Nucleation and thickening of shear bands in nano-scale twin/matrix lamellae of a Cu–Al alloy processed by dynamic plastic deformation

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Abstract

Microstructural evolution associated with the shear banding in nano-scale twin/matrix (T/M) lamellae of a Cu–Al alloy processed by means of dynamic plastic deformation was investigated using transmission electron microscopy (TEM) and high-resolution TEM. The development of a shear band was found to be a two-stage process, namely a nucleation stage resulting in a narrow band composed of nano-sized (sub)grains intersecting the T/M lamellae, followed by a thickening stage of the narrow band into adjacent T/M lamellae regions. The nucleation stage occurred within a narrow region of an almost constant thickness (100–200 nm thick, referred to as “core” region) and consisted of three steps: (1) initiation of localized deformation (bending, necking, and detwinning) against the T/M lamellae, (2) evolution of a dislocation structure within the detwinned band, and (3) transformation of the detwinned dislocation structure (DDS) into a nano-sized (sub)grain structure (NGS). On the two sides of a core region, two transition layers (TRLs) exist where the T/M lamellae experienced much less shear strain. The interface boundaries separating the core region and the TRLs are characterized by very large shear strain gradients accommodated by high density of dislocations. Increasing shear strains leads to thickening of shear bands at the expense of the adjoining T/M lamellae, which is composed of thickening of the core region by transforming the TRLs into the core region with DDS and NGS, analogous to steps (2) and (3) of the nucleation process, and outward movement of the TRLs by deforming the adjoining T/M lamellae. Grain sizes in the well-developed shear bands are obviously larger than the lamellar thickness of original T/M lamellae.

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1. Introduction

Strain localization in the form of shear bands, i.e., narrow sheet-like regions of concentrated plastic flow, is an important mode of inhomogeneous deformation for a wide range of metals and alloys with different microstructures. In materials of low stacking fault energy (SFE), shear bands develop within a highly twinned structure character-
grains at large strains. For the former effect, some detailed microtextural aspects of the shear bands formed against T/M lamellae in Cu, Cu–2% Al and Ag have been analyzed [4–6]. It is generally accepted that the extensive shear banding has a decisive effect on the later stage of the development of the brass-type texture during cold rolling [7–9].

For the latter effect, earlier studies [7,10] have shown that shear bands formed in a cold-rolled 70:30 brass consist of very small, elongated crystallites that are separated by high-angle boundaries. The significance of the shear banding on the development of ultrafine or nano-grained structures has been demonstrated in cold-rolled austenite steels [11,12] and Cu alloys subjected to dynamic plastic deformation (DPD) [13,14]. However, the detailed microstructural aspects as to the development of an ultrafine or nano-grained structure associated with the shear banding are not well understood.

Most of the previous observations of the microstructure within shear bands were made in well-developed bands where the original T/M lamellae have been completely destroyed. Furthermore, a common observation is that the size scale of the ultrafine or nano-grained structure developed in the shear bands is much coarser than the twin boundary (TB) spacing in the original T/M lamellae, indicating that shear banding is a coarsening mechanism rather than a refining mechanism although intensive shear strain is introduced within the bands. These observations raise several fundamental questions:

1. How does a shear band initiate or nucleate within the nano-scale T/M lamellae?
2. How does a nano-scale T/M lamellar structure transform into an ultrafine or a nano-grained structure during shear banding?
3. Is there any characteristic size for the nascent shear bands?
4. When does a shear band start to thicken and how does the thickening occur?

In this study, we introduced a T/M lamellar structure and shear bands in a Cu–Al alloy by means of the DPD treatment. The formation of nascent shear bands induced by localized shear deformation, their subsequent transformation to nano-scale grains, and the thickening of shear bands are systematically investigated using transmission electron microscopy (TEM) and high-resolution TEM (HRTEM). The questions raised above are addressed and discussed based on experimental observations.

