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A crystal plasticity FEM study on the deformation behaviours of bicrystals composites for potential use as load-bearing implants

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Metal matrix composites have shown great application potential in biomedical materials due to their excellent integrated properties. The deformation behaviours of metal matrix composites during fabricating and service are complicated. In this study, bicrystals processed by accumulative roll-bonding (ARB) were used as a representative case, and the deformation behaviours were investigated using crystal plasticity finite element method (CPFEM). The used three bicrystals were {112}<111>–{112}<111> (C-C), {112}<111>–{123}<634> (C-S), and {112}<111>–{001}<110> (C-RoCube), and the initial misorientation angles at the interfaces were 0°, 19.4°, and 35.3°, respectively. Pole figures, crystal rotation angles, and misorientation angles were used to characterize the texture evolution, and through-thickness shear strain γ_{RD-ND} and shear strain on slip systems were adopted to present the plastic deformation. The deformation behaviours in C-S were similar to C-C, due to the small difference in crystal orientations, while the comparison between C-C and C-RoCube shows distinct differences. The texture transition between C and RoCube was observed, and this textural transition altered the activated slip systems. The influence of interfaces on the deformation behaviours of neighbouring regions was strongly dependent on the interfacial misorientation angles.

KEYWORDS

biomaterial, metal matrix composite, crystal plasticity, accumulative roll-bonding, bicrystal

1 Introduction

High-performance load-bearing biomedical implants (e.g., artificial joints and bone plates) are indispensable in modern medicine for repairing skeletal injuries and restoring joint function (Gao et al., 2019). These devices must withstand complex cyclic mechanical loads within the human body, requiring materials that simultaneously provide high strength, superior fatigue resistance, and excellent wear resistance (Bandyopadhyay et al., 2024).

Metal matrix composites with tunable microstructures show great promise in biomedical applications owing to their biocompatibility (Davis et al., 2022), high specific strength, and the advantage of eliminating secondary removal surgery (Chen et al., 2026). A comprehensive review of the preparation and performance of additively manufactured metal matrix composites is provided in Ref. (Chen et al., 2024). However, current metallic implant materials face persistent challenges. Conventional biomedical alloys often suffer from insufficient fatigue resistance and mismatched wear properties relative to bone tissue during long-term service (Davis et al., 2022; Delavar et al., 2023). Meanwhile, biodegradable alloys are hindered by non-uniform degradation rates and the premature loss of mechanical integrity (Zan et al., 2023). Therefore, addressing these limitations requires innovative material design strategies, with control of microtexture (crystallographic orientation distribution) emerging as a key pathway to optimize mechanical performance (Wu et al., 2024). The unique service environment of biomedical implants imposes stringent texture requirements. The alternating loads in joints demand specific texture orientations to mitigate stress concentration and extend fatigue life (Wang et al., 2022); the interfacial bonding performance between bone plates and bone depends strongly on the surface hardness and friction coefficient, which are governed by texture (Zan et al., 2023); and in biodegradable metallic alloys, texture further regulates the uniformity of corrosion rates in physiological environments through its influence on grain orientation (Gerashi et al., 2022). Furthermore, in biomedical metallic sheets (particularly cold-rolled FCC metals), the rolling texture, as a typical texture formed by the primary plastic processing technique of rolling (Ramkumar et al., 2024), poses additional challenges. Such textures not only hinder subsequent plastic deformation (Su et al., 2014) but also exacerbate the anisotropy of mechanical properties (Ramkumar et al., 2024). Consequently, the development of rolling texture control strategies tailored for biomedical metallic sheets represents a critical direction for overcoming the current performance bottlenecks of load-bearing implants.

Numerous techniques have been developed to optimize textures after rolling (Dabou et al., 2023). Among them, accumulative roll-bonding (ARB), a relatively recent rolling technique, has been widely employed to fabricate ultrafine-grained materials (Valiev et al., 2022). To a large extent, the through-thickness texture after ARB resembles that produced by conventional rolling (Ebrahimi and Wang, 2022). However, due to the absence of lubricants—commonly avoided in ARB to improve interfacial bonding—a significant fraction of shear-type texture forms at the surface (Semenchenko et al., 2024; Cantergiani et al., 2024). Consequently, shear-type texture typically develops near the surface, while rolling-type texture dominates at the centre (Ebrahimi and Wang, 2022). As deformation proceeds, the shear-type texture is gradually rotated and transformed into rolling-type texture once the surface layers are cycled into the centre (Ebrahimi and Wang, 2022). Because the directions of shear strain differ between the upper and lower surfaces, the shear-type textures on these two sides also differ, giving rise to a characteristic texture transition at the interface (Kashihara et al., 2014). This implies that differences in interfacial texture play a critical role in governing overall texture evolution.

Single crystals are the ideal materials for studying texture evolution during ARB, as they eliminate the complicating effects of grain interactions. Texture evolution has been investigated using both experimental approaches (Kashihara et al., 2014; Kashihara et al., 2013) and crystal plasticity modelling (Wang et al., 2019a). Direct experimental characterization of crystallographic orientations at the exact ARB surfaces remains challenging, whereas crystal plasticity modelling provides predictive insight into surface texture development. Modelling studies on ARB-processed single crystals revealed that the crystallographic orientations rotate in opposite directions on the upper and lower surfaces (Wang et al., 2019a), leading to large misorientation angles when these surfaces are stacked in the subsequent cycle. In later cycles, the misorientation angle may either increase or decrease, depending critically on both its initial magnitude and the layer's thickness position (Wang et al., 2019a). Compared to single crystals, bicrystals have been used to examine the evolution of misorientation angles during plastic deformation, as the interfacial misorientation prior to deformation is well defined, where the misorientation angle at the interface before rolling was initially well-defined. Zaefferer et al. (2003) systematically examined the influence of misorientation on the deformation on grain boundaries (i.e., interface) during plane strain compression, covering small (8.7°), transition (15.4°), and large (31.5°) misorientation cases. They demonstrated that the plastic response within bicrystals strongly depends on the orientations of the constituent crystals (Zaefferer et al., 2003). Another study on compressed bicrystals and polycrystals showed that the deformation bands were closely related to crystallographic orientation (Luan et al.). To the best of the authors' best, the ARB deformation behaviour of bicrystals has not yet been reported, forming the central motivation of this study.

