

# Finite Element Simulation of Nano-indentation of Bulk Materials

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In this present work, a nanoindentation model of bulk material was developed. A two-dimensional (2-D) axisymmetric model and a three-dimensional (3-D) model were developed by using the capacities of the ABAQUS finite element (FE) code. The indentation process under consideration involves a bulk material substrate indented by a rigid indenter under the condition of frictionless contact. For the 2-D model, the indenter has a half-angle of  $70.3^\circ$ , and thus has the same projected area-depth function as the standard Berkovich indenter. The use of a conical indenter simplifies the analysis of a 2-D axisymmetric problem. The models have the ability to simulate the loading-unloading curves, study the influence of structure and properties on indentation response and simulate the development of plastic deformation during indentation. The simulation results show that the load-displacement curve is in a good agreement between the simulation and experimental results.

**Key words:** Finite element modeling, nanoindentation, load-displacement curve and hardness.

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# การศึกษาแบบจำลองของนาโนอินเดนเตชันด้วยวิธีไฟไนต์ เอลิเมนต์

นุโรจน์ พานิช วีระศักดิ์ กรัยวิเชียร และ Sun Yong (2547)

วารสารวิจัยวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย 29(2)

ในงานวิจัยนี้ได้มีการพัฒนาแบบจำลองเพื่อศึกษาการอินเดนเตชันในระดับนาโนเมตร (nano-indentation) ของวัสดุด้วยวิธีไฟไนต์เอลิเมนต์ (finite element modeling) โดยสร้างแบบจำลองทั้งแบบ 2 มิติ (two-dimensional) และ 3 มิติ (three-dimensional) การพัฒนาแบบจำลองนี้ทำให้สามารถจำลองกราฟโหลดดิงและอันโหลดดิง (loading-unloading curves) ระหว่างการอินเดนเตชัน ศึกษาอิทธิพลของโครงสร้างและสมบัติของวัสดุโดยการอินเดนเตชัน อีกทั้งยังสามารถศึกษาการพัฒนาของการเปลี่ยนรูปร่างถาวร (plastic deformation) ระหว่างการอินเดนเตชัน เมื่อนำผลการคำนวณของแบบจำลองเช่นกราฟแสดงความสัมพันธ์ระหว่างโหลดและการเคลื่อนตัว (load-displacement curve) ไปเปรียบเทียบกับผลการทดลองจริงจะเห็นว่าผลลัพธ์มีความใกล้เคียงกันมากและส่งผลทำให้แบบจำลองที่พัฒนานี้มีความน่าเชื่อถืออีกด้วย

**คำสำคัญ** วิธีไฟไนต์เอลิเมนต์ นาโนอินเดนเตชัน กราฟแสดงความสัมพันธ์ระหว่างโหลดและการเคลื่อนตัว

## INTRODUCTION

Since many technologies have moved to ever smaller scale, characterization of the intrinsic mechanical properties of materials has become more difficult and complicated. Among the techniques to measure the mechanical properties of materials or thin films, nanoindentation techniques have been widely used to measure mechanical properties, for instance hardness, elastic modulus, scratch resistance, creep, etc.<sup>(1)</sup> Recently, different numerical techniques have been developed to use in many fields of science and engineering and can be used in indentation problems. Finite element technique is used for studying very complex stress-strain fields of thin film or bulk materials in a nanoindentation process. Some investigators have studied the indentation process using the numerical approach of finite element method.<sup>(2-7)</sup> The first example of comparison between FE analysis and experimental results was proposed by Bhattacharya and Nix<sup>(8)</sup> in which they simulated a sub-micrometer indentation test. The finite element method has been verified to be an effective tool for simulating hardness measurements.

