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A crystal plasticity study of the effect of friction on the evolution of texture and mechanical behaviour in the nano-indentation of an aluminium single crystal

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ABSTRACT

A crystal plasticity finite element method (CPFEM) model has been developed to investigate the effect of the coefficient of friction (COF) on the evolution of crystallographic texture and mechanical behaviour of the initially oriented aluminium single crystal during nano-indentation. The simulation results have been validated by comparing with the experimental observations. The load–displacement curves from the simulation with different COFs have been analysed and the calculated values of Young's moduli agree well with the real material. The indentation hardness with different COFs has been investigated and the deviation is quite small. The piling-up curve was captured on the deformed surface and it decreased when the COF increased. Sinking-in curve was also captured and it increased when the COF increased. The pole figures and the lattice rotation angles after unloading were calculated and then analysed. The analysis revealed that these lattice rotation angles in the chosen deformed zone were significantly affected by the COF during nano-indentation.

1. Introduction

Nano-indentation and micro-indentation have become more and more important when investigating the mechanical properties of materials at the micro-structural level. These methods have been used extensively by researchers [1–5] around the world to study the load–displacement curves, Young's modulus, size effects, sinking-in and piling-up, and the evolution of the microstructure et al. Both experiments and simulations have been carried out to compare with each other, but the coefficient of friction, possibly the most important parameter, was neglect during the finite element method (FEM) simulation.

The coefficient of friction between highly polished metallic surfaces and diamond lies between 0.1 and 0.15, as proposed by Tabor in 1951 [6]. Johnson [7] were the first group to research the effects of friction during indentation by recourse to the theory of the slip-line field. They found that the hardness increased by around 20% compared to the frictionless ones. Since then, people have paid more attention to this issue. Normal inelastic contact between spherical bodies was examined theoretically and numerically by Carlsson et al. [8]. The effect of Coulomb friction was analysed in some detail, by regarding global variables such as the mean contact pressure and contact area, as well as any field variables. It can be concluded that the effects of friction are essentially negligible except where cracks begin and then grow, in which case the stress and strain fields can be substantially influenced by friction. Moreover, the effects of friction are relatively independent of the actual value of the coefficient of friction. In Carlsson's research [8] it was proved that when $\mu > 0.4$ there was no essential difference when the results given by an analysis, assuming a finite value of the coefficient of friction, were compared with a corresponding one where full adhesive contact was assumed. Mesarovic and Fleck [9] performed a numerical study of the normal indentation of an elastic–plastic half-space by a rigid sphere, and where the friction was also assessed by analysing the FEM cases of frictionless contact and sticking friction. The results showed that friction strongly affected the strain field beneath the indenter and had a quantitative effect on the size of the contact, as a function of indent depth. However, it was also reported that the contact stiffness was almost the same for sticking and for frictionless indentation within a similarity regime. Mata and Alcala [6] conducted the experimental and simulated researches on the role of friction on sharp indentation. Their analyses showed that friction caused more material to pile up around the contact area, while materials that develop moderate piling-up or sinking-in are less sensitive to friction.

Although the aforementioned researchers did extensive studies on the effect of friction on materials deformed during indentation, the evolution of the microstructure of materials was never investigated. Meanwhile, a crystal plasticity finite element method

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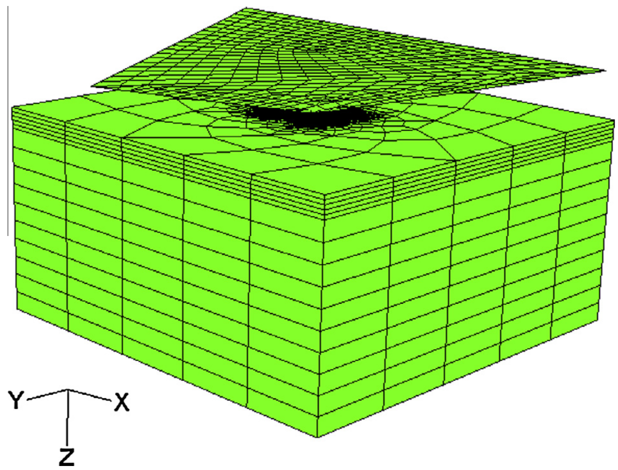

Fig. 1. 3-D nano-indentation model setup.

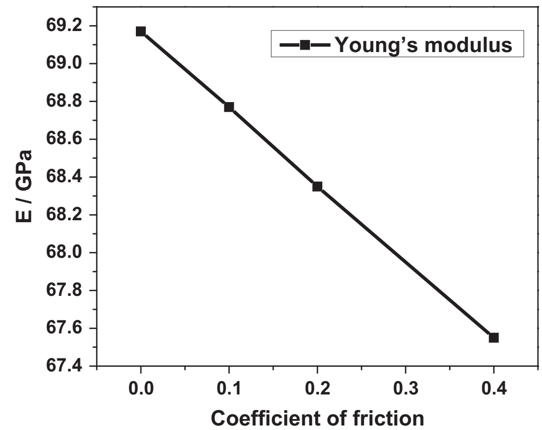

Fig. 3. Comparisons of Young's modulus for different COFs.