In this study, bicrystals were deformed by ARB. The starting orientations of crystals corresponded to either rolling-type or shear-type textures. The texture evolution and plastic deformation behaviour were systematically analysed, with particular emphasis on the effect of interfacial misorientation angle. These insights contribute to a better understanding of the mechanisms underlying texture evolution during ARB.

2 Crystal plasticity modelling

The crystal plasticity finite element method (CPFEM) was employed to model the deformation behaviour of bicrystals during ARB (Figure 1). This CPFEM–ARB framework successfully reproduced the experimentally observed textures in ARB-processed single crystals for up to nine cycles (Wang et al., 2019a; Wang et al., 2019b), thereby demonstrating its predictive capability when applied to bicrystals.

Figure 1 illustrates the simulation model of three bicrystals during the ARB process. In the C-S bicrystal, the initial orientations of the upper and lower sheets are $\{1\ 1\ 2\} \langle 1\ 1\ 1 \rangle$ and $\{1\ 2\ 3\} \langle 6\ 3\ 4 \rangle$, respectively (Figure 1a). For the C-RoCube bicrystal (Figure 1b), the starting orientation are $\{1\ 1\ 2\} \langle 1\ 1\ 1 \rangle$ and $\{0\ 0\ 1\} \langle 1\ 1\ 0 \rangle$. The selection of these three orientations was based on their relevance to texture evolution in ARB. During ARB, shear textures formed at the surfaces are transported to mid-thickness, where they gradually transform into rolling textures. Accordingly,

FIGURE 1
A schematic shows the ARB process. The bicrystals are (a) C-S, (b) C-RoCube, and (c) C-C.

TABLE 1 Notation of 12 slip systems.

Slip plane	(1 1 1)			$(\bar{1} \ 1 \ 1)$			$(1 \ \bar{1} \ \bar{1})$			$(1 \ 1 \ \bar{1})$		
Slip direction	$[0 \ \bar{1} \ 1]$	$[\bar{1} \ 1 \ 0]$	$[1 \ 0 \ \bar{1}]$	$[0 \ 1 \ 1]$	$[1 \ \bar{1} \ 0]$	$[1 \ 0 \ 1]$	$[0 \ 1 \ 1]$	$[1 \ 1 \ 0]$	$[1 \ 0 \ \bar{1}]$	$[0 \ 1 \ 1]$	$[\bar{1} \ 1 \ 0]$	$[1 \ 0 \ 1]$
Slip System	a1	a2	a3	b1	b2	b3	c1	c2	c3	d1	d2	d3

$$\text{The } \text{sgn}(x) = \begin{cases} 1 & \text{for } x \geq 1 \\ -1 & \text{for } x < 1 \end{cases} \quad (3c)$$

The $\tau_c^{(\alpha)}$ represents the strength of slip system α , and its value was calculated according to the Bassani-Wu hardening model (Wu, 2024). The hardening model was given in detail in Ref. (Wang et al., 2019b). In FCC structured aluminum, 12 slip systems were assumed, as listed in Table 1. The slip plane and direction are $\{1 \ 1 \ 1\}$ and $\langle 1 \ 1 \ 0 \rangle$, respectively.

3 Results

Excluding the two ends, only the steady-rolling region was considered for calculating the simulation results.

3.1 Texture evolution

Simulations of the three bicrystals during the ARB process were carried out for up to three cycles. The initial and final textures of the steady-rolling region are presented as $\{1 \ 1 \ 1\}$ pole figures in Figure 2, while the through-thickness crystal rotation angles (relative to the initial orientation) are shown in Figures 3, 4.

For the C-C bicrystal (Figures 2a, 3), the crystal orientations rotated about the TD after 1-, 2-, and 3-ARB, with rotations occurring in both clockwise and anticlockwise directions (Figure 2a). The crystal rotation angles were very small after 1-ARB, with a maximum of 10° observed on the upper surface (Figure 3a). The distribution of crystal rotation angles was asymmetric about the mid-thickness because of the asymmetry of the C orientation. Because the crystal rotation angles on the upper and lower surfaces were different, a large misorientation angle developed at the interface before 2-ARB (Figure 3b). This interfacial misorientation angle, however, became negligible after 2-ARB. A different trend emerged in 3-ARB. A large misorientation angle developed at the mid-thickness interface before 3-ARB, and this angle increased significantly after 3-ARB. This maximum rotation angle was located on the upper surface after 1-ARB but shifted to the lower surfaces after both 2-ARB and 3-ARB. This indicates that the previously developed texture strongly influenced subsequent textural evolution.

