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COMPARISON OF FINITE ELEMENT SIMULATION OF TUNGSTEN NANOINDENTATION WITH BERKOVICH AND CONICAL INDENTER

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Abstract: *Finite Element Method (FEM) was used to study the difference between using Berkovich and conical indenters in nanoindentation test of tungsten specimen. The study was aimed to determine the modulus of elasticity of a tested specimen and how it changes with different indenter. The FEM analysis also revealed that the modulus of elasticity was sensitive to the dimensions of both specimen and the indenter for which were made several numerical calculations with different dimensions.*

Keywords: Nanoindentation, FEM, Berkovich indenter, Conical indenter, Tungsten.

1. Introduction

The nanoindentation test is mostly used to determine the mechanical properties of thin films. Most frequently determined quantities are modulus of elasticity and hardness. Principle of this test is to press the indenter into the specimen and then measuring of the dependence of the force on the indentation depth. From this dependence, the maximum force P_{max}, the maximum indentation depth h_{max} and the contact stiffness S are determined.

According to the method introduced by W. C. Oliver a G. M. Pharr (Oliver, 2004), which is commonly used to determine the modulus of elasticity and hardness from nanoindentation tests, the relation between the contact stiffness, effective modulus of elasticity and contact area is given by equation (1).

$$S = \beta \cdot \frac{2}{\sqrt{\pi}} \cdot E_{eff} \cdot \sqrt{A_c} \tag{1}$$

In this equation, β is parameter that depends on indenter geometry, A_c is projection of contact area into upper surface of undeformed specimen and E_{eff} is an effective modulus of elasticity that expresses the relationship between modulus of elasticity and Poisson ratio of both specimen and indenter according to the equation (2),

$$\frac{1}{E_{eff}} = \frac{1-\nu_i^2}{E_i} + \frac{1-\nu_s^2}{E_s} \tag{2}$$

where index i is for indenter and index s is for specimen. Projection of contact area A_c can be determined directly from a numerical model (or from experiment), or by the analytical relationship $A_c = 24.56 \cdot h_c^2$, which is based on plastic indentation depth, defined as $h_c = h_{max} - \varepsilon \cdot P_{max}/S$ (Oliver, 2004).

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The indenters were modelled as perfectly sharp, which caused, that the pure elastic part of the loading is negligible, and the loading is mostly elasto-plastic. These plastic deformations result in residual stresses that make the unloading curve nonlinear and can be fitted with a power function in eq. (3) (Oliver, 2004).

$$P = \alpha(h - h_f)^m \tag{3}$$

Parameters α, m and h_f are characterizing the unloading curve. Contact stiffness corresponds to derivative of the force according to the indentation depth in its maximum values, $S = \left.\frac{\mathrm{d}P}{\mathrm{d}h}\right|_{h=h_{max}}$.

Berkovich indenter (triangular pyramid) is commonly used in nanoindentation. However, parameters β and ε are used to determine modulus of elasticity, which were derived provided that the Berkovich indenter can be replaced by a conical indenter with a half-angle of $70.3\,°$, which has the same ratio between the area and the depth of indentation as the Berkovich indenter (Shim, 2007). The parameter β expresses the difference in contact stiffness between the Berkovich and the conical indenter. For the conical indenter $\beta = 1$, and for the Berkovich indenter $\beta = 1.034$ (Oliver, 2004). The ε parameter depends on the indenter geometry. Recommended value is $\varepsilon = 0.75$, which corresponds to the shape of the paraboloid. Experimentally, it was found that this shape, due to the blunting of the indenter, best approximates the unloading curve (Oliver, 2004).

This paper deals with the comparison of numerical calculation of the nanoindentation of a tungsten specimen with the 3D model of Berkovich indenter and the 2D model of conical indenter and the influence of specimen and indenter size on the resulting values is discussed.

2. Finite element models

The FEM models of Berkovich and conical indentation were done. For the Berkovich indenter, only one-sixth was modelled, and the conical indenter was modelled as 2D using axisymmetry. The elastic model of diamond with elastic modulus $E_d = 1050$ GPa and Poisson ratio $\mu_d = 0.2$ (Klein, 1993) was used for indenters. The indentation specimen was made from tungsten, for which an elasto-plastic model of a material with elastic modulus $E_W = 407$ GPa and Poisson ratio $\mu_W = 0.28$ was used. Multilinear isotropic hardening was used as a plasticity model with parameters taken from (Volz, 2017).

In the nanoindentation test, the standard is given by how far apart the individual indentations can be and how thick the material must be in order not to affect results by the edge based on ČSN EN ISO 14577-1. These values are proportional to the indentation depth, which was 715 nm. For the first calculation, dimensions were used to be larger than the permissible values in the standards. The indenter height was chosen as ten times the indentation depth, i.e. 7.15 µm.

