Materials Science and Engineering A 404 (2005) 179–187

MATERIALS SCIENCE & ENGINEERING A

www.elsevier.com/locate/msea

Modeling nano-indentation tests of glassy polymers using finite elements with strain gradient plasticity

S. Swaddiwudhipong [a,*], L.H. Poh [a], J. Hua [a], Z.S. Liu [b], K.K. Tho [a]

[a] *Department of Civil Engineering, National University of Singapore, E1A-07-03, 1 Engineering Drive 2, Singapore 119260, Singapore*
[b] *Institute of High Performance Computing, 1 Science Park Road #01-01, Singapore 117528, Singapore*

Received in revised form 14 May 2005; accepted 14 May 2005

Abstract

It is widely reported that when an indentation test is carried out at the submicron level, the materials display strong size effects, which alter the mechanical properties from their bulk characteristics. Classical plasticity theory is unable to account for this phenomenon. It has been shown that introducing the strain gradient plasticity theory in the analysis is able to capture successfully the size effects of various materials. The present study adopts a constitutive model for the viscoelastic–plastic deformation of glassy polymers, incorporates the effects of strain gradient plasticity and implements them via user subroutines in the commercial general purpose finite element package, ABAQUS. It is demonstrated that the strain gradient effect has to be considered into the adopted constitutive model in order to better describe the viscoelastic–plastic response of polymers at submicron indentations. The study also covers the two approaches of deriving the values of the effective strain gradient (i) via indentation geometry and (ii) directly from finite element nodal displacement parameters. Comparison of results obtained from both approaches show good agreement with existing experimental values in all cases covered in the present study. The latter, as expected, provides slightly more accurate solutions as compared to the test results than the former but at marginally higher computing time and resources.

Keywords: Finite element method; Glassy polymers; Nano-indentation; Size effects; Strain gradient plasticity; Viscoelastic–plastic materials

1. Introduction

Material characterization based on indentation techniques has gained popularity in the past decade, largely due to the improved capabilities of indentation instruments and the necessity to perform the tests on a small volume of materials such as those on thin film coatings, MEMS and NEMS. Numerical analyses are able to model the indentation experiments with reasonable accuracy and are thus used extensively in the extraction of mechanical properties from the indentation curves. Some examples using finite element simulations in material characterization are those by Giannakopoulos and Suresh [1] and Dao et al. [2]. The latter proposed a forward and reverse analysis scheme, which was extended by Swaddiwudhipong et al. [3] who suggested employing results from dual indenters to ensure unique solutions in material characterization.

A group of materials, which commands a vast interest is the polymeric group. Polymers have been widely adopted to replace traditional materials such as metals and ceramics in various applications. The materials have been employed extensively, especially those in optical-electronics, computing and chemical industries. They have also gained importance in biomaterials applications, where the properties of materials are of primary concern to ensure no premature failure in the human's body. The growing maturity of material characterization techniques using indentation experiments, coupled with the rising importance of polymers in small volume applications leads to a surge in interest in indentations of polymers [4–7]. Larsson and Carlsson [8] and van Melick et al. [9,10] have employed indentation finite element simulations in the investigation of polymeric material properties.

* Corresponding author. Tel.: +65 68742173; fax: +65 67791635.
E-mail address: cvesomsa@nus.edu.sg (S. Swaddiwudhipong).

0921-5093/$ – see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.msea.2005.05.063

Many researchers have reported the presence of strong size effects in crystalline materials when the material length scale is of the same order of magnitude as the characteristic length associated with non-uniform plastic deformation. For example, when diameters of copper wires are reduced from 170 to 12 μm, the torsional resistance increases significantly while changes in the tensile strength are negligible [11]. Similar phenomena are reported by Stolken and Evans [12] and Haque and Saif [13] in micro-bend tests. Size effects are also observed in indentation tests at submicron level [14,15].

Dislocations formed during the deformation of crystalline materials have been proposed to account for the size effects. Fleck and Hutchinson [16] as well as Arsenlis and Parks [17] reported the dependence of dislocations on the effective plastic strain gradient. Such gradient type of theories require the determination of intrinsic material length scales [18]. Aifantis and co-workers [19–21] studied and proposed the elasto-viscoplasticity for the constitutive equations of clay. The theoretical concept for single-crystal viscoplasticity incorporating strain gradient plasticity was developed by Gurtin [22]. The framework for small-deformation viscoplasticity was presented by Gurtin [23] and then by Saczuk et al. [24] for large-deformation problems. Abu Al-Rub and Voyiadjis [25] employed a micromechanical model that assesses a non-linear coupling between statistically stored dislocation and geometrically necessary dislocation densities, linking the microscopic strain gradient effects to plastic deformations of an equivalent macroscopic continuum. Expression for the intrinsic length-scale parameter is obtained in terms of measurable microstructural parameters.