Figure 4 compares the through-thickness distribution of crystal rotation angles in the C-S and C-RoCube bicrystals with that of the C-C bicrystal. After 1-ARB (Figure 4a), the texture evolution

behaviour of the C-S bicrystal was similar to that of the C-C bicrystal, except near the two surfaces. This similarity arose because the C orientation was close to the S orientation, with a misorientation angle of 19.4°. In the upper half of the sheet (Figure 4a), the initial orientation was C in all three bicrystals, and the crystal rotation angles exhibited similar distribution patterns. In contrast, the distributions of crystal rotation angles in the lower half of the sheet showed distinct differences among the three bicrystals, particularly in the RoCube region. The crystal rotation angles in the RoCube were significantly higher, reaching ~30° (Figure 4a), with the final orientations closely aligning with the C orientation (Figure 2c). The misorientation angle between C and RoCube was 32.3°. Before 2-ARB, a small misorientation angle developed at the interface of the C-S bicrystal, and this misorientation increased substantially after 2-ARB. For the C-RoCube bicrystal after 2-ARB, the crystal rotation angles in the RoCube region were markedly higher than those in the neighbouring C layers (Figure 4b), resulting in large misorientation angles at all three interfaces. After 3-ARB, the distribution of crystal rotation angles in the C-S bicrystal resembled that of the C-C bicrystal, except for the large misorientation angles at the 1/4 and 3/4 thickness interfaces (Figure 4c), which originated from the previous mid-thickness interface after stacking. Additionally, the crystal rotation angles in the fifth layer (C) and sixth layer (RoCube) were unexpectedly high compared to the adjacent layers.

It is well known that RoCube is a component of shear-type texture, which remains unstable even on the surface under lubricated rolling in this study. In contrast, the C and S orientations are components of rolling-type texture and therefore exhibited smaller rotation angles during rolling. Interestingly, the crystal orientations of the C-C bicrystal were found to be close to the RoCube orientation at both the interface and lower surface (Figures 2a, 4c). This observation contradicts the fact that RoCube is generally unstable during rolling. This suggests that the RoCube orientation became stabilized under this bicrystal configuration, most likely due to the influence of interfaces.

Figure 5 illustrates the evolution of interface misorientation angles. In the C-C bicrystal (Figure 5a), the misorientation angles after 1-ARB were very small. Consequently, the initial misorientation angles at 0.25 mm and 0.75 mm in 2-ARB were also very low. During 2-ARB, the initial misorientation angle at the mid-thickness (0.5 mm) decreased dramatically from 11.7° to 0.5°. A large misorientation angle (30.5°) developed at the mid-thickness interface before 3-ARB, due to the substantial difference in crystal rotation angles between the upper and lower surfaces during 2-ARB. This misorientation angle further increased to 47.8° after 3-ARB. The evolution of misorientation angle in the C-S bicrystal (Figure 5b) was markedly different from that in the C-C bicrystal. The initial

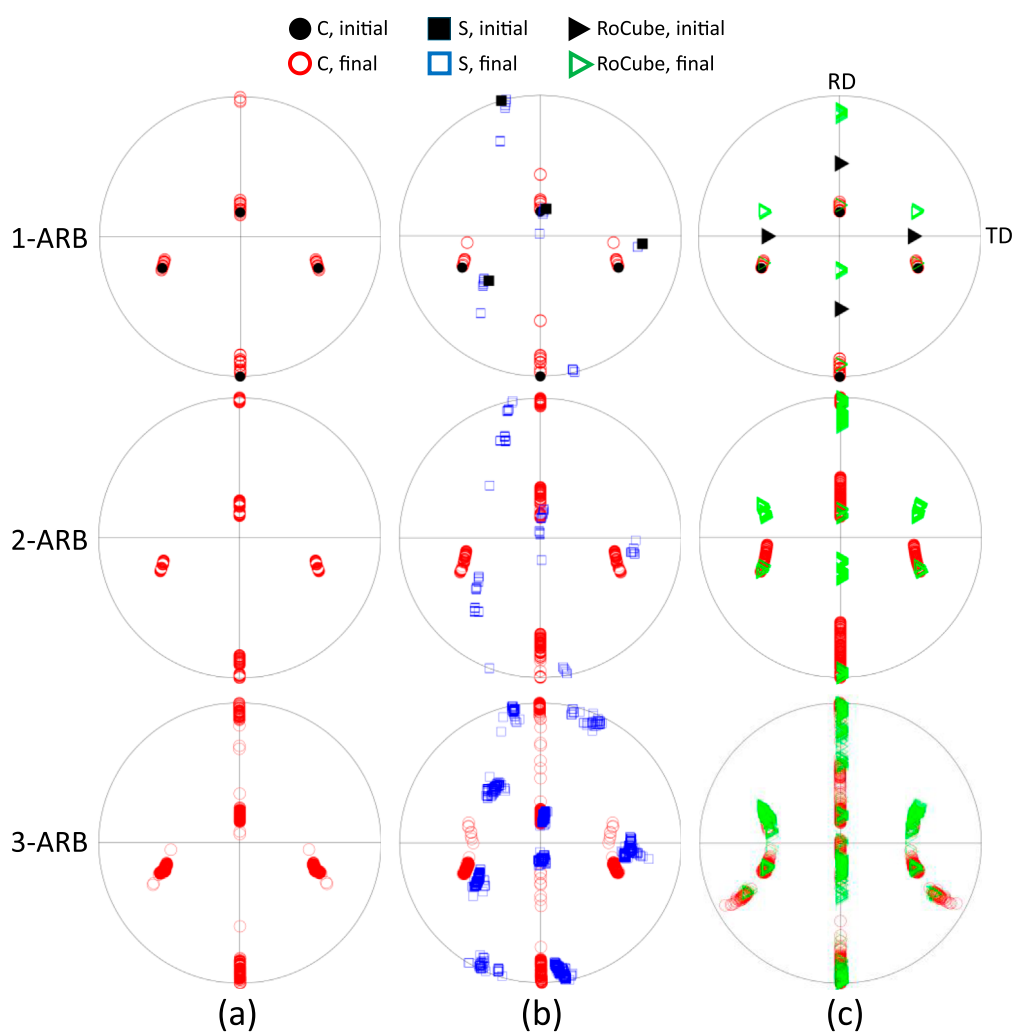


FIGURE 2
{111} pole figures after 1-ARB, 2-ARB, and 3-ARB of the (a) C-C, (b) C-S, and (c) C-RoCube bicrystals.