(CPFEM) model, which incorporates crystal plasticity constitutive equations (crystallographic slip, lattice rotation, rate-dependent hardening model, etc.) into a finite element framework, was never used to investigate friction caused by indentation. Therefore in this study, a CPFEM model is used to study the effect of friction on aluminium single crystal during indentation.

2. Finite element implementation

Crystal plasticity theory is based on an assumption that plastic deformation is the sum of crystalline slip in all activated slip systems. This is the very popular theory to be used to explain the plastic deformation of single crystals [10–12]. The crystal plasticity constitutive model used here follows the line described by Asaro [13] and it was incorporated into the implicit finite element code ABAQUS/Standard through the user material subroutine (UMAT). The noticeable functions of UMAT are to provide the material with the Jacobian matrix $\partial\Delta\sigma/\partial\Delta\varepsilon$ for the constitutive model, and to update the stresses and the solution dependent state variables. In this study, we followed the UMAT framework initially developed by Huang [14] and used Bassani Wu's formulation [15] as the hardening model.

The commercial software Abaqus 6.9 was used to simulate the deformation of nano-indentation. A three dimensional model was created to describe the behaviour of nano-indentation, as shown in Fig. 1. The indenter used here is a Berkovich with a radius of 200 nanometres. The specimen consisted of 17,040 eight-node brick elements and 18,352 nodes with reduced integration (element id: C3D8R) to make sure the mesh was fine enough, especially the area that makes contact with the indenter, which is much finer than the other regions. The total number of nodes and elements are about 7 times more than those used in most published papers [16,17], because the depth of indentation in this study is much bigger (1000 nm and 2000 nm) than in the literature (300 nm) [16,17]. The *X*, *Y*, and *Z* coordinates represent the rolling direction (RD), the transverse direction (TD), and the normal direction (ND), respectively. In this model the cube orientation is set as the initial orientation, namely the normal of slip plane (001) parallel to the *Z* axis and the [100] slip direction parallel to the *X* axis. The tangent stiffness matrix (Jacobian matrix) is not symmetric because the latent hardness is considered. It must be declared "unsymm" in the input file at the user material card.

The dimensions of the work piece in the FEM model are $40 \times 40 \times 20\ \mu m^3$. The height of the 3D model is much larger than the maximum depth of indentation of 2 μm. This satisfies the rule that the specimen should be 10 times thicker than the depth of indentation in order to avoid the influence from the substrate.

An aluminium single crystal was used to investigate the micro-scale behaviour under nano-indentation because it is easier to study plastic deformation in a single crystal and eliminate the effects of grain boundaries and second phase particles. All the nodes on the bottom surface and four surrounding surfaces of the work piece were constrained along three axes by considering the real conditions of indentation (the metal sample is mounted inside a piece of resin with only the top surface free). A Coulomb friction model was chosen in the simulation because it is suitable for a low friction (lubricated cold processes) [18]. Four different coefficients of friction (μ = 0, 0.1, 0.2, and 0.4) were used in the simula-

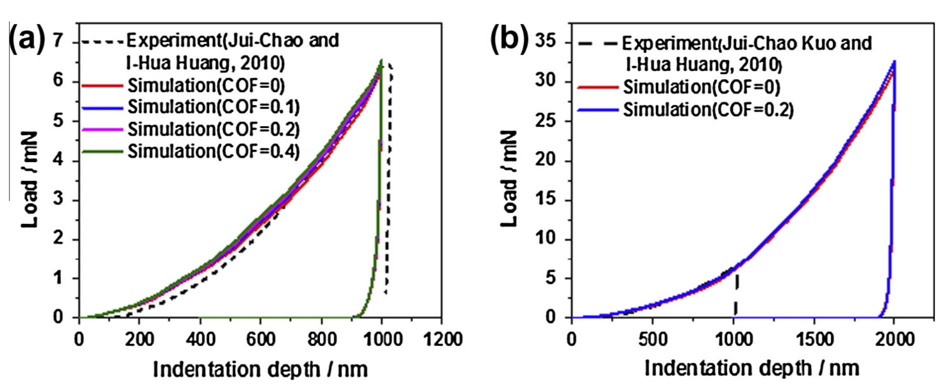

Fig. 2. Simulated and experimental load–displacement curves for aluminium: (a) 1000 nano and (b) 2000 nano.