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Crystal Plasticity Finite Element Modelling of Surface Roughness and Texture of Metals

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Abstract

A crystal plasticity finite element method (CPFEM) model was developed to analyse the surface roughness transfer and texture of metals during metal forming. In order to investigate the crystal slip mechanism and influence of different polycrystalline models (Taylor-type model and finite element polycrystalline model) on finite element modelling, the uniaxial compression of FCC pure aluminium was carried out in laboratory, and the Taylor-type and finite element polycrystalline models are separately employed in the finite element software ABAQUS to simulate the development of the deformation texture by rate dependent crystal constitutive equations during three different deformation modes (free compression, uniaxial planar compression and uniaxial tensile). The results obtained from the three different deformation modes show the same tendency that, with an increase of strain, the silk texture tends to be stronger and sharper. Both Taylor-type and finite element models can predict the tendency and silk texture. The simulation result is in good agreement with the experimental result in the surface asperity flattening process, and with an increase of reduction, the surface roughness tends to decrease significantly, lubrication can hinder the surface asperity flattening process effectively.

Keywords: Surface roughness, Texture, CPFEM, Uniaxial compression

Introduction

Surface roughness is an important parameter of surface quality, and it is also an interesting topic in cold metal manufacturing. In general, there are many reasons which result in surface roughness variation, such as the original surface roughness of the product, grain size, crystal structure, crystal orientation, texture distribution, loading path, stress-strain state (deformation mode) and tool surface etc. There are literatures in terms of the surface asperity flattening. The effect of bulk plasticity on asperity flattening has investigated when the lay of the roughness is parallel to the bulk straining direction (longitudinal roughness) (Sheu and Wilson, 1983; Wilson and Lee, 2001). They found that the rate of asperity flattening with bulk straining was related to the spacing and pressure of asperities. Makinouchi et al. (1988) have presented some elastic-plastic finite element solutions for the case of transverse roughness. Sheu and Wilson (1983) also found out that a large increase of contact area with bulk strain and a reduction in load needed for bulk yielding. Sutcliffe (1988) tested and developed Wilson and Sheu’s theories, he pointed out that the high pressure between contacting asperities and deformation of bulk material will affect the asperity deformation. Raabe et al. (2003) studied the grain-scale micromechanics of polycrystal surface. However, there are few reports studied the interaction between the surface asperity flattening and grain parameters (grain structure, orientation and size) and friction. In order to figure out the relationship between the sample surface asperity flattening, grain parameters and friction, a finite element model is employed in the commercial finite element software ABAQUS to simulate the surface asperity flattening of aluminium plate along the rolling direction during uniaxial planar compression. Based on the finite element polycrystal model, a 2D rough surface model is generated in this study. Influence of friction in the surface asperity flattening process is also analysed. Texture development in different deformation modes (free compression, uniaxial planar compression and uniaxial tensile) are also studied. Influences of different polycrystal models on the texture development are also discussed in this study.

Crystal Plasticity Models

Single grain model. The crystal plasticity constitutive model and the associated numerical procedures are applied to the commercial finite element code ABAQUS. Due to the simple relationship between the single crystal plasticity model and the polycrystal plasticity model, the single crystal model is selected to describe the stress response of polycrystal plasticity deformation. The single crystal plasticity model that is utilised in this study is summarised as follows.

Following Kalidindi and Anand (1992), the total deformation gradient ($F$) can be decomposed into elastic and plastic deformation as

$$F = F^p : F^P \quad \text{det} \; F > 0,$$

The constitutive equation for stress in the crystal can be expressed as

$$T^{(l)} = L : E^{(l)} = F^{*-1} \left\{ \text{det} \; F^* \right\} T^* F^{*-T},$$

$$E^{(l)} = \frac{1}{2} \left( F^* T^* F^* - I \right),$$

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where \( T^{(i)} \), \( F^{(i)} \) are a pair of work conjugate stress and strain measures. The velocity gradient of plastic deformation can be expressed as

\[
F^{(p)} = \sum_{\alpha=1}^{n} \mathbf{\dot{\gamma}}^{\alpha} \mathbf{u}_0^\alpha \otimes \mathbf{v}_0^\alpha,
\]

\[
S_0^\alpha = \mathbf{u}_0^\alpha \otimes \mathbf{v}_0^\alpha,
\]

where \( \mathbf{u}_0^\alpha \) indicates the slip direction of the slip system \( \alpha \),
\( \mathbf{v}_0^\alpha \) is the slip plane normal of the slip system \( \alpha \).