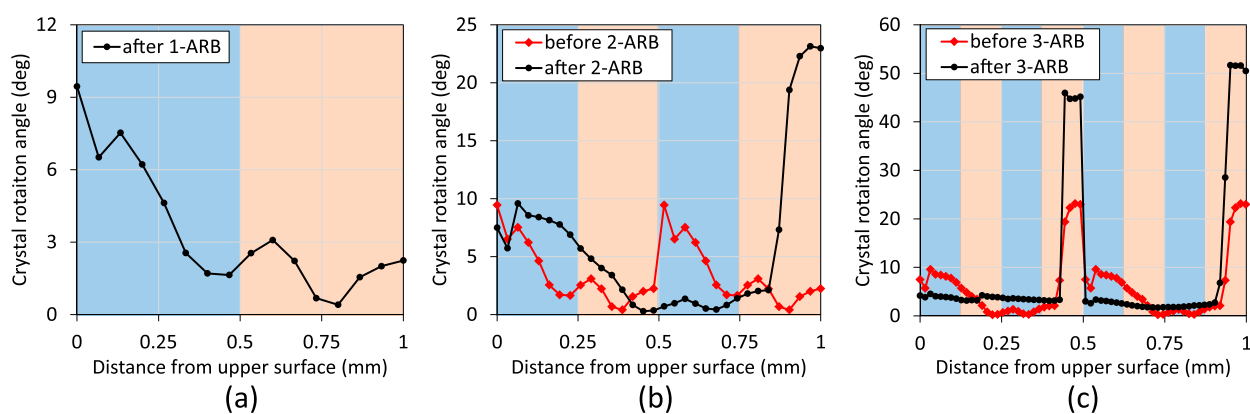


FIGURE 3
Distribution of crystal rotation angles along the thickness of C-C bicrystal after (a) 1-ARB, (b) before and after 2-ARB, and (c) before and after 3-ARB.

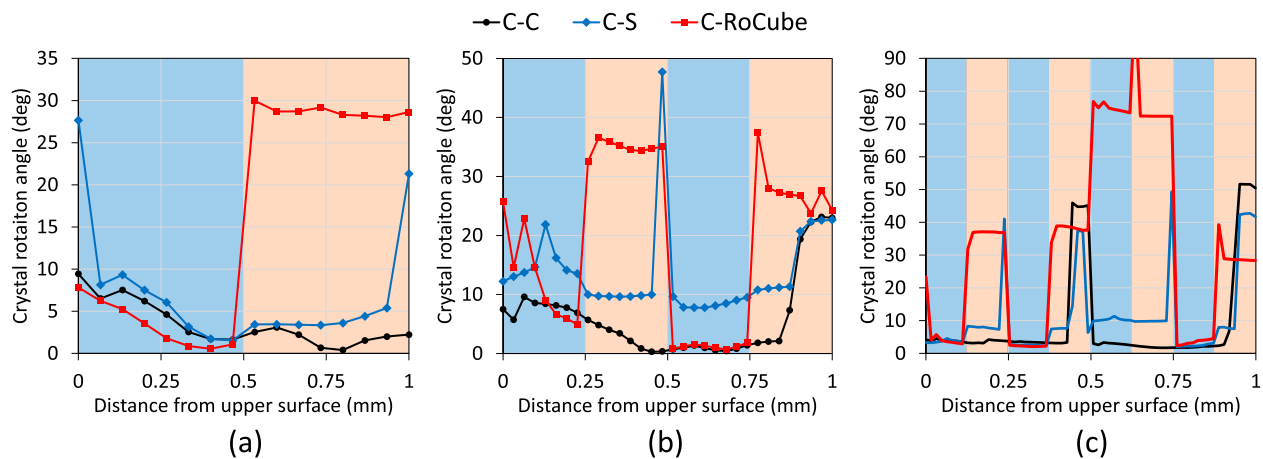


FIGURE 4 Distribution of crystal rotation angles along the thickness of C-C, C-S, and C-RoCube after (a) 1-ARB, (b) 2-ARB, and (c) 3-ARB.