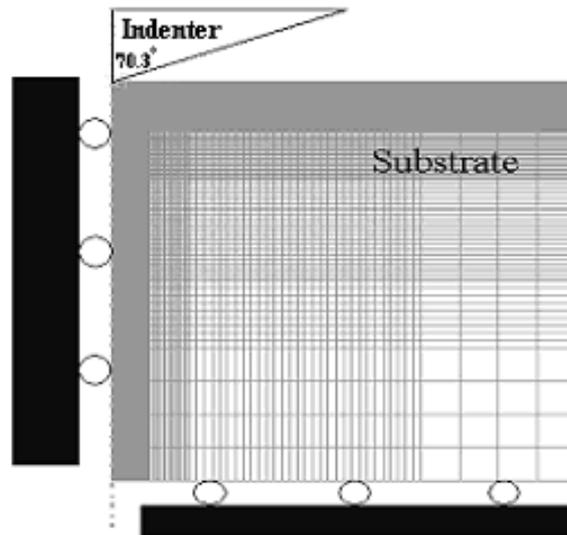
In order to gain a better understanding of the mechanical behaviour of the nanoindentation procedure, finite element modeling (FEM) was performed and discussed. The indentation modeling was performed with a commercial ABAQUS software.<sup>(9)</sup>

In this present work, the attempt has been to develop a nanoindentation model by finite element method of the bulk material. The model has the ability to simulate the loading-unloading curves, simulate the development of plastic deformation during indentation and extract intrinsic material properties from the examination.

## THE MODELLING PROCEDURE

In this model, the indentation process of bulk materials with isotropic elastic and plastic properties was simulated by the capability of the *ABAQUS* finite element (FE) code as mentioned above. The conical rigid indenter is used in the model in order to define an axisymmetric model (semi-angle = 70.3°). The specimen is modeled with 7,841 four-node axisymmetric reduced integration elements (CAX4R element type<sup>(9)</sup>), as shown in Figure 1. A fine mesh is used around the contact area and near the tip of the indenter. The mesh is continuously coarser further away from the tip, as shown in Figure 2.

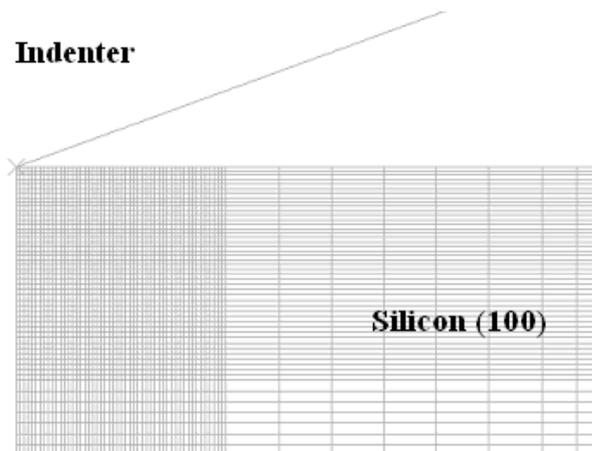
The indentation process is simulated both during the loading and unloading step. During the loading process the simulation is performed to a depth of 300 nm in the y-direction (U-2) into the specimen; during the unloading process the indenter tip returns to the initial position (0, 0, 0).



**Figure 1. Mesh of the entire silicon specimen with the indenter.**

The contact constraint is defined by the master and the slave surfaces. Because only the master surface can penetrate into the slave surface, the contact direction is then determined by the master surface. The model chooses the indenter as the master surface and the specimen as the slave surface. The boundary conditions are applied along the original point, centerline and bottom of the specimen.

The nanoindentation model developed was based on the following assumptions, there is no strain hardening of the materials used in model and there is perfect interface between the indenter and the substrate so that the indenter and the substrate will not be separated during the indentation process and the friction between the indenter tip and the specimen surface is assumed to be zero.



**Figure 2. Details of the mesh in the region near the tip of the indenter.**

In the calculation, the elastic deformation occurs in the beginning of the process. The Mises yield criterion is

applied in the occurrence of the plastic deformation. The Mises stress equation is given by the expression

$$\sigma_{Mises} = \sqrt{\frac{(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2}{2}}$$

where  $\sigma_1$ ,  $\sigma_2$  and  $\sigma_3$  are the three principle stresses. When the  $\sigma_{Mises}$  reaches the yield strength ( $\sigma_0$ ), the specimen starts to deform plastically. There is no strain-hardening behaviour of the specimen considered in the model.

since this was the only available single crystal material in the laboratory, it was thus selected to verify the model. The results of the simulation by assuming isotropic properties will surely be affected by this anisotropic behaviour. But since Si (100) was used in the experiment, using the Si (100) properties gave the best approximation. The results of the simulation are discussed later.

