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3D versus 2D finite element simulation of the effect of surface roughness on nanoindentation of hard coatings

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ABSTRACT

Indentation with a spherical indenter tip into CrN coatings with an arithmetic surface roughness (Ra) ranging between 2.6 and 11.1 nm is modelled with the finite element method. Results are compared for a 2D axisymmetric model (published earlier) and a true 3D model for three different coatings within that roughness range. Both models predict a significant underestimation of the evaluated Young's modulus due to the effect of surface roughness. They give comparable results for Ra<3 nm, but differ considerably for higher roughness values. The axisymmetric setup of the 2D model leads to increased scatter of the load–displacement data and higher stiffness on average compared to the 3D model and therefore a 3D simulation seems preferable.

1. Introduction

Surface roughness can be a severe source of error in the determination of properties from indentation experiments [1–6]. The contact area is not measured directly in the indentation experiment but it is usually calculated from the depth of contact and the indenter tip geometry. This implies the assumption that the contacting surfaces are smooth and in continuous contact within the contact depth. However, the presence of asperities can change the area of contact between the indenter tip and the sample and this is generally not accounted for in the analysis of load displacement curves. This especially applies when the indentation depth is very limited, e.g. during indentation of thin films, but has also been observed for high indentation depths [3].

The indentation of thin films with an inapt ratio of surface roughness to thickness results in highly scattered data which inhibits a reliable determination of properties such as Young's modulus. This is a frequently encountered problem which, in practice, is often handled by polishing of the rough surfaces before indentation, silently accepting all possible effects on the material properties of this surface manipulation. Recently, the influence of roughness on the evaluated data from indentation experiments has attracted interest for a number of different materials. Investigations aim towards a criterion for reliable results independent of the surface roughness. As a general guideline it is suggested that the indentation depth should exceed the arithmetic surface roughness Ra by a factor of 20 in the European standard for instrumented indentation testing for hardness and materials parameters [EN ISO 14577-1]. This applies to the indentation of metallic materials with a Berkovich tip. Rico et al. established that the ratio of arithmetic surface roughness to elastic displacement should be lower than 3% for consistent results measuring the mechanical properties of ceramic materials [4]. For cement paste 5 times the RMS roughness measured over a scanning size of 200 times the indentation depth was stated as a criterion for a unique set of measured properties by Miller et al. [5]. Measuring cancellous bone with nanoindentation, Donnelly et al. found that the variability in material properties increased substantially as the ratio of indentation depth to surface roughness decreased below ~3:1 [6]. For rock materials it has been shown experimentally by Bobji et al. that the scatter decreases with higher loads and softer materials and that it can be described with a power law relation as a function of the penetration depth and roughness [7,8]. Quasmi and Delobelle arrived at similar results investigating the influence of roughness on the precision of Young's modulus and hardness determination using nanoindentation with a Berkovich indenter [9]. Berke and Massart

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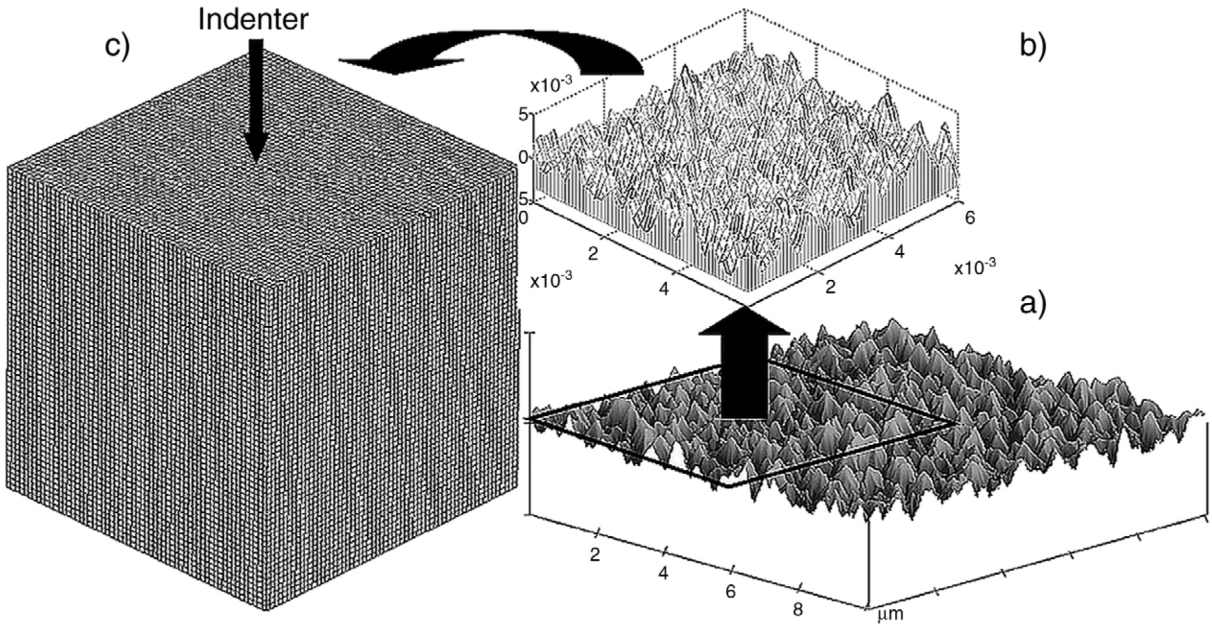