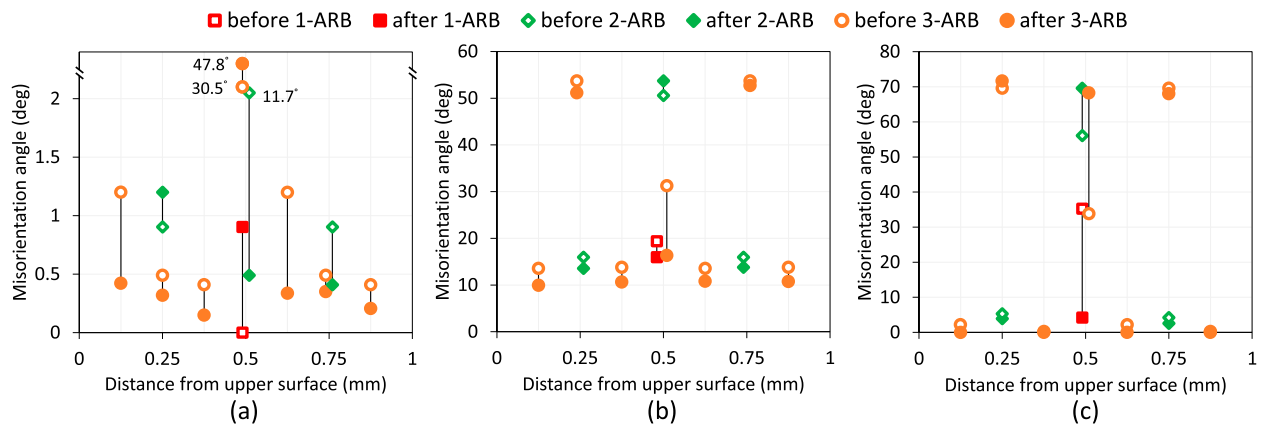


FIGURE 5 Misorientation angles at interface of (a) C-C, (b) C-S, and (c) C-RoCube bicrystals.

and final misorientation angles at the mid-thickness interface of 2-ARB were very high, and these high misorientation angles persisted at the 0.25 mm and 0.75 mm interfaces of 3-ARB. The changes in the misorientation angles at the other interfaces remained within the range of the initial misorientation angle (at the mid-thickness interface of 1-ARB).

In the C-RoCube bicrystal (Figure 5c), the initial misorientation angle at the mid-thickness interface after 1-ARB dropped sharply from 35.3° to 4.2°, and this angle remained low after this interface was shifted to the 0.25 mm and 0.75 mm positions in 2-ARB, and to the 0.125 mm, 0.375 mm, 0.625 mm, and 0.825 mm interfaces of 3-ARB. A newly developed misorientation angle at the mid-thickness interface of 2-ARB increased from 56.1° to 69.6°, and this high misorientation angle was retained at the 0.25 mm and 0.75 mm interfaces of 3-ARB. Another newly developed misorientation angle at the mid-thickness interface of 3-ARB also increased substantially.

3.2 Plastic deformation

It is well known that plastic deformation and texture evolution are mutually interdependent. To correlate with the through-thickness crystal rotation angles in Figure 4, the distribution of shear strain γ_{RD-ND} in the three bicrystals is shown in Figure 6, where the shear strain represents the deformation generated in a single ARB cycle rather than the cumulative value. After 1-ARB, the C-C and C-S exhibited similar deformation patterns along the thickness, and the upper half sheet of the C-RoCube bicrystal also underwent comparable deformation, but the lower half sheet showed distinct differences. After 2-ARB, the variation of shear strain in C-C was relatively smooth, whereas a large variation was observed at the mid-thickness interface of C-S. In contrast, pronounced changes were observed at all three interfaces (1/4, 1/2, 3/4) in the C-RoCube bicrystal. This indicates that the large variation of shear strain at the 1/2 interface after 1-ARB was preserved at the 1/4 and 3/4 interface

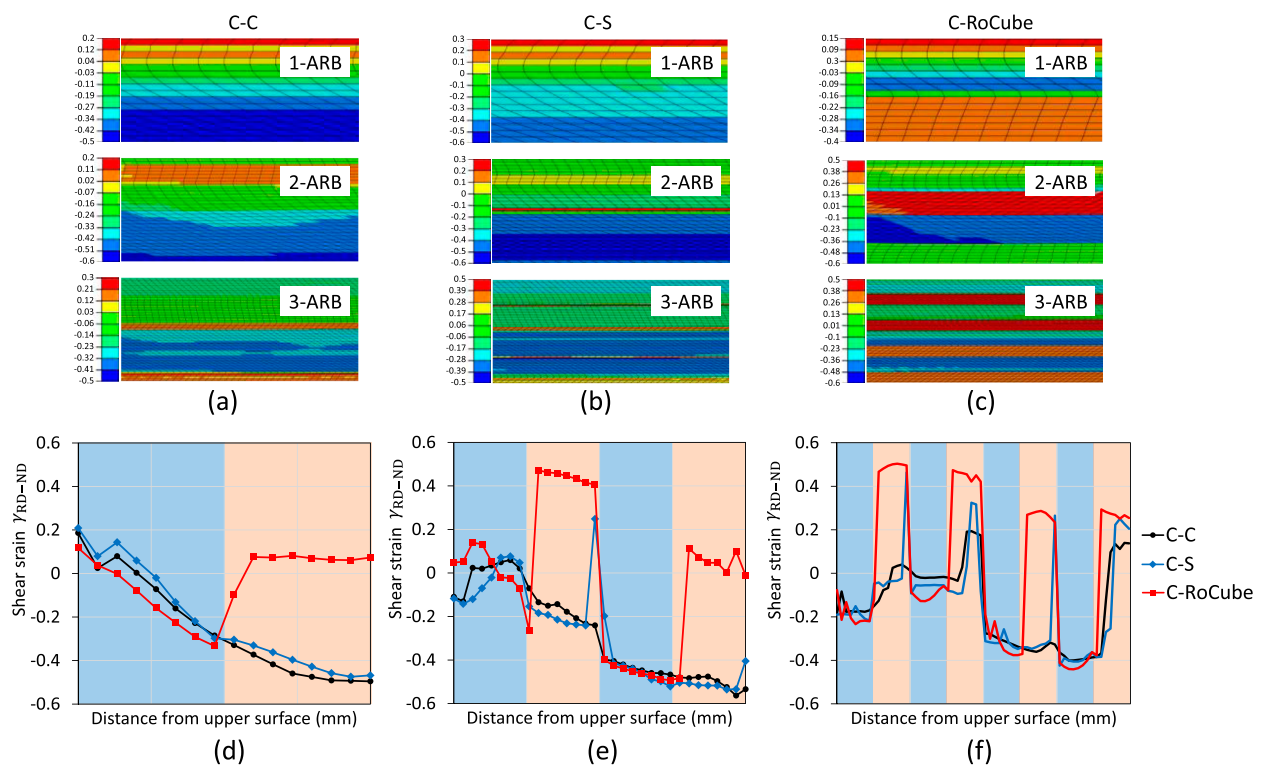


FIGURE 6 Contour of shear strain γ_{RD-ND} (evolved in a single cycle, not cumulative value) in the three ARB cycles of (a) C-C, (b) C-S, and (c) C-RoCube bicrystals. Distribution of through-thickness shear strain γ_{RD-ND} after (d) 1-ARB, (e) 2-ARB, and (f) 3-ARB.