The shearing rate on each slip system depends on the resolved shear stress \( \tau^\alpha \) and the slip resistance \( s_\alpha \) of that slip system. From Kalidindi et al. (1992), it can be expressed in a power-law relationship as

\[
\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \text{sgn}(\tau^\alpha) \left[ \frac{\tau^\alpha}{s_\alpha} \right]^{1/t},
\]

\[
\tau^\alpha \approx T^\alpha \cdot S_0^\alpha
\]

In this simulation, \( \dot{\gamma}_0 \) is taken as 0.001s\(^{-1}\) and \( t \) is 0.001. The slip system resistance rate can be expressed in the following general form.

\[
s^{\alpha} = \sum_{\beta=1}^{n} h_{\alpha\beta} \left| \dot{\gamma}^{\beta} \right|,
\]

The rate of strain hardening \( h_{\alpha\beta} \) can be expressed as

\[
h_{\alpha\beta} = q_{\alpha\beta} h^{\beta},
\]

where \( h^{\beta} \) is the single slip hardening rate, and \( q_{\alpha\beta} \) is a matrix describing the latent hardening behaviour of a crystallite. The single slip hardening rate can be obtained as

\[
h^{\beta} = h_0 \left( \frac{1 - s^{\beta}/s_s}{1} \right)^l,
\]

where \( h_0 \), \( l \) and \( s_s \) are the hardening parameters of the slip system.

**Taylor averaging procedure.** In Reference (Kalidindi and Anand, 1992), the stress response at each macroscopic continuum material point is given by the volume-averaged response of the multitude of microscopic single crystalline grains comprising the material point. The essential as-

sumptions in the Taylor-type polycrystal model are that all grains have equal volume, and that the local deformation gradient in each grain is homogeneous and identical to the macroscopic deformation gradient \( F \) at the continuum material point level. Then, with \( T^{(k)} \) denoting the Cauchy stress in \( k \)th crystal, these assumptions lead to:

\[
\bar{T} = \frac{1}{N} \sum_{k=1}^{N} T^{(k)},
\]

where \( \bar{T} \) is the volume averaged stress, and \( N \) is the total number of grains comprising the material point.

**Finite element averaging procedure.** In our study, finite element calculations are employed to make the transition from the response of a single grain (or a region within a grain) to the response of a polycrystalline aggregate. It is assumed that each element represents one crystal and is assigned an orientation as the initial texture. So each grain is modelled to allow non-uniform deformation between the grains and within the grains, and both equilibrium and compatibility are satisfied in the weak finite element sense. In this study, a 2D rough surface model is generated from the finite element averaging procedure. The influence of friction has also been taken into account. The influence of Taylor model (free deformation) and finite element model (uniaxial planar deformation) on the simulation results are analysed separately.

**Experimental**

The workpiece was polished by the auto polishing machine along the transverse direction, and the surface roughness distribution along the rolling direction was also polished with the sand papers of grade P220. All the workpieces have been restricted to have a surface roughness of about 0.7\( \mu m \). A 2D profilometer (Hommel Tester T1000 surface profile meter) is used to measure the sample surface roughness. Before the compression, a central line is drawn on the top surface of the sample, and surface roughness is measured along this line. After the compression, the surface roughness is measured along the same line. Three dimensional surface roughness can be measured by the AFM (Atomic Force Microscopy). All the parameters for AFM scanning are shown as: scan size is 60\( \mu m \), scan rate 1.00 Hz, number sample is 512, image data is height, and data scale is 6.140\( \mu m \). Before compression, a certain area of the sample is marked by colourful pen. After compression, the surface roughness is measured in the same area. When the compression takes place, the sample is constrained in the transverse direction. The workpiece’s deformation develops along the rolling direction. The compression test has been carried out in the Instron MTS. The workpiece size is 10\( mm \times 10\)mm\times 6mm. The surface roughness of workpiece is shown in Fig. 1a. Reduction ranges from 5-40%. Two groups of workpieces are carried out in the compression. One group of samples are compressed with lubricant, the other are compressed by the tool directly. The lubricant used in this experiment
is Molykote BR2-plus. At 40°C/104°F, the base oil viscosity is 114 mm²/s.

