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Crystal plasticity FEM study of nanoindentation behaviors of Cu bicrystals and Cu–Al bicrystals

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A crystal plasticity finite element constitutive model combined with Bassani and Wu hardening law has been developed to investigate the effects of grain/phase boundary (GB/PB) on mechanical properties and microtexture evolution of Cu bicrystals and Cu–Al bicrystals during nanoindentation process. The simulated load–displacement curve for the Cu single crystal with Goss initial orientation has been analyzed and compared with the result from the experiment to validate the parameters. The numerical results indicate that the effects of GB/PB on load–displacement curves, indentation Young's moduli, Mises stresses, pile-up patterns are insignificant for Cu bicrystals while they are significant for Cu–Al bicrystals. The main reason is that PB works as a very effective barrier to resist the plastic slip propagation of the deformed material. The effects from different misorientations of GBs/PBs are insignificant for both Cu bicrystals and Cu–Al bicrystals. The effects of GB/PB on lattice rotation angles for both Cu bicrystals and Cu–Al bicrystals are significant.

I. INTRODUCTION

Nanoindentation of materials is the most popular method to determine their mechanical properties at both micro- and nanoscales. The load–displacement curve, the Young's modulus, and the indentation size effect have been widely studied by both experimental and modeling methods (e.g., Refs. 1–6). However, most of the studies have focused on discovering the mechanical properties of a single grain by using single-crystal materials or polycrystalline materials due to the fact that the indent is quite small and can be located within a grain of the materials. In polycrystalline materials, two adjoining crystals that are dissimilar in orientation or structure form an interface. The interface formed by two crystals with the same structure but different orientations is often called grain boundary (GB); while the interface formed by two crystals of different lattice structures is called phase boundary (PB).⁷ Recently, there has been an increasing concern about the interface effects of polycrystalline materials on their nanoindentation behaviors.

Britton et al.⁸ studied the slip transfer phenomenon at GBs by nanoindentation tests. A pop-in event which is a sudden displacement jump was observed in the loading

part of load–displacement curve for body-centered cubic (BCC) materials but not face-centered cubic (FCC) materials. Ohmura et al.⁹ investigated dislocation-GB interactions in martensitic steel through in situ nano-indentation in a transmission electron microscopy (TEM). It was found that the dislocations produced by the indentation were simply absorbed into the boundary, without dislocation pileup or the transmission of strain. Wang and Ngan¹⁰ found the pop-in phenomenon by doing indentation near GB in niobium. Its occurrence was rationalized in terms of slip transmission across the GB. Wo and Ngan¹¹ investigated the influence of GBs on material deformation in Ni₃Al by carrying out nano-indentation tests near its GB. They found that hardness is not a sensitive parameter to measure GB strengthening effects. Ohmura et al.¹² found the same phenomenon by performing the nanoindentation tests in the vicinity of single GB of interstitial-free steel. Lee et al.¹³ reported a significant change of hardness close to GB of the Ni₃Al bicrystal. However, their results could not be reproduced by other researchers.¹¹ A few studies showed that there is a weak dependence of hardness on the distance from the GB when using low maximum loads for hardness measurement.^{14–17} Eliash et al.¹⁸ did a systematic investigation of it and found that the trend vanished when the indentation loads exceeded 10 mN using a Berkovich indenter. Furthermore, Nilsen and Subramanian¹⁹ performed indentation studies on two-phase bicrystals of alpha-beta brass with various geometries of the PB to discover its role in the propagation

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of deformation. The PB acted as a very effective barrier for slip propagation, irrespective of its geometry.

However, the nanoindentation tests cannot capture the detailed three-dimensional (3D) microstructure information including misorientation map of deformed materials. Thus, 3D crystal plasticity finite element method (CPFEM) simulation has been used to study the nanoindentation behaviors extensively. It is different from the conventional FEM which cannot capture the anisotropy and orientation evolution in crystalline materials during indenting process. The conventional FEM does not contain the constitutive model based on the fact that plastic deformation occurs by crystallographic slipping on slip systems and the rotations of the crystal lattices. Therefore, 3D CPFEM which considers dislocation slips and lattice rotations as the only deformation mechanism plays an important role in investigating mechanical properties of single-crystal and polycrystal materials.

The 3D CPFEM study of the mechanical behavior, microstructure and microtexture evolution for single-crystal materials via nanoindentation modeling was frequently reported for the last decade.²⁰ Kalidindi et al.²¹ simulated the load-indentation depth curve of the forging process and the result agrees with that from the experiment. A combination of 3D discrete dislocation simulation and the FEM was developed by Fivel et al.²² to study the formation of an indent-induced plastic zone during nanoindentation on copper single crystal. The simulated microstructure has been directly compared to that obtained from TEM observations. It showed that both the simulated dislocation microstructure and the corresponding indent-induced plastic volume were quite realistic. Liu et al.²³ determined the mesoplastic parameters for CPFEM model by fitting the simulated load-displacement curves to the experimental data and used them to determine the stress-strain relationship of a single-crystal copper at meso-scale. They also conducted the simulations using a commercial finite element code (ABAQUS) with a user-defined subroutine (VUMAT) that incorporates crystal plasticity constitutive model to discuss the orientation effects in nanoindentation of single-crystal copper.²⁰ Zaafarani et al.²⁴ used 3D CPFEM to investigate the texture and microstructure below a nanoindent in a Cu single crystal and compared the results with those from electron backscatter diffraction (EBSD) tests. Although the simulations failed to predict the fine details of the patterning of the rotation directions with the frequent changes in sign observed in the experiment and overemphasize the magnitude of the rotation field tangent to the indenter, they showed a similar pattern for the absolute orientation changes and provided details of the shear distribution in the deformation zone on the different slips systems. Zaafarani et al.²⁵ also used a CPFEM which is based on a dislocation density-based constitutive model to study the plastic deformation-induced rotation patterns below