in 2-ARB. Similarly, in the C-S bicrystal, the large shear strain at the mid-thickness interface of 2-ARB was also maintained at the 1/4 and 3/4 interfaces of 3-ARB. In the C-RoCube bicrystal, the shear strain in the RoCube layer was exceedingly higher than that in the C layer in all three ARB cycles.

It is known from the crystal plasticity theory (i.e., Equations 1 and 2) that the crystal rotation angles (Figure 4), macroscopic plastic deformation (shear strain in Figure 6), and slip activities (Figure 7) are correlated. In 1-ARB and 2-ARB of C-C bicrystals, only two sets of slip systems were activated, i.e., a1-a3 and b2-c2 (Figure 7a). The most highly activated slip system set alternated from the upper surface to the lower surface. Another slip system set, d1-d3, was activated at the mid-thickness interface and lower surface of 3-ARB (Figure 7a), where the local crystal orientation approached the RoCube component. In Figure 7b, the behaviour of slip activity in the C layer of the C-S bicrystals was similar to that in the corresponding layer of C-C bicrystals in 1-ARB and 2-ARB, while the slip activity in the S layer was markedly different. Due to the asymmetry of the S orientation, the shear strains on the four most highly activated slip systems differed significantly. In 1-ARB of C-S bicrystals, the shear strain on a1 slip system was exceedingly higher than that on the other three slip systems, and a similar behaviour occurred in the second S layer (0.75 mm–1 mm) of 2-ARB. The difference in shear strain between these four slip systems was small in the first S layer (0.25 mm–0.5 mm) of 2-ARB. The behaviours of

slip activities became more complex in 3-ARB, with the dominant slip system alternating among the 4 S layers.

As for C-RoCube in Figure 7c, the slip activities in the C layers of 1-ARB, 2-ARB, and 3-ARB were similar to the corresponding layers of C-C bicrystals (Figure 7a), though slight deviations were observed near the interfaces. This indicates that the interface, and more specifically the misorientation angles across the interfaces, significantly influence slip activities. In the RoCube layer of C-RoCube bicrystals, the d1-d3 slip system set was exceedingly activated compared to the a1-a3 set, which clearly demonstrates the inherent instability of the RoCube orientation. The activated slip systems in the RoCube layer were the same as the interface and lower surface of C-C bicrystals in 3-ARB (Figure 7a). In addition to the d1-d3 slip system set, another slip system set, b2-c2, was also activated in the RoCube layer of C-RoCube during 2-ARB (Figure 7c), since the initial RoCube rotated toward the C orientation. After 3-ARB, three slip system sets (a1-a3, b2-c2, and d1-d3) were activated in the first C layer and the last RoCube layer, while only two sets of slip systems were activated in the other layers.

4 Discussion

The texture evolution and plastic deformation of three bicrystals after ARB were numerically investigated using CPFEM. The