The mesh for the 3D Berkovich model had 200 000 SOLID 186 elements and for the 2D conical model had 10 000 PLANE 183 elements. When creating the mesh, the effort was to create the most regular and fine mesh under the indenter, and at the same time to create a coarser mesh at the edges of the specimen. The elements directly under the tip of the indenter were created intentionally larger, because due to the ideally sharp tip problems with distortion and convergence occurred during loading process (Fig. 1).

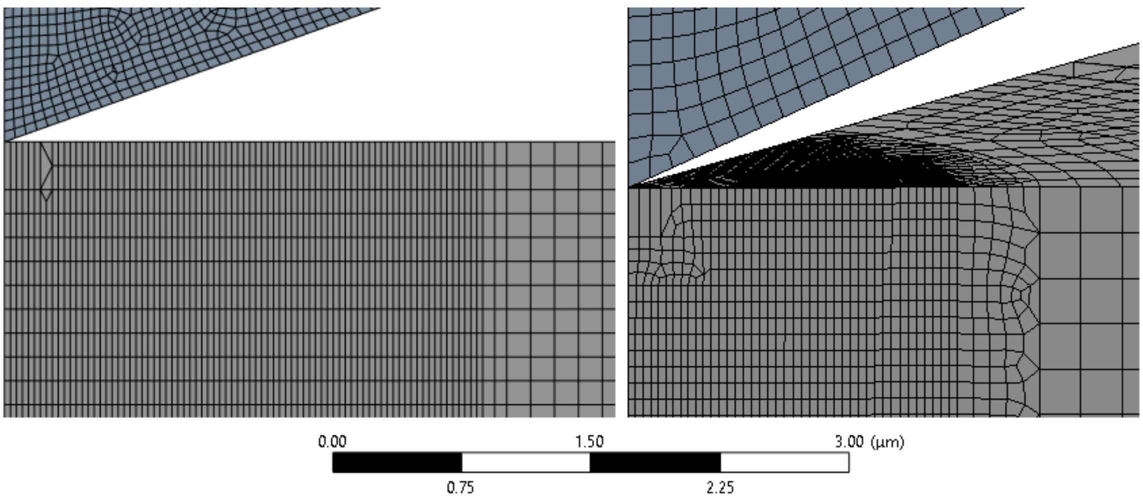

Fig. 1: Detail of the FEM models of conical indenter (left) and the Berkovich indenter (right).

In the 3D model, normal displacement on the symmetry surfaces was prevented for both the specimen and the indenter. In the 2D model, radial displacement on symmetry axis was prevented by axisymmetry. In both models a displacement was set on the upper surface of indenter to achieve imprinting of indenter to specimen, which was supported on the bottom side. The contact was modelled without friction, which is possible because there is no significant pile-up during indentation (Kovář, 2020). Penetration was corrected to be in the order of tenths of nanometers, which did not significantly affect results.

3. Results

When analysing results, it was found that for a model with dimensions given by the standard of ČSN EN ISO 14577-1, the modulus of elasticity comes out significantly higher than it is. This was due to the small, modelled part of the indenter and the specimen, which caused to the high stress values at the edges of the specimen and indenter, and therefore the dimensions were gradually increased. Dependence of the slope of the unloading curve on the size of the model is shown in Fig. 2. The curves are determined from the model of Berkovich indenter and for the conical indenter results were similar.