nanoindents. By comparing to the experiment, it was found that the complex rotation pattern induced during conical indentation was well predicted. Lee and Chen²⁶ observed the size effect in the microindentation of FCC single-crystal copper modeled by the employment of mechanism-based strain gradient crystal plasticity. Recently, Eidel²⁷ found experiments and CPFEM simulations were in agreement about predicting pile-up during indentation on the surface of a single crystal material. However, the modeling of nanoindentation behavior with polycrystal materials is much more complicated due to the complex nature of the polycrystals and the challenges in modeling 3D grains. Thus, most of the CPFEM modelings were carried out on either polycrystals in 2D or single crystal in 3D.²⁸

Recently, Li et al.²⁸ are the first and only group that proposed an approach to study 3D CPFEM simulation of nanoindentation on aluminum alloy. It was found that high angle GBs act as barriers to cause local stress concentrations. However, it contradicted with previous experimental reports indicating there is little resistance to slip transfer across GBs for FCC metals.⁸ Besides, the study only discussed the effects of GB from one-phase FCC metal. Does the grain/phase boundary (GB/PB) affect a one-phase FCC bicrystal and a two-phase FCC bicrystal differently? Do GBs/PBs with different misorientations affect the same material significantly? To answer above questions, the 3D bicrystal CPFEM model has been established to investigate the effects of GBs on nanoindentation behaviors. The Voronoi tessellation method has been used to develop the 3D bicrystal model, which is exactly the same as developing 3D polycrystal. However, comparing to the polycrystal, the bicrystal is able to provide much more details to define the GB/PB. To the best knowledge of authors, it is the first work to simulate the behavior of GB/PB in both one-phase bicrystalline material and two-phase bicrystalline material during nanoindentation deformation through crystal plasticity theory.

II. CONSTITUTIVE MODELS AND FINITE ELEMENT SIMULATIONS

A. Kinematics of crystalline deformation

The quantitative description of kinematical theory for the mechanics of elastic-plastic deformation of crystals is derived from the earlier work done by Taylor²⁹ and Hill.³⁰ It is found that material flows through the crystal lattice via dislocations gliding along the corresponding slip systems. The constitutive models used here follows the earlier works by Asaro,³¹ Asaro and Rice³² and Huynh.^{33–35}

The crystalline material under load undergoes crystallographic slip due to dislocation motion on the active slip systems and elastic deformation including stretching and rotating of the crystal lattice,^{31–33,36,37} which leads to a hypothesis that the crystallographic slipping may be supposed to firstly occur from the reference configuration

to the intermediate configuration, followed by the elastic stretching and rotation from the intermediate configuration to the current configuration. Therefore, three configurations have been proposed to describe the deformation process. The initial configuration corresponds to the original undeformed state of the element and the current configuration corresponds to the deformed state of the element. The intermediate configuration is obtained from the current configuration when relaxing the lattice elastic stretching and rotation. The total deformation gradient $\mathbf{F}$ can be decomposed into two different components, namely $\mathbf{F}^*$ and $\mathbf{F}^P$ as

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \mathbf{F}^* \cdot \mathbf{F}^P, \quad (1)$$

where $\mathbf{X}$ represents the position of material points in the reference configuration and $\mathbf{x}$ denotes the position of material points in the current configuration. Here, $\mathbf{F}$ is the total deformation gradient, $\mathbf{F}^*$ describes the elastic deformation gradient including the stretching and rotation of the crystal lattice, and $\mathbf{F}^P$ indicates the crystallographic slip on the slip system, which can be written as

$$\mathbf{F}^P = \sum_{\alpha=1}^N \mathbf{F}^{(\alpha)P} = \sum_{\alpha=1}^N \mathbf{I} + \gamma^{(\alpha)} (\mathbf{s}_0^{(\alpha)} \otimes \mathbf{m}_0^{(\alpha)}), \quad (2)$$

where $\mathbf{F}^{(\alpha)P}$ is the contribution of the α -th slip system to $\mathbf{F}^P$, $\gamma^{(\alpha)}$ is the shear strain of α -th slip system, $\otimes$ indicates the dyadic product of two tensors or vectors, $\mathbf{I}$ is a second-order unit tensor, and N is the number of activated slip systems. The Green strain tensor can be written as