Acharya and Bassani [26] proposed a constitutive model incorporating gradient type non-local measures for rate independent plasticity through the instantaneous hardening moduli. Based on the balance laws in non-local theory, Chen et al. [27–29] adopted C^0 finite elements with both translational and rotational nodal displacements. The numerical results of thin wire torsion, micro-bend tests and micro-indentation with size effects are identical to classical local theories presented earlier by Eringen [30,31]. Recently, Huang et al. [32] presented a meso-scale conventional theory of mechanism based strain gradient (CMSG) plasticity theory taking into account the size effects for crystalline materials.

Compared to crystalline materials, there are limited studies on polymeric deformations at nano-scale. This may be due to the time dependent mechanical properties of polymeric materials, which complicate the testing procedures as well as the accuracy and interpretation of results. From the literature review, however, there is a general trend that the hardness of polymeric materials increases with decreasing indentation depth. This phenomenon is observed near the surface of the polymeric materials. Above a certain threshold indentation depth, the hardness remains fairly constant [33–37]. Lam and Chong [38] proposed a strain gradient plasticity theory for polymers to explain the above phenomenon. Based on the polymer model proposed by Argon [39], an analogy was made between the dislocations in metals and kink bands in polymers. The results based on their plasticity law for glassy polymers were later compared with experimental data showing a satisfactory agreement [40].

In this paper, the finite element method is used to simulate the indentation tests on glassy polymeric materials. The behavior of materials at micron and submicron indentations is investigated. The viscoelastic–plastic constitutive model for glassy polymers by Govaert et al. [41] is adopted in the analyses. Size effects are incorporated in the constitutive relation through the strain gradient plasticity. Both approximate strain gradient expressions based on the geometry of the indenter and the indentation depth proposed by Lam and Chong [38] and those derived directly from displacement field in finite element analyses [42] are employed in the study. The latter involves the strain gradient expressions explicitly evaluated from the appropriate displacement shape functions. The results from the two different approaches in obtaining the values of the effective strain gradient are compared and discussed.

2. Constitutive model for glassy polymers

The yield behavior of polymers under a multiaxial state of stress based on the Eyring equation [43] was proposed by several researchers including Ward [44] and Duckett et al. [45]. Govaert et al. [41] and Tervoort et al. [46,47] adopted the above approach and the compressible Leonov model to propose the viscoelastic–plastic constitutive relation for glassy polymers. The Govaert's constitutive model is adopted and incorporated in the user subroutine of the finite element package ABAQUS [48], which was employed in the analyses of the simulated indentation tests carried out in the present study. For completeness, a brief description of this constitutive relation is summarized in this section.

The total Cauchy stress $\boldsymbol{\sigma}$ of the model is decomposed into a driving stress $\boldsymbol{s}$ and a hardening stress $\boldsymbol{r}$:

$$\boldsymbol{\sigma} = \boldsymbol{s} + \boldsymbol{r} \tag{1}$$

The hardening stress $\boldsymbol{r}$ based on a neo-Hookean strain hardening relationship is expressed as:

$$\boldsymbol{r} = G_{\mathrm{R}}\tilde{\mathbf{B}}^{\mathrm{d}} \tag{2}$$

where G_{R} is the strain hardening modulus and $\tilde{\mathbf{B}}^{\mathrm{d}}$ is the deviatoric component of the left Cauchy–Green strain tensor. This hardening stress is to account for the hardening behavior of glassy polymers and is dependent on the total deformation.

The driving stress $\boldsymbol{s}$ can be decomposed into hydrostatic $\boldsymbol{s}^{\mathrm{h}}$ and deviatoric $\boldsymbol{s}^{\mathrm{d}}$ components.

$$\boldsymbol{s} = \boldsymbol{s}^{\mathrm{h}} + \boldsymbol{s}^{\mathrm{d}} = K(J-1)\mathbf{I} + \mathrm{G}\tilde{\mathbf{B}}_{\mathrm{e}}^{\mathrm{d}} \tag{3}$$

$$J = \sqrt{\det(\mathrm{G}\tilde{\mathbf{B}}_{\mathrm{e}}^{\mathrm{d}})} \tag{4}$$

$$\overset{\circ}{\tilde{\mathbf{B}}}_{\mathrm{e}} = (\mathbf{D}^{\mathrm{d}} - \mathbf{D}_{\mathrm{p}}) \cdot \tilde{\mathbf{B}}_{\mathrm{e}} + \tilde{\mathbf{B}}_{\mathrm{e}} \cdot (\mathbf{D}^{\mathrm{d}} - \mathbf{D}_{\mathrm{p}}) \tag{5}$$