2. Experimental

The material used in the present investigation was a single phase Cu–4.5 wt.% Al alloy with a SFE of about 12 mJ m⁻² [15]. Prior to the DPD treatment, the alloy was annealed at 1123 K for 2 h, resulting in a coarse-grained structure with an average grain size of about 200 μm. Cylinders 9 mm in diameter and 12 mm in height were subjected to the DPD treatment on a dynamic compression facility; the cylindrical specimen on a lower anvil was impacted by an upper anvil at a high loading rate at room temperature (RT). The plastic strain was controlled to be 0.2–0.3 at each impact with a strain rate in the range of 10²–10³ s⁻¹. The strain is defined as \( \varepsilon = \ln (L_0/L_f) \), where \( L_0 \) and \( L_f \) are the heights of the cylinder before and after the impact, respectively. The samples used for TEM observations were deformed to a high accumulative strain of \( \varepsilon = 1.7 \), in which shear bands developed to different stages can be observed.

TEM samples were cut from the longitudinal section containing the compression axis. Thin sheets of about 0.5 mm thick were sectioned by spark-cutting, ground on both sides, and then electropolished using a twin-jet polisher. TEM observations were carried out on a JEOL 2010 electron microscope operating at 200 kV and HRTEM observations were carried out on a FEI Tecnai F30 electron microscope operating at 300 kV.

To measure the shear strain and shear strain gradient associated with a given shear band, the curved twin boundaries (TBs) that run through the shear band are used as markers, as shown in Fig. 1a. A fiducial line is drawn following a TB and it is divided into a series of segments of equal width, \( \delta \), in the direction perpendicular to the shear banding direction (Fig. 1b). The average shear strain associated with each segment could be calculated according to the equation \( \gamma = d/\delta = \cot \theta - \cot \theta_0 \), where the parameters \( d, \theta, \theta_0 \) are defined in Fig. 1b. Apparently, the associated

![Fig. 1. (a) A TEM image of a typical shear band in the DPD Cu–Al sample in which the original TBs are deformed; (b) geometric relation for calculating shear strain within the shear band: \( \theta_0 \), the angle of shear direction \( AA' \) to the original direction of TB \( BB' \); \( \theta \), the angle of the shear direction \( AA' \) to the reoriented direction of TB \( CC' \); \( \delta \), the width (transverse to the shear direction) of a unit segment; \( d \), the shear displacement of a unit segment.](image-url)
shear strain varies across a given shear band. To evaluate and compare the microstructural evolution inside different shear bands, the maximum shear strain $\gamma_{\text{max}}$ calculated by the method described above was taken as a measure of the shear strain of a shear band.

3. Results and analysis

3.1. Development of shear bands: an overview

The microstructural evolution in the DPD Cu–Al sample is typical of the cold-deformed fcc metals with low SFEs. Deformation twins were formed inside many grains at low strains ($\gamma \sim 0.15$). As the DPD strain increases, the density of deformation twins increases and the TBs gradually rotate towards the compression plane, i.e., the plane perpendicular to the loading direction. Fig. 2 shows a typical image of high-density nano-scale T/M lamellae, in which TBs are straight and parallel to the compression plane. The corresponding selected area electron diffraction (SAED) pattern (inset) indicates a regular twin relationship. The T/M lamellae have a narrow thickness distribution with a mean thickness of about 10 nm.

A large number of shear bands of various thicknesses were observed inside the areas of high-density T/M lamellae in the deformed samples, with the associated maximum shear strains varying from $\gamma_{\text{max}} = 0.3$ to $>7$. Typical examples of TEM observations are shown in Fig. 3a–d to demonstrate the general evolution of shear bands as a function of shear strain. The initiation of shear banding is revealed at the low strain levels $\gamma_{\text{max}} < 2$ (Fig. 3a), which is characterized by an obvious bending of T/M lamellae inside a narrow localized shear region. When $2 < \gamma_{\text{max}} < 4$ (Fig. 3b), intensive shear deformation separates the T/M lamellae inside the band from those outside. In Fig. 3b, the detailed structural features within the shear band are not resolved when the T/M lamellae outside are near [0 1 1] zone axis, indicating a large deviation of the [0 1 1] zone axis from the beam direction inside the band. At $4 < \gamma_{\text{max}} < 7$ (Fig. 3c) a narrow shear band consisting of a well-developed (sub)grain structure is formed. Extensive TEM observations showed that during the course of transformation from an initial shear localization zone (Fig. 3a) to a shear band composed of well-developed ultrafine or nano-sized (sub)grains (Fig. 3c), the shear band thickness remains almost constant, being typically 100–200 nm.