$$\mathbf{E} = \frac{1}{2} (\mathbf{F}^T \mathbf{F} - \mathbf{I}). \quad (3)$$

$$\mathbf{s}_0^{(\alpha)} \cdot \mathbf{m}_0^{(\alpha)} = 0. \quad (4)$$

Both $\mathbf{s}_0^{(\alpha)}$ and $\mathbf{m}_0^{(\alpha)}$ will not be changed during crystallographic slip from the initial configuration to the intermediate configuration but converted with the lattice when the lattice is stretched and rotated from the intermediate to the current configuration. The slip direction vector $\mathbf{s}_0^{(\alpha)}$ can be given in the deformed configuration by

$$\begin{aligned} \mathbf{s}^{(\alpha)} &= \mathbf{F}^{(\alpha)} \cdot \mathbf{s}_0^{(\alpha)} = \mathbf{F}^* \left[\sum_{\alpha=1}^N \mathbf{I} + \gamma^{(\alpha)} (\mathbf{s}_0^{(\alpha)} \otimes \mathbf{m}_0^{(\alpha)}) \right] \mathbf{s}_0^{(\alpha)} \\ &= \mathbf{F}^* \cdot \mathbf{s}_0^{(\alpha)}, \end{aligned} \quad (5)$$

and the normal to the slip plane $\mathbf{m}_0^{(\alpha)}$ after deformation can be written as

$$\mathbf{m}^{(\alpha)} = \mathbf{s}^{(\alpha)-1} = (\mathbf{F}^* \cdot \mathbf{s}_0^{(\alpha)})^{-1} = \mathbf{m}_0^{(\alpha)} \cdot \mathbf{F}^{*-1}. \quad (6)$$

It should be noted that $\mathbf{s}^{(\alpha)}$ and $\mathbf{m}^{(\alpha)}$ are not in general unit vectors but remain orthogonal as

$$\mathbf{s}^{(\alpha)} \cdot \mathbf{m}^{(\alpha)} = 0. \quad (7)$$

In the crystalline coordinate system, for an FCC crystal, $\mathbf{s}^{(\alpha)}$ and $\mathbf{m}^{(\alpha)}$ are given by

$$\begin{aligned} \mathbf{s}^{(1-3)} &= \frac{1}{\sqrt{3}} (1, 1, 1), \mathbf{s}^{(4-6)} = \frac{1}{\sqrt{3}} (-1, 1, 1), \mathbf{s}^{(7-9)} \\ &= \frac{1}{\sqrt{3}} (1, -1, 1), \mathbf{s}^{(10-12)} = \frac{1}{\sqrt{3}} (1, 1, -1), \end{aligned} \quad (8)$$

$$\begin{aligned} \mathbf{m}^{(1)} &= \frac{1}{\sqrt{2}} (0, -1, 1), \mathbf{m}^{(2)} = \frac{1}{\sqrt{2}} (1, 0, -1), \mathbf{m}^{(3)} = \frac{1}{\sqrt{2}} (-1, 1, 0), \mathbf{m}^{(4)} = \frac{1}{\sqrt{2}} (1, 0, 1), \\ \mathbf{m}^{(5)} &= \frac{1}{\sqrt{2}} (1, 1, 0), \mathbf{m}^{(6)} = \frac{1}{\sqrt{2}} (0, -1, 1), \mathbf{m}^{(7)} = \frac{1}{\sqrt{2}} (0, 1, 1), \mathbf{m}^{(8)} = \frac{1}{\sqrt{2}} (1, 1, 0), \\ \mathbf{m}^{(9)} &= \frac{1}{\sqrt{2}} (1, 0, -1), \mathbf{m}^{(10)} = \frac{1}{\sqrt{2}} (0, 1, 1), \mathbf{m}^{(11)} = \frac{1}{\sqrt{2}} (1, 0, 1), \mathbf{m}^{(12)} = \frac{1}{\sqrt{2}} (-1, 1, 0). \end{aligned} \quad (9)$$

In the initial configuration, the crystal slip system α consists of a slip direction vector $\mathbf{s}_0^{(\alpha)}$ lying in a slip plane with normal vector of $\mathbf{m}_0^{(\alpha)}$. Both $\mathbf{s}_0^{(\alpha)}$ and $\mathbf{m}_0^{(\alpha)}$ are unit vectors and should satisfy the orthogonal relationship, namely

The velocity gradient $\mathbf{L}$ can be uniquely decomposed into a symmetric part $\mathbf{D}$ (stretching rate tensor) and a skew-symmetric $\mathbf{\Omega}$ (spin tensor) part as

$$\mathbf{L} = \mathbf{D} + \mathbf{\Omega} \quad , \quad (10)$$

$$\mathbf{D} = \frac{1}{2}(\mathbf{L} + \mathbf{L}^T) \quad , \quad (11)$$

$$\mathbf{\Omega} = \frac{1}{2}(\mathbf{L} - \mathbf{L}^T) \quad , \quad (12)$$

where $\mathbf{D}$ is, in general, called the rate of deformation. Both tensors $\mathbf{D}$ and $\mathbf{\Omega}$ can also be decomposed into the elastic stretching and lattice rotation component ($\mathbf{D}^*$ and $\mathbf{\Omega}^*$) and the plastic component ($\mathbf{D}^P$ and $\mathbf{\Omega}^P$) as follows,