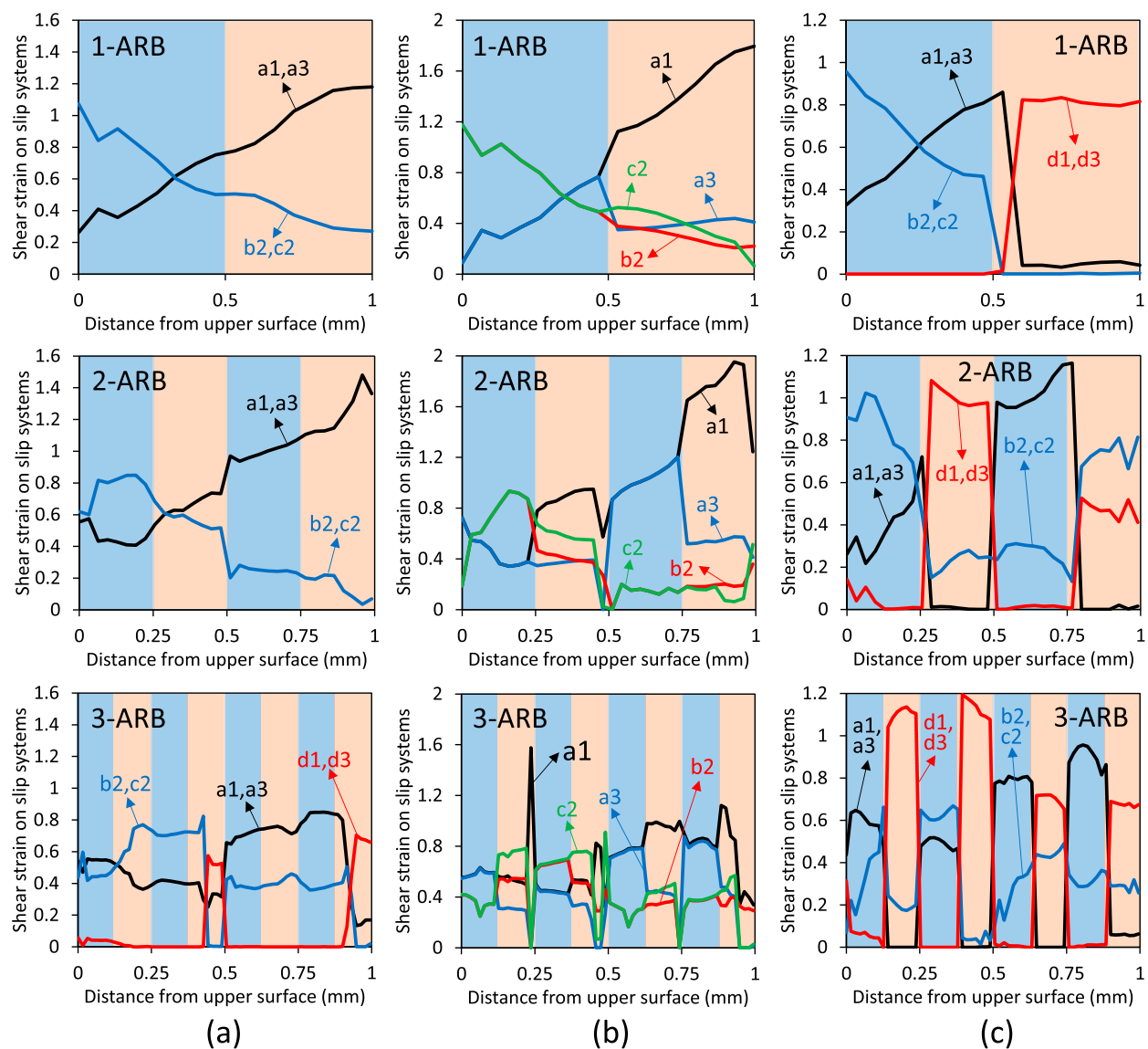


FIGURE 7 Distribution of shear strain on slip systems along the thickness after 1-ARB, 2-ARB, and 3-ARB of the (a) C-C, (b) C-S, and (c) C-RoCube bicrystals.

comparative study clearly demonstrates the effect of misorientation angles at grain interfaces on the deformation behavior.

The adopted CPFEM model is the so-called full-field method, since no homogenization is theoretically assumed (Wang et al., 2019b). The crystal plasticity (CP) constitutive law was incorporated into FEM framework, where the FEM was used as the solver and the CP constitutive law was used to determine the deformation and texture in each element after every FEM increment (Feather et al., 2021). Therefore, the crystal orientations and plastic deformation are fully coupled in CPFEM, ensuring the strain compatibility and stress equilibrium are reached (Siddiq and Schmauder, 2024). The CPFEM model is well-suited for predicting deformation behavior of single crystals and bicrystals, which show significant anisotropy, because the textural anisotropy also influences the distribution of imposed strain (Wang et al., 2019a). Another factor determining

the textural prediction accuracy is the choice of hardening model. In this study, the adopted Bassani-Wu model is a rate-dependent phenomenological model, which accurately describes the three-stage hardening behavior in FCC single crystals during straining (Siddiq and Schmauder, 2024). This hardening model was regarded the best texture predictors among the five compared hardening laws (Lin and Havner, 1996).

The coupling between plastic deformation and crystal rotation in CPFEM was investigated using the case of C-C during 3-ARB (Figure 8a). The evolved values of through-thickness shear strain γ_{RD-ND} , shear strain on slip systems, and crystal rotation angles in a single cycle (not cumulative ones) are shown in Figure 8a, where the crystal rotation angles were calculated based on the crystallographic orientations at the beginning of 3-ARB. In the first layer (i.e., C, 0–0.125 mm), the a1-a3 and b2-c2 were almost equally activated and

