ELSEVIER

Materials Science and Engineering A 390 (2005) 233–239

MATERIALS SCIENCE & ENGINEERING A

www.elsevier.com/locate/msea

FEA study on nanodeformation behaviors of amorphous silicon and borosilicate considering tip geometry for pit array fabrication

S.W. Youn[a], C.G. Kang[b,*]

[a] *Department of Precision and Mechanical Engineering, Pusan National University, P/Busan, South Korea*
[b] *National Research Laboratory of Thixo/Rheo Forming, School of Mechanical Engineering, Pusan National University, P/Busan 609-735, South Korea*

Received 3 May 2004

Abstract

In order to predict the nanodeformation behaviors (piling-up, sinking-in, and elastic recovery) of hard-brittle materials such as amorphous silicon and Pyrex 7740 glass (borosilicate) indentation simulations were performed for various tip radii (40, 100, 200 nm), half-angle of conical indenter (55, 60, 65°), and indenter geometries (conical, Berkovich, spherical) by the numerical method with ABAQUS finite element software package. The result for conical indenter showed the smallest elastic recovery. The amorphous silicon showed higher pile-up than the Pyrex glass 7740 because it has a larger value of E/σ_y. It was also observed that the height of pile-up decreased with increasing amount of the elastic recovery. For a given indentation depth, the applied load and elastic recovery increased with a tip radius and half-angle due to the increase of the contact area. In addition, a larger plastic zone size formed with shaper indenter due to the higher stress concentration exerted.

Keywords: Borosilicate; Amorphous silicon; Nanoindentation; Indenter geometry; Elastic recovery; Pile-up

1. Introduction

Nanoprobe-based lithographic technologies using a diamond particle or tip of nanosize have been studied by many researchers on the grounds of advantages such as the free selection of materials, the easy alternation of designs and convenient initial facilities [1–6]. The nanoprobe-based lithography itself is not suitable for mass production since it is a time-consuming method and not economical for commercial applications. This problem can be improved by fabricating a mold for mass production processes such as nanoimprint lithpgraphy (NIL). The key advantage of nanoimprint is the ability to pattern nanostructures with high-throughput and low cost [7,8].

From this point of view, the authors consider that an indentation experiment using a nanoindenter is one of the most promising methods of nanomachining for pattern fabrication [3]. Commonly, nanoindentation experiments are performed to measure the mechanical properties of very thin films such as the hardness, elastic modulus, and the friction coefficient [9]. In addition, quantitative data for the elastic recovery of materials can be investigated from the load–displacement curve. These mechanical properties are very important data in order to quantitatively understand the nanomachining process and to validate the FEM analysis result. Additionally, this process is suitable for obtaining nano/micrometer scale features on a large size specimen because it has a very wide working area and load range.

Up to date, numerous FEM techniques have been applied to nanoindentation experiment, generally as tools to help understand the indentation itself, to develop improvements in the analytical methods commonly used to extract mechanical properties from the data, and to develop a flexible set of tools which use FEM for routine analysis of materials [10–15]. These techniques have mainly been carried out only focusing on the mechanical properties, and performed using two-dimensional models because it has been reported that 2D

* Corresponding author. Tel.: +82 51 510 2335; fax: +82 51 512 1722.
E-mail addresses: yswonny@pusan.ac.kr (S.W. Youn), cgkang@pusan.ac.kr (C.G. Kang).

0921-5093/$ – see front matter
doi:10.1016/j.msea.2004.08.041

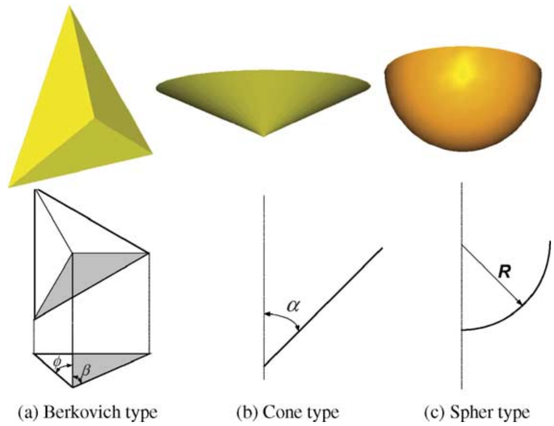

Fig. 1. Geometries of the indenters used for nanoindentation simulations.

and 3D models show almost the same results for mechanical properties.