Figure 1. Surface roughness under different conditions: (a) original surface roughness, (b) surface roughness after 40% (with lubrication), (c) surface roughness after 40% (without lubrication).

During the compression, it is obvious that with an increase of reduction (reduction refers to the reduction of the height in the compression), the workpiece surface tends to be flattened (Figs. 1 and 2). Under the condition of without lubrication, if the reduction increases from 0 to 40%, the surface roughness of workpiece decreases rapidly from 0.7 to 0.1 µm (Figs. 1c and 2c). When the workpiece is compressed with lubrication, the surface asperity flattening process takes place slowly. If the reduction increases from 0 to 40%, the surface roughness will decrease from 0.7 to 0.2 µm (Figs. 1b and 2b). After the compression, the workpiece surface qualities are also different. It is obvious that, under the same reduction, the workpiece compressed with lubrication has a much smoother surface. It has no obvious surface scratches. While the workpiece compressed without lubrication, it has flat surface with some surface scratches. During the compression, the lubrication can constrain the surface asperity flattening process effectively. It can also reduce the friction between the workpiece and tool significantly. Then the surface scratches could not be formed easily. During the compression, if the workpiece contacts with tool directly, its surface will be dependent upon the tool surface. In our study, the tool is smooth, and its surface roughness is only about 10 nm. Therefore, after compression, the workpiece surface will be about 10 nm. When reduction is 5-30%, a lubricant layer will be formed. This will hinder the contact of compressing tool and sample, and reduce the decrease of sample surface roughness. Before the compression, the lubricant layer thickness is about 2-3 mm, after more than 30% reduction, the lubricant layer will be destroyed and disappeared.

Figure 2. 3D surface asperity under different conditions: (a) original surface, (b) after 40% height reduction with lubrication and (c) after 40% height reduction without lubrication.

Simulation

The workpiece material is 6061 T5 aluminium alloy. Size of the two-dimensional model is 500 µm x 500 µm. The original surface roughness of the three workpieces is
0.72μm. The reduction of workpieces ranges from 5 to 40%. Contact friction coefficient between the workpiece and rigid compressing tool and mold ranges from 0.001 to 0.35. The reduction is applied to the top of the workpiece by the rigid compressing tool. Due to symmetry, all the nodes on edge ab (Fig. 3) have no displacement in direction 1. A finite element polycrystal model is employed in this study. The two dimensional model has 902 CPE4R reduced integration elements, and one grain set with one element. The rigid tool and mold both have 20 discrete rigid elements. Kalidindi’s method (Kalidindi and Anand, 1992; Kalidindi et al., 1992) was used to incorporate crystal plasticity into FEM. The constitutive model and time-integration procedures were implemented into the implicit finite element code ABAQUS by employing the user material subroutine UMAT. The combinations of slip systems were taken into account during modelling, including 12 \{110\}<111>. It was assumed that the shearing rate is equal on each slip system. 902 random Euler angle triplets was input into ABAQUS as the initial crystallographic condition of the model. From Brandes (1999), the components of the elasticity tensor were taken as $C_{11} = 106750\,\text{MPa}$, $C_{12} = 60410\,\text{MPa}$, $C_{44} = 28340\,\text{MPa}$. We followed Asaro and Needleman (1985), and took the parameters as, $q_{ab} = 1.0$ for coplanar systems and $q_{ab} = 1.4$ for non-coplanar slip systems. The other material parameters were according to Raabe et al. (2005) work.

![Figure 3. Two dimensional model and mesh.](image)

**Texture Development under Different Deformation Conditions**

Pi (2006) simulated texture development in free compression and tensile test. He did not consider the influence of friction and roughness on the deformation. The deformation of his models was free deformation. In our study, a 2D rough model is built up based on the theory of crystal plasticity finite element method, and the influence of friction is also employed in the simulation. Compared to his simulation results, the situation for texture development in our study is more complicated and applicable. Simulation results are in good agreement with Pi’s results. No matter what the deformation is, the silk texture will be stronger and sharper with an increase of strain (load). Then the preferred textures <111>, <110> and <100> will be more obvious. In the simulation of uniaxial planar compression, friction can constrain the forming of the preferred silk texture <100>, and promote the forming of silk texture <110>.

