44' 08''

Sample results of the Pd-C film, obtained by nanoindentation



H_1 = 0,3-1 GPa
Er_1 = 5-30 GPa

H_2 = 8-14 GPa
Er_2 = 75-125 GPa

Fig.3 a) AFM image with indent peak load 2mN, b) load–displacement curve for application to a Pd-C film, c) nanohardness and reduced modulus versus depth

FEM ANALYSIS

Finite Element Method (FEM) and ANSYS program (Ansys, Inc) were used for numerical simulation of nanoindentation experiment of Pd-C film. Model of the C-Pd film is presented in Fig.4a. Spherical objects are palladium nanograins. Ratio of nanograins size and tip diameter determined a scale of problem.

Tip rounding becomes important when one wishes to perform nanoindentations on a thin film of a thickness more than ~500nm and when the maximum depth of the penetration of tip is ~50nm. A real indenter can therefore be modeled as a spherical indenter. For example, a model of spherical shaped tip in the simulated nanoindentation experiment for the C-Pd film is shown in Fig.6.

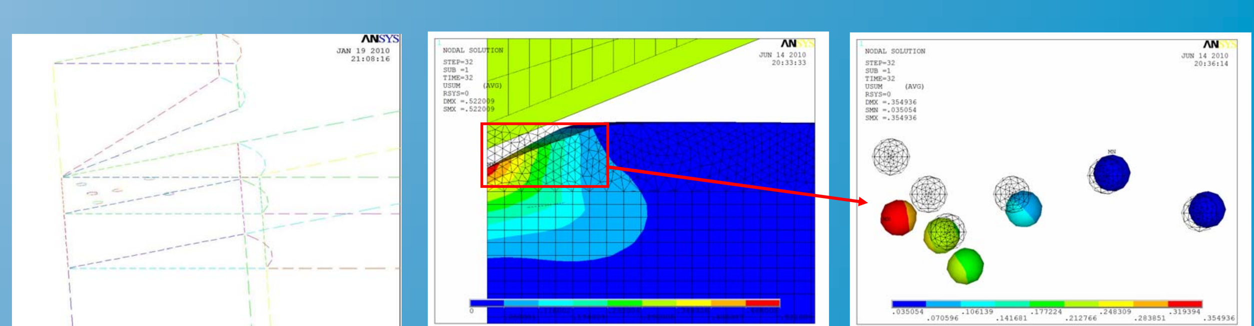


Fig.4 a) Model of the C-Pd film, b) plastic deformation of the film after unloading c) displacement vector sum Pd nanograins

$$A_c(h) = C_0h^2 + C_1h + C_2h^{\frac{1}{2}} + C_3h^{\frac{1}{4}} + C_4h^{\frac{1}{8}} + C_5h^{\frac{1}{16}} + \dots$$
$$A_c = \pi R^2$$
$$R^2 = r^2 - (r-h)^2$$
$$A_c = -\pi h^2 + 2\pi rh$$

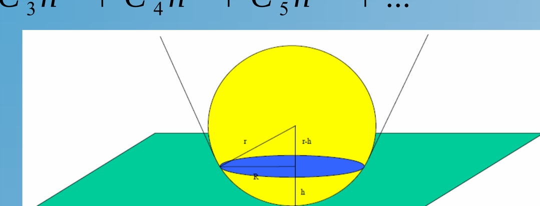
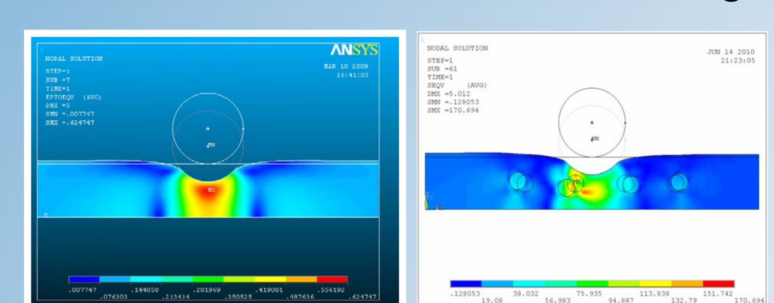