$$\mathbf{D} = \mathbf{D}^* + \mathbf{D}^P \quad , \quad (13)$$

$$\mathbf{\Omega} = \mathbf{\Omega}^* + \mathbf{\Omega}^P \quad , \quad (14)$$

and the tensor $\mathbf{D}^P$ in Eq. (13) can be expressed as

$$\mathbf{D}^P = \frac{1}{2}(\mathbf{L}^P + \mathbf{L}^{P^T}) = \sum_{\alpha=1}^N \mathbf{p}^{(\alpha)} \dot{\gamma}^{(\alpha)} \quad , \quad (15)$$

where $\mathbf{p}^{(\alpha)}$ can be defined as

$$\mathbf{p}^{(\alpha)} = \frac{1}{2}(\mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)} + \mathbf{m}^{(\alpha)} \otimes \mathbf{s}^{(\alpha)}) \quad . \quad (16)$$

Similar to $\mathbf{D}^P$, the tensor $\mathbf{\Omega}^P$ in Eq. (14) can be expressed as

$$\mathbf{\Omega}^P = \sum_{\alpha=1}^N \mathbf{w}^{(\alpha)} \dot{\gamma}^{(\alpha)} \quad , \quad (17)$$

where $\mathbf{q}^{(\alpha)}$ can be defined as

$$\mathbf{w}^{(\alpha)} = \frac{1}{2}(\mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)} - \mathbf{m}^{(\alpha)} \otimes \mathbf{s}^{(\alpha)}) \quad , \quad (18)$$

B. Rate-dependent hardening model

The crystal plasticity constitutive model used in this study follows the line described by Asaro³¹ and it is incorporated into the implicit finite element code ABAQUS/Standard through the user material subroutine (UMAT). The prominent functions of UMAT are to provide the material with the Jacobian matrix for the constitutive model, and to update the stresses and the solution dependent state variables. In this study, we adopt the UMAT framework initially developed by Huang³⁸ and use the formulations established by Bassani and Wu³⁹ as the hardening model, which has been specifically described by Liu et al. and Lu et al.^{35,40} The formulations of the rate-dependent hardening model used in the present study can be expressed as

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0^{(\alpha)} \operatorname{sgn}(\tau^{(\alpha)}) \left| \frac{\tau^{(\alpha)}}{\tau_c^{(\alpha)}} \right|^n \quad , \quad (19)$$

with

$$\operatorname{sgn}(x) = \begin{cases} -1, & x < 1 \\ 1, & x \geq 1 \end{cases} \quad , \quad (20)$$

where $\dot{\gamma}_0^{(\alpha)}$ is the reference (initial) value of the shear strain rate, which is a constant for all the slip systems. Here, n is the strain rate sensitive exponent. Both $\dot{\gamma}_0^{(\alpha)}$ and n are the material parameters. Here, $\tau_c^{(\alpha)}$ is the critical resolved shear stress of the slip system α , which represents the strength of the material.

The rate of change of the critical resolved shear stress is expressed by³⁰

$$\dot{\tau}_c^{(\alpha)} = \sum_{\beta=1}^N f_{\alpha\beta} h_{\alpha\beta} \dot{\gamma}^{(\beta)} \quad , \quad (21)$$

$$h_{\alpha\alpha} = \left[(h_0 - h_s) \sec h^2 \left(\frac{(h_0 - h_s) \gamma^{(\alpha)}}{\tau_1 - \tau_0} \right) + h_s \right] \left[1 + \sum_{\substack{\beta=1 \\ \beta \neq \alpha}}^N f_{\alpha\beta} \tanh \left(\frac{\gamma^{(\beta)}}{\gamma_0} \right) \right] \quad , \quad \text{for } \alpha = \beta \quad , \quad (22a)$$

$$h_{\alpha\beta} = q h_{\alpha\alpha} \quad , \quad \text{for } \alpha \neq \beta \quad , \quad (22b)$$

where $\mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)}$ is the Schmid factor. Here, $\mathbf{p}^{(\alpha)}$ and $\mathbf{w}^{(\alpha)}$ are symmetric and asymmetric part of the Schmid factor, respectively.

where $h_{\alpha\beta}$ is the hardening modulus including the self-hardening of each system ($\alpha = \beta$) and latent hardening ($\alpha \neq \beta$), the constant q is the latent hardening parameter, the constant γ_0 is the reference value of slip, γ is the shear strain, τ_0 is the initial critical resolved shear stress, τ_1 is the breakthrough stress where large plastic flow initiates, h_0 is the hardening modulus just after initial yield, h_s is the hardening modulus during easy glide, and $f_{\alpha\beta}$ is the magnitude of the strength of a particular slip interaction between two slip systems α and β . The factor $f_{\alpha\beta}$ depends on the geometric relation between two slip systems. There are five constants for $f_{\alpha\beta}$, namely α_1 (no junction), α_2 (Hirth lock), α_3 (coplanar junction), α_4 (glissile junction), and α_5 (sessile junction).