In this study, the effects of nanoindentation experiment parameters (such as indenter geometry, half-angle of conical indenter, and tip radius) on the deformation behaviors of materials were analyzed by the numerical method with ABAQUS S/W. Hard-brittle materials, such as amorphous silicon and amorphous borosilicate (Pyrex 7740 glass), were used as specimens because they are feasible for ductile-regime nanomaching and are widely used in the filled of nano/micro technology. Indentation simulations were performed using a 3D model to consider the effect of the bluntness of tip corner and of tip end. In order to evaluate the validity of the model, the nanoindentation simulation results were compared with experimental ones. From the simulation results, indentation process conditions to reduce the elastic recovery and piling-up (or sinking-in) were proposed. The obtained analysis results will be applied to the fabrication of the nano/micro pit array by the nanoindentation process.

2. FEM modeling and experiments

Three types of rigid indenters (conical $\alpha = 65^\circ$, Berkovich $\beta = 70.3^\circ$, and spherical $R = 2\,\mu$m) [16] were used in order to define models, as shown in Fig. 1. The finite element mesh is shown in Fig. 2. Since very small indentations were being simulated, the meshes near the indenter needed to be very fine to be able to describe the deformation and stress gradients associated with indentation with sufficient accuracy. Thus, extremely fine mesh sizes of 1–10 nm were used under the indenter. Fig. 2(a) shows the model with the Berkovich indenter. The Berkovich indenter was modeled with 663 rigid elements (R3D4 element type). The specimens were modeled with 123208-node reduced integration elements (C3D8R element type). The thickness and width of the specimens were 5 and 6 μm, respectively. The indenter and the specimens were treated as revolving bodies to avoid the difficulty of modeling the real pyramidal indenter with a non-zero tip radius. The nodes along the axis of rotation can move only along the y-axis, and all the nodes on the bottom of the mesh were fixed. Fig. 2(b) shows the cases with the conical indenter and the spherical indenter. The specimens were modeled with 69508-node reduced integration elements (C3D8R element type) for the conical indenter and 75008-node reduced integration elements (C3D8R element type) for the spherical indenter. Both the conical and the spherical indenter were modeled with 120 rigid elements (R3D4 element type). Contact between two contacting surfaces, in this case the indenter surface and the specimen surface, was assumed. The friction coefficient between the tip and the specimen surface was assumed to be 1. The indentation procedure was simulated in two alternating steps, loading and unloading. During loading, the rigid surface or the modeled tip moves along the y-direction and penetrates the specimen up to the maximum depth. During unloading, the tip returns to the initial position. Since strain hardening was not considered in this study, all specimens were assumed to be isotropic, linear elastic, perfectly plastic materials. Generally, amorphous materials are not expected to show hardening behavior. For isotropic materials, elastic deformation ceases and yielding commences when the von Mises yield criterion is satisfied. To predict the elastic recovery and pile-up of hard-brittle materials (amorphous silicon and borosilicate) that occur during a nanoscale indentation process, simulations were performed for various tip radii (40, 100, and 200 nm), half-angle of conical indenter ($\alpha = 55$, 60, and 65°), and tip geometries (conical, Berkovich, and spherical) using the large-strain elastoplastic feature of the ABAQUS finite element code. The materials used in the calculations are given in Table 1. The yield strength and Poisson's ratio are the values of bulk materials. In order to measure the elastic modulus and the hardness of the materials, a depth-sensing indentation experiments were performed on a Nanoindenter® XP using the continuous stiffness measurement (CSM) method. This method measures hardness and elastic modulus as a continuous function of depth into the specimen. For the experiments in this study, the CSM imposed a 1 nm oscillation at 45 Hz on the loading curve. A detailed description of the theory behind this procedure was given by Oliver and Pharr [9]. The rest of the experimental conditions are summarized in Table 2.

The diamond Berkovich having a tip radius of about 40 nm was used for the experiments. Prior to experiment, five indents were made in pure Al to clean up the tip, and then

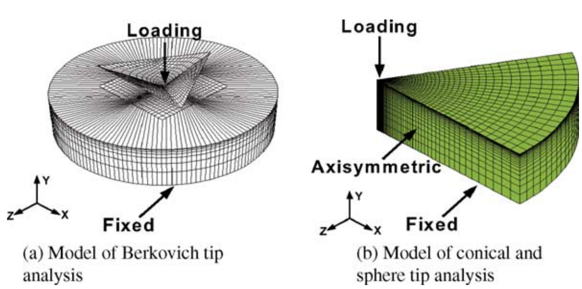

Fig. 2. Finite element models.