As a case study, Si (100) was chosen as the sample material. Although Si is an anisotropic material with mechanical properties varying with crystal directions as shown in Table 1,

**Table 1. The mechanical properties of silicon.**

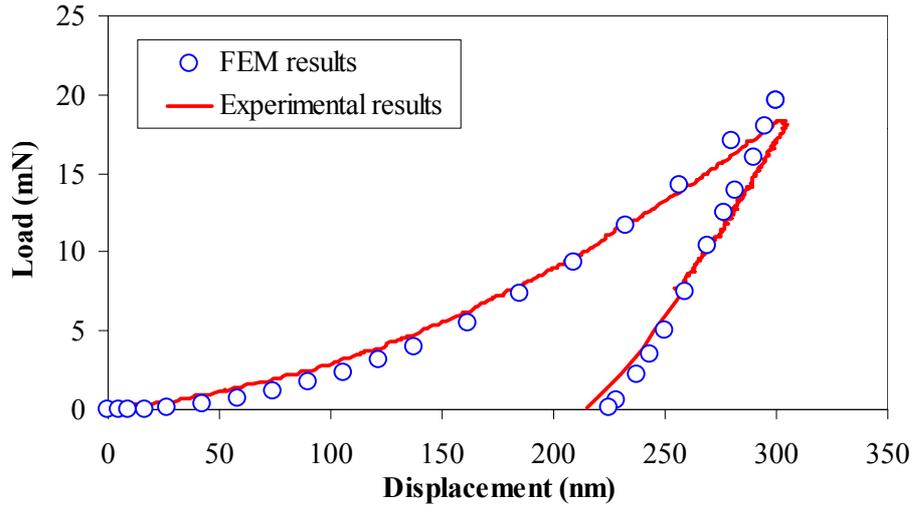
Material	Young's Modulus E (GPa)	Yield Strength Y (GPa)	Poisson's ratio	Reference
Silicon (100)	130	1	0.28	10
Silicon (110)	170	2.3	0.27	10
Silicon (111)	187	1.3	0.26	10

Regarding the experimental work, nanoindentation testing involves indenting a specimen by a very low load using a high precision instrument which records the load and displacement continuously. The mechanical properties, such as hardness and elastic modulus, can be derived from the measured load-displacement loading/unloading curve through appropriate data analysis.<sup>(11)</sup> The experiment was performed using the NanoTest™ (Micro Materials Limited, UK), at a constant loading rate of 0.2 mN/s and to a maximum depth of you mention a depth of 300 nm. Under heading the modelling procedure, we these the same 500 nm. The unloading curves were used to derive the hardness and modulus values by the analytical

technique developed by Oliver and Pharr.<sup>(11)</sup>

**RESULTS AND DISCUSSIONS**

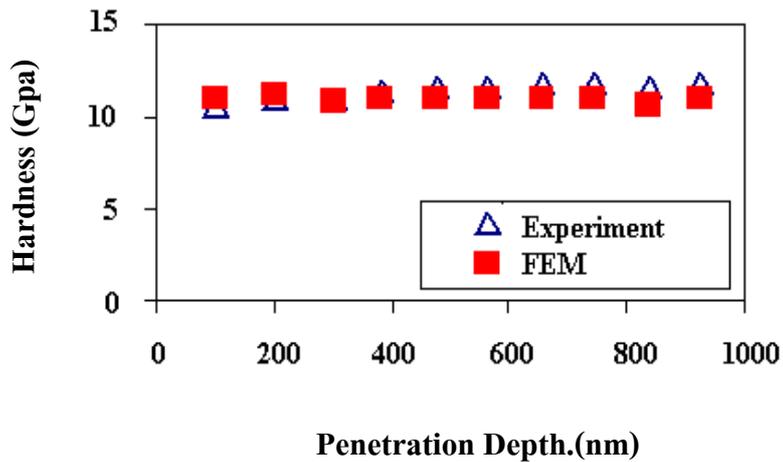
With the performance of finite element (FE) analysis, the nanoindentation loading-unloading process of bulk material, silicon (100) was simulated. Figure 3 shows the load-displacement curves that resulted from the experiment using silicon (100) together with the prediction from the simulation modelling, and the input data from Table 1. Since the experimental data were used as the basis of the simulation, such as the yield strength and Poisson's ratio, it is not surprising that there is a good agreement between the simulation and experimental results.



