Computers and Mathematics with Applications 64 (2012) 2775–2786

Contents lists available at SciVerse ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

Modelling and parameter re-identification of nanoindentation of soft polymers taking into account effects of surface roughness

Zhaoyu Chen *, Stefan Diebels **

Chair of Applied Mechanics, Saarland University, PO Box 151150, 66041, Saarbrücken, Germany

ARTICLE INFO

Article history:
Received 1 February 2012
Received in revised form 3 April 2012
Accepted 12 April 2012

Keywords:
Numerical modelling of nanoindentation
Soft polymer
Surface roughness
Parameter identification

ABSTRACT

In this paper the characterisation of polymers by nanoindentation is investigated numerically by the use of the inverse method. Effects of the surface roughness are explicitly considered. The boundary value problems of the nanoindentation of two polymers, PDMS and silicone rubber, are modelled with the FE code ABAQUS®. The model parameters are re-identified by using an evolution strategy based on the concept of the numerical optimisation. The surface roughness effects are investigated numerically by explicitly taking into account the roughness profile in the model. At first the surface roughness is chosen to have a simple representation considering only one-level of asperities described by a sine function. The influence of the surface roughness is quantified as a function of the sine parameters as well as of the indentation parameters. Moreover, it is verified that the real surface topography can be characterised by using multi-level or simple one-level of protuberance-on-protuberance sinusoidal roughness strain-energy function. profiles. The effects of the surface roughness are investigated with respect to the force–displacement data and the identified model parameters. These numerical results are expected to offer a deep insight into the influence of the real surface roughness at the results of indentation tests.

1. Introduction

Over the last decades, the nanoindentation testing technique has continuously been improved. Now it is widely applied in metallic and ceramic engineering materials to determine the mechanical properties such as hardness and modulus. Since this technique is able to measure the properties of extremely small volumes with sub-μm and with sub-μN resolution, it also became one of the primary testing techniques for the mechanical characterisation of polymeric materials and biological tissues. The analysis of individual indentation tests by using the conventionally applied Oliver and Pharr method (abbreviated as O&P method) [1,2] is limited with regard to capture the hyperelastic and the rate-dependent properties of polymers and some metals. Therefore, numerical approaches in combination with the experimental testing, i.e. the finite element simulations and numerical optimisation have been used and evolved [3–13]. In this method, the difference between the experimental data and the numerical prediction is minimised with respect to the material model parameters by using numerical optimisation. The parameters are identified as the optimised solution.

Nanoindentation has the considerable advantage to measure the local properties of small volume materials from the continuously sensed force–displacement curve. However, it includes various error contributions, e.g. friction, adhesion, surface roughness and indentation process associated factors. These contributions generate the systematic errors between

* Corresponding author. Tel.: +49 0 681 302x2169.
** Corresponding author. Tel.: +49 0 681 302x2887.
E-mail addresses: zh.chen@mx.uni-saarland.de (Z. Chen), s.diebels@mx.uni-saarland.de (S. Diebels).

0898-1221/$ – see front matter © 2012 Elsevier Ltd. All rights reserved.
doi:10.1016/j.camwa.2012.04.010

the numerical model and the experiments, and this often leads to large errors in the parameter identification [9,14–16]. Therefore, basic investigations and the certain knowledge about the influence of these factors are indispensable to characterise the materials accurately from nanoindentation based on the inverse method.