Fig. 1. a) 10×10 µm^2 AFM surface image of CrN coating with Ra = 11.1, b) 6×6 µm^2 section of this AFM image after interpolation at the node positions (node spacing 0.1 µm), and c) 6×6×6 µm^3 3D FEM submodel with rough top surface.

used finite element modelling (FEM) simulations to investigate the influence of the experimental uncertainties of the nanoindentation experiment [10]. They found that roughness does have an influence but could not identify a clear relation with respect to Ra.

This work applies FEM to study the influence of the surface roughness on the Young's modulus determined from nanoindentation with a spherical indenter tip. The study has relevance to applications since it focuses on the example of a typical hard coating deposited by physical vapour deposition (PVD). The central point is a comparison between the results of the newly developed 3D model and 2D simulations which have been published previously [11].

2. FEM simulation

The general model consists of a spherical indenter tip with a radius of 50 µm on top of a sample. The top 3 µm of the sample represent the CrN coating with a Young's modulus E of 323.6 GPa and a Poisson's ratio v of 0.25 [12]. Below the coating follows the Si substrate (E = 164.4 GPa, v = 0.224 [13]). Plasticity has been shown to be negligible for the applied load of 15 mN [11]. Plastic deformation occurs to a small extent locally at the asperity tips but has no significant effect on the load–displacement behaviour. The diamond indenter is assumed to be rigid and driven into the sample by a defined load. The surface roughness for the finite element models was taken from experimental atomic force microscopy data of sputter-deposited CrN coatings with an arithmetic roughness Ra between 2.6 and 11.1 nm [11]. To evaluate the arithmetic roughness, an area of 10×10 µm was scanned with 512×512 sampling points. The measured surface profiles were mapped to the FEM model by interpolation at the top surface node positions of the sample mesh repositioning these nodes in axial direction. Fig. 1 shows a) a measured surface profile from which b) a section is selected and interpolated at the node positions of the mesh and then introduced as top layer into c) the FEM model of the sample. In the zone of contact the node spacing is 0.1 µm in both, the 2D and the 3D model. The 2D model is axisymmetric and has been described in detail earlier [11]. The particulars about the 3D model are given in the following.

The challenge of 3D modelling is to keep the number of degrees of freedom (DOF) within feasible limits for computation. Since the size of the elements has to be small in order to represent the actual roughness profile sufficiently well, the viable overall dimensions of the model are limited, too. To ensure that the effect of the interpolation of the measured roughness profile remains below 0.1 Ra, the maximum node spacing was constrained to 0.1 µm for the cubic elements. This node spacing limits the size of the model that can be comfortably calculated on the available facilities to a block of 6×6×6 µm (219,722 elements, 692,112 DOFs, ~40 increments, ~70,000 s wall clock time, IBM Power5 Chip, 8 GB memory, 73 GB storage). These dimensions are too small to represent the continuous volume of material as seen by the real indenter. Therefore, the boundary conditions become very important for the accuracy of the simulations.

Fig. 2 shows schematically the four different scenarios for the boundary conditions that have been tested and compared to the theoretical solution according to Hertzian contact mechanics for indentation of a perfectly smooth Si sample [14]. For the given case of a rigid indenter the Hertzian equations reduce to $h = \left(\frac{3P(1-\nu^2)}{4E\sqrt{R}}\right)^{2/3}$ as an expression for the penetration depth h as a function of the load P, the indenter radius R, the elastic modulus E and Poisson ratio v of the

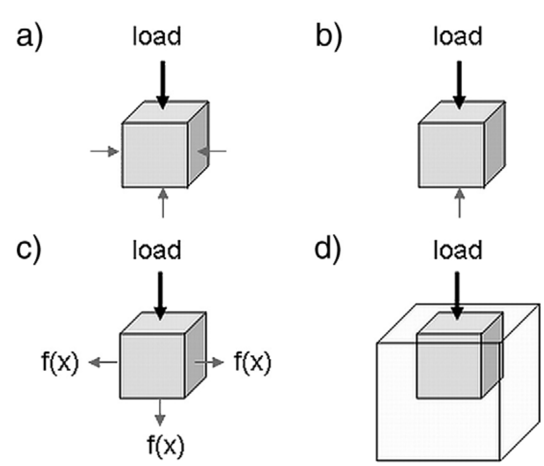

Fig. 2. Schematic of FEM model with different boundary conditions: a) nodes fixed in normal direction on side and bottom surfaces, b) nodes fixed in normal direction only on bottom surface, c) node displacements described according to Boussinesq [9] on side and bottom surfaces, and d) submodelling.