C. Finite element implementation

The aforementioned crystal plasticity constitutive model is implemented into the implicit finite element code ABAQUS/Standard by using the UMAT which are able to provide the material Jacobian matrix $\partial\Delta\sigma/\partial\Delta\varepsilon$, for the constitutive model and to update the stresses and the solution dependent state variables.

The commercial software Abaqus6.9, Pro/ENGINEER Wildfire 4.0, and CUBIT 13.1 have been used to simulate

the deformation procedure of nanoindentation. A 3D model has been built to describe the behavior of nanoindentation, which is shown as Fig. 1. The Voronoi diagram is the most popular method to generate polycrystalline material structure⁴¹ in the present. In this study, the 3D Voronoi diagram has been used to generate two 3D cells. Firstly, the input file of 3D nanoindentation setup was generated by Abaqus6.9. Secondly, the input file was implemented into a MATLAB program to construct two 3D cells (grains). Each Voronoi cell corresponds to one seed and the number of seeds will be controlled to determine the average size of the cells. The generated two Voronoi cells are then assigned with different crystallographic orientations and implemented into the CPFEM model. In the CPFEM simulation, each Voronoi cell represents a virtual grain. The detailed description for constructing poly-crystal CPFEM model has been given in our earlier work.³⁴

The indenter is a Berkovich indenter with a 200 nm radius round tip. 13,024 eight-node brick elements and 14,463 nodes with reduced integration (element id: C3D8R) are used in the CPFEM model. A refined mesh is generated in the contact area [Figs. 1(b) and 1(c)] directly underneath the indenter to obtain the accurate

FIG. 1. 3D nanoindentation model setup: (a) the whole model; (b) the upper surface of Cu single crystal; (c) the upper surface of Cu bicrystals (or Cu–Al bicrystals) and (d) through thickness view of Cu bicrystals (or Cu–Al bicrystals).

contact solution while a coarser mesh is created in the rest region to decrease the elements number in the model and to keep the computer time within limits. The importance of having an appropriate mesh density in the contact area has been proposed by Liu et al.^{20,23} The size of the smallest element is about 0.1 μm in all three directions.

The X , Y , and Z coordinates represent the rolling direction, transverse direction, and normal direction, respectively. In this model, the specific Goss orientation is set as the initial orientations, namely the (011) slip plane parallels to the Z axis, and the [100] slip direction parallels to the X axis, to validate the model by comparing the numerical result with the experimental observation. Figure 1(c) shows the upper surface of the sample for Cu bicrystal or Cu–Al bicrystal. For Cu bicrystals, the orientations of Grain 2 are always set as Goss orientations while the orientations of Grain 1 are set as Cube, Brass and R, respectively. For a Cu–Al bicrystal, Grain 2 is set as Cu and its orientations are always set as Goss orientations. Grain 1 is set as Al and its orientations are set as Cube, Brass and R, respectively. The misorientation between Grain 1 and Grain 2 for both Cu bicrystals and Cu–Al bicrystals is listed in Table I. Clearly, all the GBs between Grain 1 and Grain 2 are high angle GBs.

The dimensions of the sample in the FEM model are 60 $\mu\text{m} \times 60 \mu\text{m} \times 30 \mu\text{m}$. The height of the sample is much larger than the maximum indentation depth (1 μm)

TABLE I. Misorientations for Cu bicrystal and Cu–Al bicrystal between Grain 1 and Grain 2.

Grain 1 (orientation)	Grain 2 (orientation)	Misorientation (axis/angle)
Cube (001)[100]	Goss (011)[100]	45°, [0, 1, 0]
Brass (111)($\bar{1}\bar{1}0$)	Goss (011)[100]	46°, [5, 0, -1]
R (124)[21 $\bar{1}$]	Goss (011)[100]	41.5°, [3, -2, -2]

TABLE II. Parameters in the constitutive model for copper.^{43,44}

n	$\dot{\gamma}_0$ (1/s)	h_0 (MPa)	h_s (MPa)	τ_1 (MPa)	τ_0 (MPa)	γ_0	q
2	0.001	90	1.5	1.3	1	0.001	1

TABLE III. Parameters in the constitutive model for aluminum.^{35,40}

n	$\dot{\gamma}_0$ (1/s)	h_0 (MPa)	h_s (MPa)	τ_1 (MPa)	τ_0 (MPa)	γ_0	q
300	0.0001	100	0.01	6.3	6	0.001	1

TABLE IV. Notation of the slip systems for the FCC materials considered in this study.

System	$a1$	$a2$	$a3$	$b1$	$b2$	$b3$	$c1$	$c2$	$c3$	$d1$	$d2$	$d3$
Plane	(111)	...	...	($\bar{1}\bar{1}\bar{1}$)	...	...	($\bar{1}\bar{1}1$)	...	...	($\bar{1}\bar{1}1$)	...	...
Direction	[0 $\bar{1}1$]	[10 $\bar{1}$]	[$\bar{1}10$]	[011]	[101]	[110]	[0 $\bar{1}1$]	[101]	[110]	[011]	[10 $\bar{1}$]	[110]

to avoid the influence from the sample.⁴² In addition, the length and the width are bigger enough as the stress contour never reaches four surrounding surfaces of the sample.