**Figure 3. Comparison of simulated results with experimental data.**

A further study was conducted in order to extract the intrinsic mechanical properties such as hardness using the developed FE model. From the load-displacement curves, the unloading curves were used to derive the hardness values by the analytical technique developed by Oliver and Pharr.<sup>(11)</sup> Figure 4 shows the

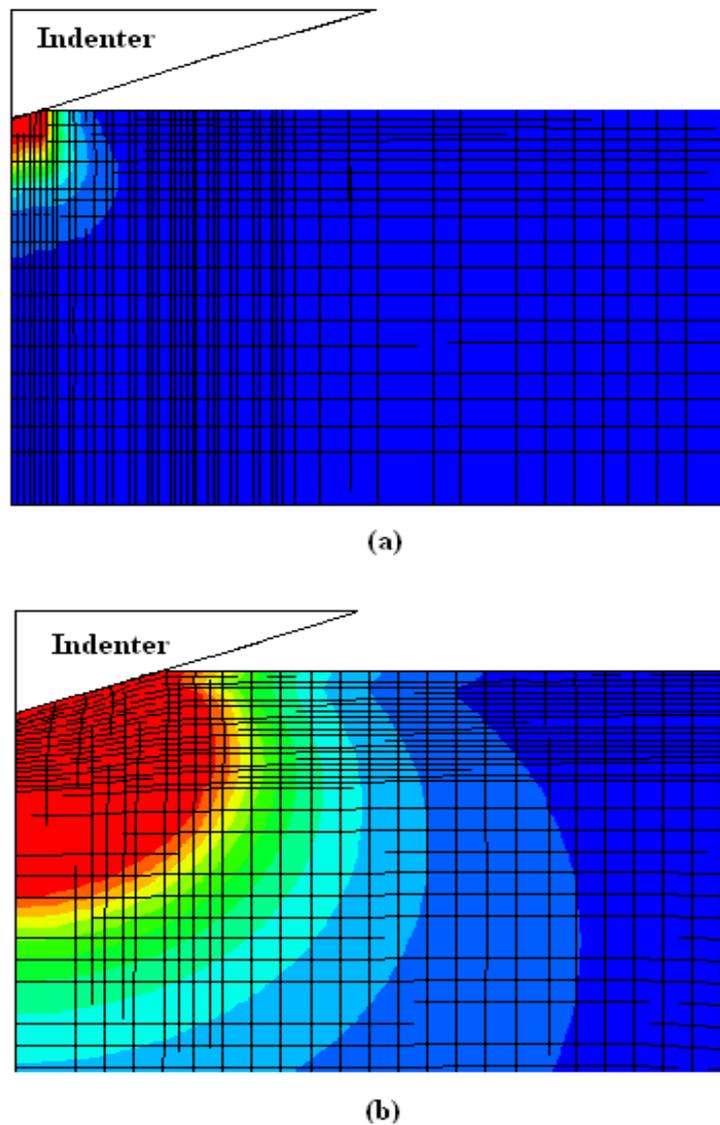
comparison of hardness between the experiment and FEM. It is noted that FEM is able to extract intrinsic material properties such as hardness. The calculated hardness is about 11.5 GPa which is in good agreement with the experiment.