![Figure 4. Pole figure {111} of different conditions: (a) Free compression without friction, (b) Uniaxial planar compression with friction.](image)
texture lies in the centre of the pole figure. At the same
time, a few grains distribute along the axis <110> and
<113>. With an increase of reduction, the silk textures
<110> of two models tend to be stronger (Fig. 4a). This
result agrees with the EBSD experimental result. In the
uniaxial compression, silk textures <110> and <111> are
formed, but not concentrate in the pole figure centre.
The texture shape is not snowflake. As shown in Fig. 4b,
the centre of pole figure is the symmetrical centre of silk
texture. With an increase of strain, the texture also tends to
be stronger and sharper. The difference between the two
different compression modes is that in the free compres-
sion, the majority of grains will rotate along the compres-
sion axis. However, in the uniaxial planar compression,
the deformation could not take place along the transverse
direction 3. Friction also influences the grain rotation. In
this process, with an increase of friction coefficient, the
snowflake shape texture is not significant. When the com-
pression takes place, the contact friction will constrain the
rotation of grains along a certain axis. It can hinder the
forming of planar strain silk texture.

Comparison with the texture development of uniax-
ial tension. For the uniaxial planar compression, the de-
formation takes place along the longitudinal and normal
directions. This process is similar to the uniaxial tension.
As shown in Fig. 5a, the finite element model and Taylor
model show a good agreement, they both predict the
<111> silk texture and <100> silk texture well. The silk
texture <111> is much stronger than that of silk texture
<100>. In the uniaxial tension, <111> orientation of some
gains rotate and distribute along the tensile axis. <100>
orientations of other grains rotate and distribute along the
tensile axis. In the uniaxial planar compression, the silk
textures <111> and <110> can be obviously predicted. As
shown in Fig. 5b, when the strain is 0.25, the deformation
is small, and only a few grains can be activated and rotate.
So when the true strain is 0.25, the silk texture is not very
strong and obvious. In the uniaxial planar compression,
only silk textures <111> and <110> are formed. While in the
uniaxial tensile, silk textures <111> and <100> are
formed.

Analysis of Surface Roughness Development

The effect of reduction and surface roughness is shown
in Fig. 6. It can be seen that the experimental results are
close to the simulation results. Both results show that, with
an increase of reduction, the surface roughness of work-
piece decreases quickly, and lubrication can delay the
process of surface asperity flattening. On the other hand,
there is difference between the experimental and simulated
results. The simulated result has the large decreasing rate
of surface roughness than that of the experimental result.
In Fig. 6a, when the reduction is less than 10%, the two
results keep the same tendency of surface asperity flatten-
ing. When the reduction exceeds 10%, though the two
curves keep the similar tendency, the decreasing rate of
surface roughness from simulation is a bit larger than that
obtained from experiment. In the experiment, when the
reduction exceeds 10%, the lubrication layer can play a
remarkable role in delaying surface asperity flattening.
However, in the simulation, we just use the penalty fric-
tion coefficient to replace. When the reduction is between
10 and 40%, the lubrication layer can keep its function
properly. So the difference between the simulated and
experimental results is significant. When the reduction
exceeds 40%, the lubrication layer will be damaged, and
cannot continue to hinder the surface asperity flattening.

Figure 5. Pole figures {111} and {100} of different condi-
tions: (a) uniaxial tensile without friction (ε=0.25) and (b)
uniaxial planar compression with friction (ε=0.25).

Conclusion

From the comparison of experimental and simulation
results, the following conclusion can be obtained.
(1) The experimental and simulation results both pre-
dict the same tendency that, an increase of reduc-
tion, surface roughness decreases greatly. Lubri-
cation can hinder the decrease of surface roughness in the compression.

(2) Different deformation modes play an important role on the texture development: in free compression (without lubrication), only silk texture $<110>$ is formed. In the uniaxial compression, silk textures $<111>$ and $<110>$ are formed. In the uniaxial tensile, silk texture $<111>$ and $<100>$ are formed.

(3) Both the results of two polycrystal models show a good agreement that, with an increase of strain (load), the texture will be stronger and sharper. Silk texture from the Tay-model is much stronger than that from the finite element model.

(4) Friction can hinder the development of silk texture in the uniaxial compression process.

![Graphs showing surface roughness vs. reduction with and without lubrication.]

Figure 6. Relationship between the surface roughness and reduction: (a) with lubrication, (b) without lubrication.

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