All nodes on the bottom surface and four surrounding surfaces of sample are constrained along three axes considering the real indentation condition (the metal sample was mounted inside a piece of resin and just the top surface is free). Liu et al.²³ found that both the indentation depth and the load–displacement curve are not affected by the coefficient of friction. Therefore, a frictionless contact pair is defined by two contact surfaces with associated nodes between the indenter and sample. The time step increment is set for the convergence of modeling. In this study, a fixed time step increment 0.01 s is chosen and a total time step increments of 24,062 in the simulation are used, including contact, loading, and unloading.

According to the report from Bassani et al.⁴³ and Huang,³⁸ the factor $f_{\alpha\beta}$ for single-crystal copper is taken as: $\alpha_1 = \alpha_2 = \alpha_3 = 8$, $\alpha_4 = 15$ and $\alpha_5 = 20$ in this study. Three elastic moduli can be used as $C_{11} = 168,400$ MPa, $C_{12} = 121,400$ MPa, and $C_{44} = 75,400$ MPa, respectively.⁴³ Other material parameters in the hardening models (Eqs. 19–22) are listed in Table II.^{43,44} Franciosi et al.⁴⁵ and Lu et al.⁴⁰ have reported that the factor $f_{\alpha\beta}$ for aluminum can be chosen as: $\alpha_1 = \alpha_2 = \alpha_3 = 1.75$, $\alpha_4 = 2$ and $\alpha_5 = 2.25$. Other material parameters in the hardening models are listed in the Table III.^{35,40} All of these parameters were evaluated by fitting the simulated stress–strain curve with the experimental results of single-crystal aluminum under plane strain compression.^{46,47} Aluminum has an FCC structure with elastic moduli $C_{11} = 112,000$ MPa, $C_{12} = 66,000$ MPa, and $C_{44} = 28,000$ MPa. There is only one set of slip systems for FCC metals, $\{111\}\langle 110 \rangle$, which includes 12 different slip systems shown in the Table IV. In the deformed single-crystal copper and aluminum, slips occur on the $\{111\}$ planes and in the $\langle 110 \rangle$ directions. All of aforementioned parameters for copper were evaluated by both experiments and simulations^{38,48,49} and all parameters for aluminum were validated in the simulations of nanoindentation, rolling, tensile, and ECAP deformation.^{33,35,40,50,51}

III. RESULTS AND DISCUSSIONS

Figure 2(a) shows the comparison between numerical and experimental load–indentation depth curves.⁵²

FIG. 2. Comparisons of load–displacement curves between: (a) numerical and experimental results for Cu single crystal; (b) the Cu single crystal and Cu bicrystals via simulation and (c) the Cu single crystal and Cu–Al bicrystals via simulation.

The depth controlled modeling has been carried out to achieve the same maximum depth (1000 nm) as the experiment.⁵² The maximum load in our simulation is 26.08 mN, while it is 26.28 mN in the experiment. Clearly, the simulated result is in a reasonable agreement with that from the experiment.⁵² It is noteworthy that all the initial condition of simulation is the same as that of experiment, including the same Goss orientation for indented sample, the same indented sample (Cu single crystal) and the same indenter (Berkovich indenter). Figure 2(b) shows the comparison of load–indentation depth curves between the Cu single crystal and Cu bicrystals. Clearly, there are only slight differences between the Cu single crystal and Cu bicrystals, which suggest that the GB affects the load–indentation depth curves of the one-phase material insignificantly. The result is consistent with the work done by Li et al.²⁸ who investigated the nanoindentation behavior by 3D CPFEM simulation of polycrystal aluminum. Figure 2(c) shows the comparison of load–indentation depth curves between the Cu single crystal and Cu–Al bicrystals. Clearly, there is a significant difference between the Cu single crystal and Cu–Al bicrystals although all of these indents locate in the grain of Cu. It suggests that the PB affects the mechanical behavior of nanoindentation significantly. The present study agrees with the observations by Nilsen and Subramanian¹⁹ who performed indentation

TABLE V. Simulated Young's modulus for Cu samples and Cu–Al bicrystals.

Materials	Young's modulus (GPa)
Cu single crystal (Goss)	119.3
Cu Goss-cube bicrystal	120.6
Cu Goss-brass bicrystal	118.7
Cu Goss-R bicrystal	120.2
Cu–Al interface 1	102.9
Cu–Al interface 2	102.6
Cu–Al interface 3	102.3

tests on two-phase bicrystals of alpha-beta brass with various geometries of PB. Besides, Fig. 2(c) also shows that the difference in misorientation between the Cu grain and the Al grain does not affect the load–indentation depth curves significantly.

The simulated elastic modulus E_s along indented surface normal can be calculated via the Oliver–Pharr (O & P) method¹:

$$h_c = h_{\max} - k \frac{P_{\max}}{S}, k = 0.75, S = \left(\frac{dP}{dh} \right)_{h=h_{\max}}, \quad (23)$$

FIG. 3. The distributions of the Mises stress on the upper surfaces of Cu samples: (a) the Cu single crystal with Goss orientation; (b) the Cu bicrystal with Goss-Cube GB; (c) the Cu bicrystal with Goss-Brass GB and (d) the Cu bicrystal with Goss-R GB.