**Figure 4. The comparison of hardness between the experiment and the FE method.**

The simulation of the development of plastic deformation in silicon (100) was investigated in order to gain a better

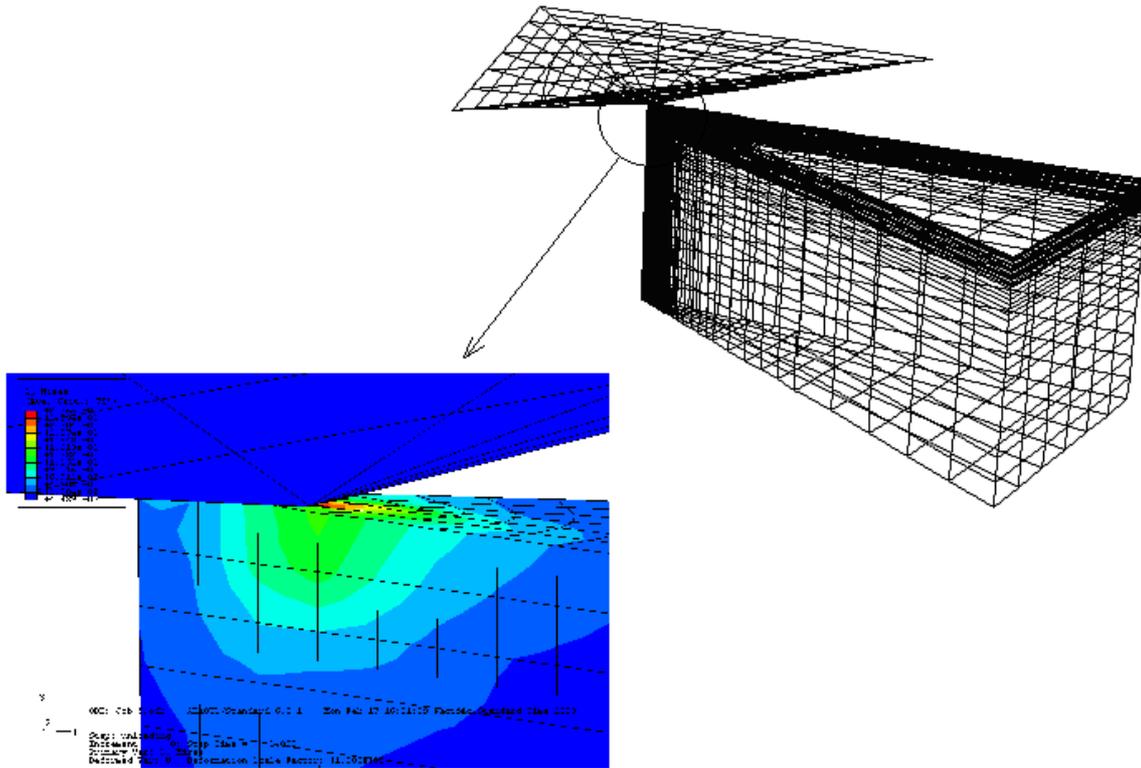
understanding of the deformation behaviour in the material as the indentation depth is increased.



**Figure 5. Development of the plastic zone in bulk material as the indentation depth is increased.**

Figure 5 shows the propagation of the plastic deformation zone in silicon (100) material. At the beginning, plastic deformation in the specimen at the interface (between indenter and specimen) is initiated and then propagated. At small indentation depths the plastic deformation takes place around the indenter tip region and propagates both vertically and laterally as a round shape (Figure 5 (a)). At larger indentation depths, plastic

deformation also propagates both vertically and laterally. A further increase in depth results in the further lateral propagation of the plastic zone in the substrate as shown in Figure 5 (b). In order to gain a better understanding of the developed plastic deformation, Figure 6 shows the propagation of the plastic deformation zone in the three-dimensional (3-D) model.



**Figure 6. The development of the plastic deformation zone as shown in 3-D FE model.**

## CONCLUSIONS

- (1) The FE model has been developed to simulate the nanoindentation response of bulk material. The model is capable of simulating the loading and unloading stages of the plastic deformation behaviour during the indentation process.
- (2) The applicability of the model has been investigated through nanoindentation of bulk silicon. The simulation result is in good agreement with the experimental results.

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