Fig.6 Scheme of spherical shaped tip in the simulated nanoindentation experiment



Rys.7 Von Mises stress intensity; a) fullerene film, b) C-Pd film

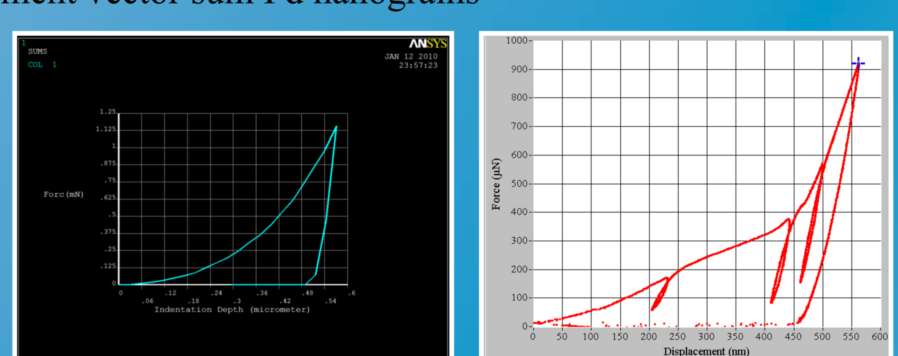


Fig.5 Load–displacement curve, a) simulation, b) experimental test

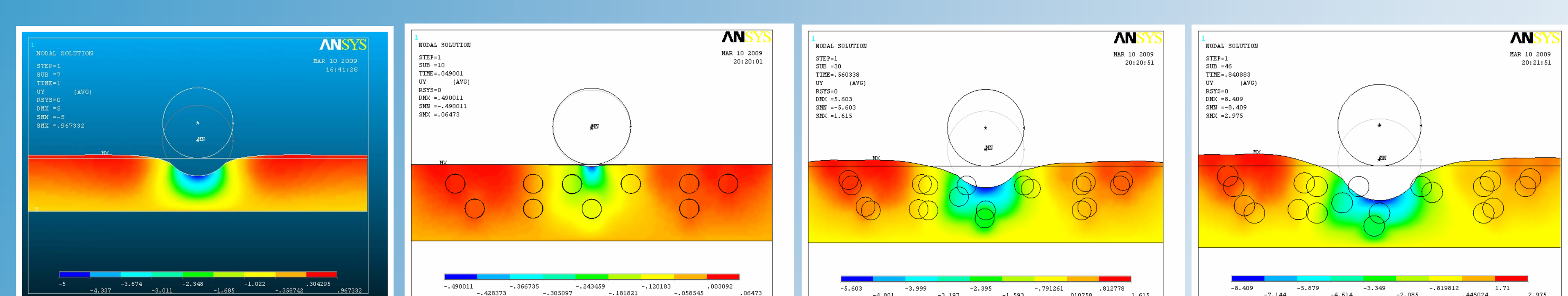


Fig.8 Plastic deformation of a) fullerene film, b-d) C-Pd film in time

CONCLUSION

The mechanical properties of the C-Pd films are connected to the nanostructure of the films. The Pd carbonaceous film have completely different mechanical properties in comparison to pure C_{60} films. It was deduced from FEM results that Pd nanocrystals are moving in carbon matrix toward the film surface due to a external stress. The influence of distribution of palladium nanograins in the film volume on the Young modulus and nanohardness was also found.

FEM simulation shows also that deformation of the carbonaceous-palladium film is not symmetrical. In the carbonaceous matrix Pd nanograins move toward the film's surface. They also create piling-up on the surface of the film in a contact area of the penetration. Deformation inside the film's volume depends on the distribution of grains in this film.

Observed effects are important because of practical applications of films. Various mechanical properties are connected to differences in the structure and the composition of studied films.

Our simulations allowed for observation of the process of migration of Pd nanograins during nanoindentation experiment.

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