FIG. 4. The distributions of the Mises stress on the upper surfaces of Cu and Cu–Al bicrystals: (a) the Cu single crystal with Goss orientation; (b) the Cu–Al bicrystal with Goss-Cube PB; (c) the Cu–Al bicrystal with Goss-Brass PB and (d) the Cu–Al bicrystal with Goss-R PB.

where P is the indentation load at the maximum load and h is the indentation depth at the maximum load. Here, h_c represents the contact depth. The factor k depends upon the indenter. For the Berkovich indenter, the factor k is equal to 0.75, while $k = 0.72$ is for the conical indenter. Here, S is the slope of the unloading curve. The elastic modulus was determined by¹

$$\frac{1}{E_r} = \frac{1 - \nu_s^2}{E_s} + \frac{1 - \nu_i^2}{E_i}, \quad (24)$$

where E_i , E_s , ν_i and ν_s are Young's modulus and Poisson's ration of the indenter and the sample, respectively. For a diamond, the variables E_i and ν_i are taken to be 1141 GPa and 0.07 (Ref. 1). However, in this study, these two parameters can be ignored as the simulated Berkovich indenter is a rigid body.

The slope of unloading curves is used to calculate E_r of the indented material:

$$E_r = \frac{\sqrt{\pi}}{2} \frac{S}{\sqrt{A_c}}, \quad A_c = 3\sqrt{3}h_c^2 \tan^2 65.3 = 24.56h_c^2, \quad (25)$$

where A_c is the contact area.

For the materials which are elastically anisotropic, Vlassak and Nix^{53,54} demonstrated that relationships in Eqs. (24) and (25) still worked and the reduced modulus could be re-defined as

$$\frac{1}{E_r} = \frac{1}{E} + \frac{1 - \nu_i^2}{E_i}, \quad (26)$$

here, the variable E is the theoretical elastic modulus, which is proved to be a complicated function of single-crystal elastic constants C_{11} , C_{12} , and C_{44} . It is also defined as indentation modulus by Wang and Lu.⁵⁵ The simulated Young's moduli for Cu samples and Cu–Al bicrystals have been calculated and shown in the Table V.

FIG. 5. The distributions of the Mises stress on the through thickness cross section of Cu samples and Cu–Al bicrystals: (a) the Cu single crystal with Goss orientation; (b) the Cu bicrystal with Goss-R PB and (c) the Cu–Al bicrystal with Goss-R PB.

FIG. 6. The pile-up patterns made on the upper surfaces of Cu samples: (a) the Cu single crystal with Goss orientation; (b) the Cu bicrystal with Goss-Cube GB; (c) the Cu bicrystal with Goss-Brass GB and (d) the Cu bicrystal with Goss-R GB.

FIG. 7. The pile-up patterns made on the through thickness cross section of Cu samples: (a) the Cu single crystal with Goss orientation; (b) the Cu bicrystal with Goss-Cube GB; (c) the Cu bicrystal with Goss-Brass GB and (d) the Cu bicrystal with Goss-R GB.

Clearly, the GB does not affect indentation Young's modulus of single-phase material significantly as the maximum difference between the Cu single crystal and Cu bicrystals is only $\sim 1.09\%$. However, the maximum difference between the Cu single crystal and Cu–Al bicrystals is $\sim 16.6\%$, which suggests that the PB affects indentation Young's modulus significantly.

Figure 3 shows the distributions of the Mises stress on the upper surfaces of Cu samples. The maximum difference in the maximum Mises stress between the Cu single crystal and the Cu bicrystal with Goss-Brass GB is only 3.53% . The difference between the Cu single crystal and Cu bicrystals is insignificant, which suggests that the GB does not become a barrier to block the plastic slip behavior. The former research revealed that there is little dislocation locking and little resistance to slip transfer across GBs for copper.⁸ Soer and De Hosson⁵⁶ concluded that slip transmission is unlikely to be observed directly during indentation tests of FCC metals.

Figure 4 shows the distributions of Mises stress on the upper surfaces of Cu samples and Cu–Al bicrystals. For Figs. 4(b)–4(d), there is a noticeable dividing line on each upper surface and the Mises stress stops propagates there. The maximum difference in the maximum Mises

stress between the Cu single crystal and Cu–Al bicrystals is 10.1% , approximately. Clearly, the PB works like a barrier which can resist the propagation of the Mises stress. It is consistent with the observations from Nilsen and Subramanian¹⁹ who demonstrated that it is not easy to propagate slip through the PB by localized stress caused by indentation.

Figure 5 shows the distributions of the Mises stress on through thickness cross section of Cu samples and Cu–Al bicrystals. Figure 5(a) displays a symmetrical distribution of the Mises stress on the through thickness cross section of the Cu single crystal under the Berkovich indenter. Figure 5(b) shows that the pattern of the stress distribution is similar as Fig. 5(a). However, the pattern is not symmetrical at the vicinity of GB. Figure 5(c) shows that the pattern of the stress distribution is significantly different from Figs. 5(a) and 5(b) as the propagation of the Mises stress is completely resisted by PB, at where the diving line is quite noticeable.