It is recognised by the use of the experimental and the numerical approaches that the surface roughness has a significant influence on the force–displacement data at a small or a moderate indentation depth, which is comparable to the height of the surface asperities [17–29]. It is known by the experimental investigation that the surface roughness impacts the Young's modulus and the hardness measurements [17,18,21,24]. The surface roughness can considerably disturb the indentation curves [22], and may, at least, be one of the main reasons for the indentation size effect [23]. The criteria to remove the surface roughness effects are found by experiments for some special materials. Miller et al. [28] found that it is possible to get a unique set of material properties if the average indentation depth is 5 times greater than the RMS roughness. For cancellous bone Donnelly et al. [29] pointed out that the variability in material properties increases substantially if the ratio of indentation depth to surface roughness decreases below 3:1. The surface roughness effects are difficult to control in an experiment, and moreover the measuring results are not easily to interpret. Nevertheless, the numerical simulation tools may help to understand the physics involved in this complex experiment. Therefore, FE simulations are widely used to interpret the experimental results if surface roughness effects are included [26,27,30,20]. The results in [26,27,30] have shown that an increasing roughness causes an increasing scatter of the data, but the mean value of a sufficiently large number of indents can still give a good approximation of the Young's modulus. Jiang et al. [20] pointed out that in order to rule out the influence of the surface morphology, the indentation depth should be much greater than the characteristic size of the surface roughness. Moreover, an indenter with a sufficiently large diameter could also be a good choice. A numerical study was conducted in [19] to understand the coupled influence of friction and surface roughness in the nanoindentation of pure nickel. Results have shown a strong interaction between these two contributions of surface effects, and their cumulative effects leads to significant variations in the force–displacement curves. The surface roughness of the bulk sample can be altered by various mechanical or electrochemical methods of polishing. However, an excessive polishing could influence the mechanical properties of soft and thin polymer films. Therefore, in practical experiments, the surface roughness of thin films can reach an average height of asperities about 30–60 nm [21,31,32]. Because of that, the surface roughness is comparable to the imposed indentation depth limited by the thin layer's thickness and the influence of the substrate. In this case, some of the criteria documented in the literature cannot be used longer. A quantified evaluation of the surface roughness effect is still required. Furthermore, it is essential to decrease the errors between the experimental settings and the numerical simulations if the inverse method is used. For this reason, more attention is paid on the numerical model of the realistic surface roughness profile. The surface roughness for the finite element models is taken from AFM data of sputter-deposited CrN within 2D and 3D in [26,27]. Pre-existing straight grooves defects are introduced on the film surface in 2D FE models in [20]. Berke et al. [19] describes the roughness with a protuberance-on-protuberance profile approximated by a sine function using axisymmetric 2D FE models.

In this present article, the behaviour of two hyperelastic soft polymers under nanoindentation is investigated numerically taking into account the effects of the surface roughness. The characterisation of the materials' properties is performed based on parameter re-identification procedure by using the inverse method. In this procedure, the virtual experimental data, which are obtained from numerical simulations with the chosen parameters, replace the real experimental measurements. In this sense, the finite element code ABAQUS® is used as a virtual laboratory. The parameter re-identification concept was used in [9,33] to validate the gradient-based material parameter identification routine. The surface roughness effects are investigated numerically based on the approach, which is mainly influenced by the work of Kumar et al. [21] and Berke et al. [19]. The surface roughness is chosen to have a simple representation considering a one-level roughness profile described in a first step by a sine function. The influence of the surface roughness is quantified phenomenological as a function of the sine curve parameters as well as of the indentation parameters. Moreover, it is verified that a real surface topography can be characterised by using a multi-level or a simple one-level of protuberance-on-protuberance sinusoidal profiles. The effects of this surface roughness are investigated with respect to the identified model parameters. The whole force–displacement curve is taken into account. The results are expected to offer a deep insight into the effects of the real surface roughness by a numerical modelling of nanoindentation.

2. FEM simulation of nanoindentation

2.1. Hyperelastic material model

In the present work we consider the nanoindentation of two nearly incompressible soft polymers by numerical simulation: polydimethylsiloxane (PDMS) 1:10 used in [34] and silicone rubber ELASTOSIL® RT 265 used in [35]. Both of the two polymers were assumed to be isotropic hyperelastic materials under isothermal conditions. Firstly in the framework of finite strain continuum mechanics, constitutive models of a nearly incompressible hyperelastic material will be recalled.

The existence of the Helmholtz free-energy function Ψ is postulated for a so-called hyperelastic material. Concerning the isotropic material under isothermal conditions, $\Psi = \Psi(\mathbf{F})$ is solely a function of the deformation gradient $\mathbf{F}$ or a strain tensor, respectively. So the Helmholtz free-energy function is referred to the strain-energy function. The general format of the constitutive equation can be derived from the second law of thermodynamics in the form of the Clausius–Planck