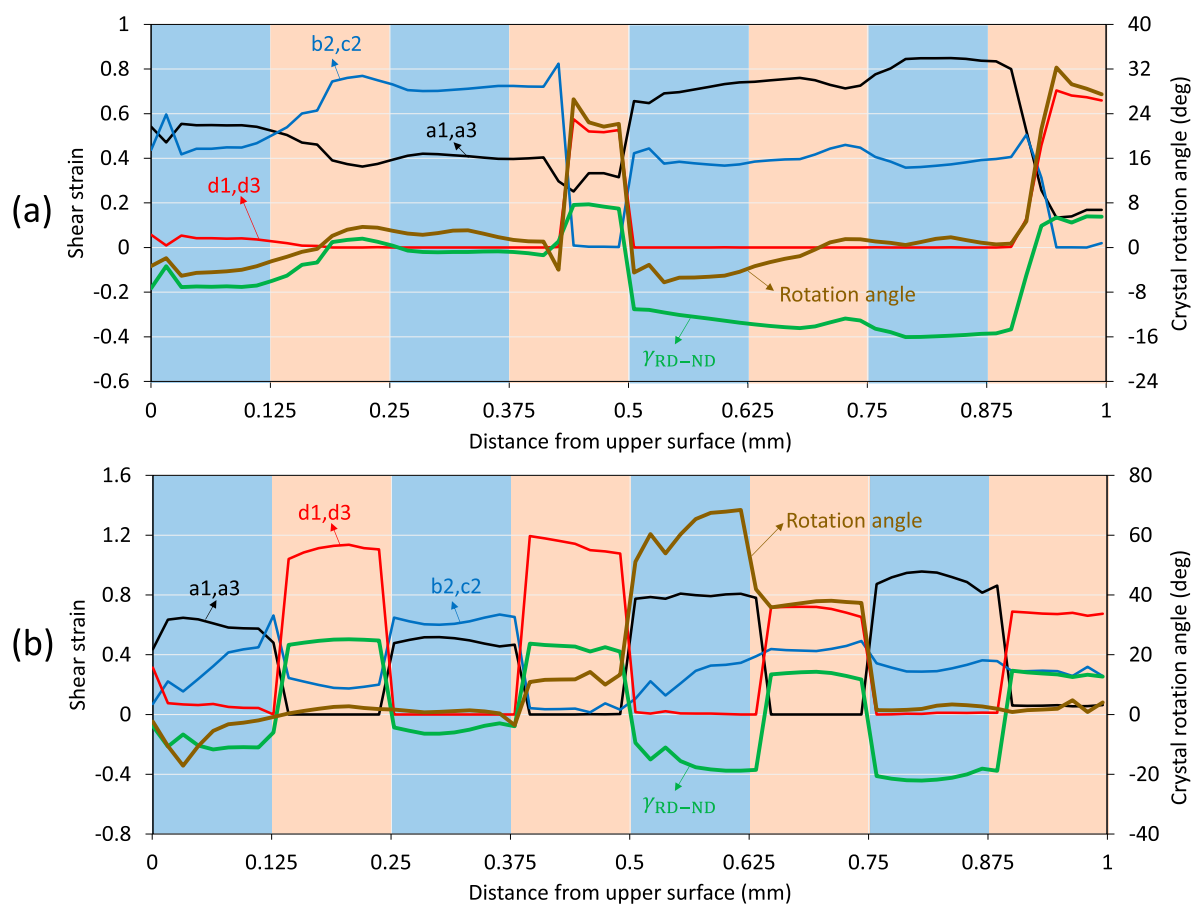


FIGURE 8 Distribution of shear strain γ_{RD-ND} , shear strain on slip systems, and crystal rotation angles in 3-ARB of (a) C-C, and (b) C-RoCube bicrystals.

thus the plastic deformation induced material rotation was very low (Equation 2). Therefore, the crystallographic rotation was required to accommodate the overall material rotation represented by the shear strain γ_{RD-ND} . A different behaviour was observed in the third C layer (0.25 mm–0.375 mm). In this layer, the b2-c2 set was highly activated over a1-a3 set, resulting in positive material rotation. To accommodate the negative material rotation (represented by γ_{RD-ND}), a positive crystallographic rotation was necessary and thus developed. In the fifth C layer (0.5 mm–0.625 mm), the shear strain on a1-a3 was obviously higher than b2-c2, which resulted in negative material rotation. In this layer, the crystallographic rotation was also negative, since the overall material rotation (γ_{RD-ND}) was strongly negative. A similar phenomenon was also observed in the sixth and seventh C layer (0.75 mm–0.875 mm). The deformation behaviour in C-RoCube (Figure 8b) can also be similarly deduced.

In Figure 8a, a sharp transition of deformation behaviour was observed in the fourth layer (0.375 mm–0.5 mm). In this layer, the primarily activated slip system set changed from b2-c2 to a1-a3, and large rotation angle and shear strain developed. This transition was due to the fact that a large misorientation angle developed at the mid-thickness interface before 3-ARB (Fig.a), which was

caused by the different crystal rotation angles at the upper and lower surfaces of 2-ARB (Figure 3c). This pre-existing misorientation angle at the mid-thickness interface increased after 3-ARB. In contrast, the misorientation angles at all other interfaces were very low before and after 3-ARB, and thus the plastic deformation varied smoothly along the thickness at these interfaces. The large misorientation angle at the mid-thickness interface before and after 3-ARB altered the plastic deformation and crystallographic rotation in this region.

Unlike the C-C single crystal, the deformation behaviour of C-S and C-RoCube bicrystals exhibited alternating patterns across their interfaces (Figures 7b, 8b). The deformation behavior of C-S was similar to that of the C-C bicrystal except for sharp changes observed at the interfaces. This was due to the small initial misorientation angle between the C and S crystals, combined with the development of large misorientation angles at the interfaces during deformation. In contrast, the C-RoCube bicrystal initially possessed a large misorientation angle, and sharp transitions in deformation behaviour were also observed at its interfaces. However, within each layer of the C-RoCube bicrystal, the deformation behaviour was primarily governed by the initial crystallographic orientation of that layer.

5 Conclusion

1. CPFEM modelling of ARB-processed bicrystals was performed for the first time, covering three configurations: C-C, C-S, and C-RoCube.
2. Differences in crystal rotation between the upper and lower surfaces during an ARB cycle led to the development of misorientation angles at the mid-thickness in the subsequent cycle, even in the C-C bicrystal.
3. In the C-C bicrystal, the misorientation angles after each ARB cycle remained negligibly low, despite initially high misorientation angles before 2-ARB and 3-ARB.
4. For the C-S bicrystal, the pre-existing interface misorientation angles decreased after ARB, due to the initially low misorientation between the C and S orientations (19.4°).
5. Misorientation angles at interfaces significantly influenced the deformation behavior on either side of the interface, with the extent of alteration depending on the magnitude of the misorientation.

Data availability statement

The raw data supporting the conclusions of this article will be made available by the authors, without undue reservation.

Author contributions

JZ: Formal Analysis, Investigation, Methodology, Writing – original draft. JW: Conceptualization, Formal Analysis, Investigation, Writing – original draft. XJ: Methodology, Project administration, Resources, Writing – review and editing. CW: Formal Analysis, Investigation, Software, Writing – original draft. HW: Conceptualization, Investigation, Supervision, Writing – original draft. GW: Conceptualization, Validation, Project administration, Writing – review and editing.

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