Figure 6(a) shows the distribution of pile-up patterns on the upper surface of the Cu single crystal with a two-fold symmetry at the maximum indentation depth. It is consistent with the numerical and experimental observations from Wang et al.⁵⁷ and Hollatz et al.⁵⁸

FIG. 8. The pile-up patterns made on the upper surfaces of Cu single crystal and Cu–Al bicrystals: (a) the Cu single crystal with Goss orientation; (b) the Cu–Al bicrystal with Goss-Cube PB; (c) the Cu–Al bicrystal with Goss-Brass PB and (d) the Cu–Al bicrystal with Goss-R PB.

FIG. 9. The pile-up patterns made on the through thickness cross section of Cu single crystal and Cu–Al bicrystals: (a) the Cu single crystal with Goss orientation; (b) the Cu–Al bicrystal with Goss-Cube PB; (c) the Cu–Al bicrystal with Goss-Brass PB and (d) the Cu–Al bicrystal with Goss-R PB.

FIG. 10. Distribution of lattice rotation angles induced by nanoindentation for: (a) the Cu single crystal with Goss orientation; (b) the Cu bicrystal with Goss-Cube GB and (c) the Cu–Al bicrystal with Goss-Cube PB.

for Cu and NiAl single crystal on (011) oriented surfaces. Figures 6(b) and 6(c) show that pile-up patterns have been slightly changed due to the effect of GBs. However, the material still flows through the GB. Figure 7 shows the through thickness view of pile-up patterns at the maximum indentation depth.

Figure 8 shows the comparison of pile-up between Cu–Al bicrystals and the Cu single crystal at the maximum indentation depth. Clearly, the pile-up patterns are significantly changed on the Cu–Al bicrystals due to the blocking of material flow by PB. Figure 9 shows the through thickness view of pile-up patterns at the maximum indentation depth.

To analyze the effect of interface on the evolution in the crystallographic orientation during the indentation process, the “misorientation” of each node relative to the initial orientation is partitioned into three components representing the rotation angles around the X (RD), Y (TD), and Z (ND) axes, individually. This method was initially proposed by Wert et al.⁵⁹ In this study, the contour map of the crystallographic rotation angle around the Y axis is investigated for the cross section along the X axis of three individual indented samples, since the GB/PB is noticeable on the chosen through thickness cross section [refer to Fig. 1(d)]. Positive values represent counter-clockwise rotation and negative values represent the clockwise rotation.

Figure 10 shows the lattice rotation angles for the Cu single crystal, the Cu bicrystal with Goss-Brass GB and the Cu–Al bicrystal with Goss-Brass PB, respectively. For the Cu single crystal, lattices on the left-hand side of the indent rotate clockwise while the ones on the right-hand side rotate oppositely. The rotation angles on both sides of indent are opposite to make the whole sample remain stable. However, for the Cu bicrystal, lattices on the left-hand side of the indent change the rotation direction. It is because that the GB works like a barrier to turn around the lattice rotation angle even the material can flow through it. The lattices which are far away from the indent rotate counter-clockwise to remain the whole sample stable. The Cu–Al bicrystal has the same tendency as the Cu bicrystal, which suggests that the PB has the same effect on the lattice rotation angle as GB does.

IV. CONCLUSIONS

(1) A CPFEM model combined with Bassani and Wu hardening law has been developed to investigate the nanoindentation behavior of Cu bicrystals and Cu–Al bicrystals with three different misorientations. The simulated load–displacement curve for the Cu single crystal with Goss initial orientation has been analyzed and compared with the result from the experiment to validate the parameters.

(2) The numerical results indicate that the interface does not affect the load–displacement curves of Cu bicrystals. However, it affects the load–displacement curves of Cu–Al bicrystals significantly. The effect on load–displacement curves from GBs/PBs with different misorientations is insignificant for both Cu bicrystals and Cu–Al bicrystals.

(3) The GB does not affect indentation Young’s moduli of Cu bicrystals significantly as the maximum difference between the Cu single crystal and Cu bicrystal is only $\sim 1.09\%$. However, the maximum difference between the Cu single crystal and Cu–Al bicrystal is $\sim 16.6\%$, which suggests that the PB affects indentation Young’s modulus of the Cu–Al bicrystal significantly.

(4) The maximum difference in the maximum Mises stress between Cu single crystal and Cu bicrystal with Goss-Brass GB is only 3.53% , which suggests that the GB does not block the plastic slip behavior as a barrier. However, the maximum difference in the maximum Mises stress between Cu single crystal and Cu–Al bicrystal is 10.1% , approximately. Clearly, the PB can resist the propagation of the Mises stress in Cu–Al bicrystals.

(5) The pile-up patterns have been slightly changed due to the effect of GB for the Cu bicrystals without blocking of the material flow. The pile-up patterns are significantly changed on the surfaces of Cu–Al bicrystals due to the blocking of the material flow by PB.

(6) The lattice rotation angles under the indent can be turned around by the GBs/PBs for both Cu bicrystals and Cu–Al bicrystals.

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