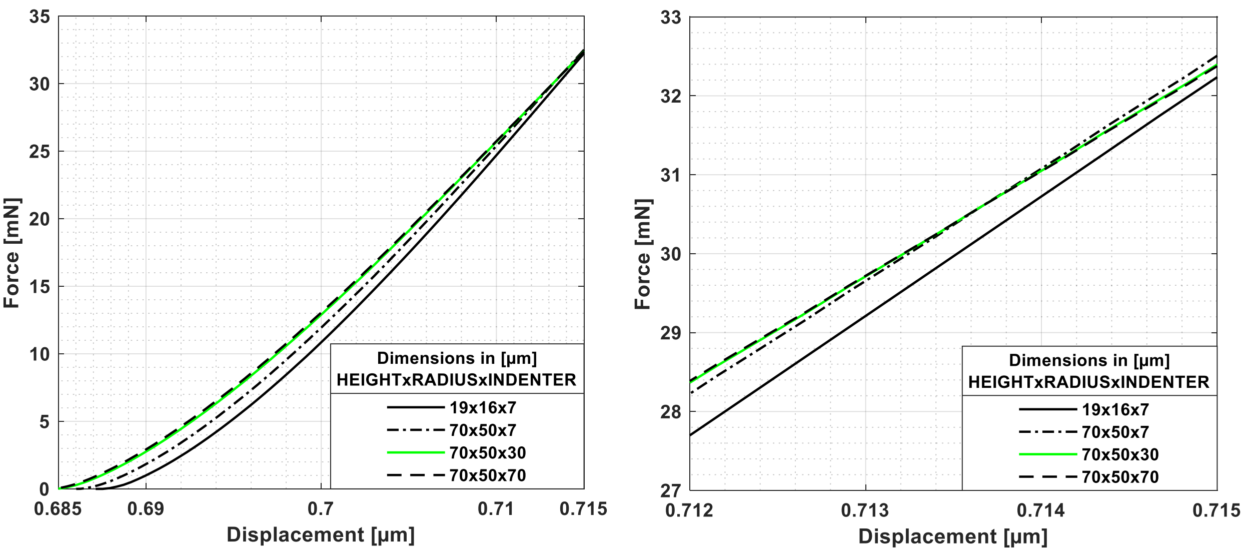

Fig. 2: The unloading curves for different dimensions (left) and detail of its beginning (right).

Even a small change in slope of the unloading curve significantly affects the contact stiffness and thus the resulting modulus of elasticity. Contact stiffness was determined by fitting equation (3) to the first half of the unloading curve and then substituting the observed parameters α, m and h_f into the derived eq. (3). The dimensions were increased until difference in resulting stiffness was lower than 1 %. This condition was met by the dimensions of the specimen 70×50 μm and the indenter height of 70 μm. For models with sufficiently large dimensions, the parameters for the Berkovich indenter were found $\alpha = 0.659\ \mathrm{mN/nm^m}$, $m = 1.17$ and $h_f = 687.5$ nm, while for the conical indenter were $\alpha = 0.604\ \mathrm{mN/nm^m}$, $m = 1.18$ and $h_f = 686.8$ nm.

The projection of the contact area was determined in two ways, namely analytically using Oliver-Pharr analysis and directly from the numerical model. The difference between results obtained by these approaches is due to the O-P analysis, which does not include radial displacements. From these contact areas the moduli of elasticity were determined (Tab 1.). Effective modulus calculated from analytically obtained projected area was corrected due to the radial displacements by parameter γ (Hay, 1999).

Tab. 1: Determined values from both indenters.

Indenter type	Stiffness	Maximal force	A_c		E	
			O-P	FEM	O-P	FEM
	[mN/nm]	[mN]	[μm^2]	[μm^2]	[GPa]	[GPa]
Berkovich	1.39	3241	11.88	13.23	412.6	415.8
Conical	1.29	32.09	11.91	13.18	410.5	409.4

The projection of contact areas obtained analytically using O-P analysis are almost identical for both models. Even for projections obtained directly from the model, the difference is minimal. The difference is in the stiffness, which is 7 % greater for the Berkovich indenter than for the conical indenter. More accurate results of Young modulus were achieved with a conical indenter, with a difference lower than 1 % from the expected value, and that is because Oliver-Pharr analysis was directly derived for this indenter. In model with Berkovich indenter results of Young modulus were in the range of 1 ÷ 2.2 % from the expected value, which can be also considered as very accurate. The indentation curves for both models are very similar (Fig. 3), which proves the similarity between the Berkovich and conical indenters with a half-angle of 70.3°. It should also be mentioned that these results were obtained using this tungsten specimen and may differ using another material (Sakharova, 2009).

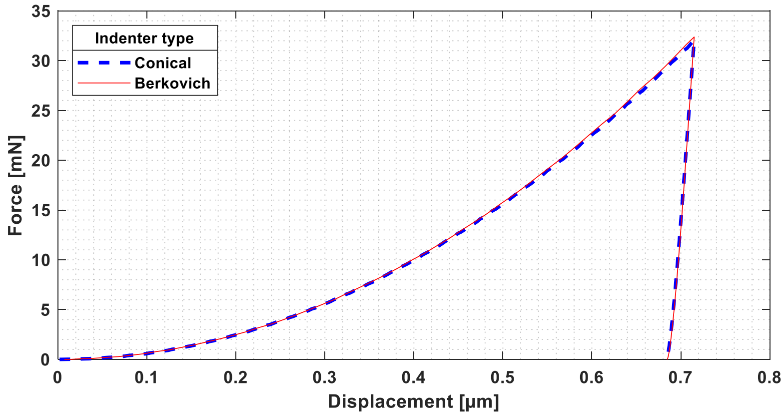

Fig. 3: Comparison of indentation curves for both indenters.

4. Conclusion

The numerical simulation of the nanoindentation test of the tungsten specimen was performed using a conical indenter and a Berkovich indenter. Calculations showed that the size of numerical model of the specimen and the indenter has large impact on determined values of the elastic modulus. To obtain correct results, the dimensions of model must be large enough, because O-P analysis assumes the indentation of the half-space i.e., the specimen has infinite dimensions. Very accurate results were obtained from both models with a difference of approximately 2 %. The model with conical indenter is more accurate, because it better corresponds to the assumptions of O-P analysis. These results were obtained from the indentation of a material that shows almost no pile-up, and therefore it would be advisable to do a similar analysis in the future for materials showing significant pile-up.

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