At $\gamma_{\text{max}} > 7$ (Fig. 3d), the shear bands composed of ultrafine or nano-sized (sub)grains increasingly erode the surrounding T/M lamellae, leading to an expansion of shear bands to thicknesses of 0.5 to several micrometers.

Based on the evolution of the band thickness and of the internal substructure within the sheared regions, the development of shear bands can be divided into two characteristic stages, nucleation stage (Fig. 3a–c) and thickening stage (Fig. 3d), which correspond to shear strain ranges of $\gamma_{\text{max}} < 7$ and $\gamma_{\text{max}} > 7$, respectively. In the following sections, the detailed microstructural evolution during the
nucleation stage and the thickening stage of shear bands will be analyzed and discussed.

3.2. Shear band nucleation ($\gamma_{\text{max}} < 7$)

The nucleation stage of a shear band is composed of three component steps: (1) localized deformation (initiation of bending, necking, and detwinning) in original T/M lamellae, (2) evolution of detwinned band into a dislocation structure (referred to as detwinned dislocation structure (DDS)), and (3) transformation of the DDS into a nano-sized (sub)grain structure (NGS).

3.2.1. Localized deformation in the original T/M lamellae ($\gamma_{\text{max}} < 2$)

Localized deformation initiates in narrow bands (hereafter referred to as the “core” region, usually 100–200 nm thick) in which crystal rotation occurs and high shear strains are introduced. An example of analysis of the crystal rotation and the shear strain distribution associated with such a band is shown in Figs. 4 and 5. The core region is bounded by two remarkable dark strips, which are diffusive in contrast and within which high density of dislocations are observed. TBs far outside the band are straight with a twin relationship as revealed by corresponding SAED pattern (Fig. 4b). Inside the core region of shear band, most T/M lamellae still remain, but are bent toward the shear direction; the corresponding SAED pattern (Fig. 4c) reveals two arrays of strong spots, which still accord with the T/M relationship. A comparison between Figs. 4b and c, as illustrated in Fig. 4d, indicates a clockwise crystallographic rotation inside the shear band, in accordance with the bending of the T/M lamellae. Fig. 4a also shows that adjacent to the core region, a transition layer (TRL) in which the T/M lamellae are bent, is identified on each side of the core region. The TRL has a thickness smaller than or comparable with the core region. It is most likely that the clockwise lattice rotation in both the twin and the matrix lamellae is caused by the geometry of the shear deformation: the sheared zone will rotate with respect to the un-sheared around a transverse direction (TD) that is parallel to the shear band plane and perpendicular to the shear direction. It is also noticed from Fig. 4c.

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Fig. 4. (a) A closer observation of a part of the shear band in Fig. 3a with $\gamma_{\text{max}} = 0.8$. The dark-gray region, labeled “Core”, refers to the core region with intensive shear strains; the light-gray region, labeled “TRL”, refers to the transition layered region with relatively small amount of shear strains. (b,c) SAED patterns from the circled areas labeled as “b” and “c” in (a). (d) Schematic illustration of relative rotation between (b) and (c). The black and gray spots correspond to the diffraction spots of (b) and (c), respectively.

Fig. 5. (a,b) Distributions of shear strain and strain gradient across the shear band, measured along the three TBs indicated by stars and three pairs of arrows in Fig. 4a. Values from three TBs are averaged for the same transverse position.
that the beam direction within the band is deviated from the [0 1 1] zone axis, indicating that there is an additional rotation component besides the rotation around the TD. Since deformation by slip is evident from the residual dislocation structures seen in shear bands (results to follow), this additional rotation component is considered to be induced by dislocation glide with the constraints of surrounding materials. The rotation axis induced by dislocation glide is determined by the active slip systems and often differs from the TD. Analogous analysis of lattice rotation in shear bands has been previously made in pure copper deformed at 77 K [6] and in cold-rolled IF steel [16].

The microstructural features of the shear band in Fig. 4a can be correlated to the measured shear strain and shear strain gradient across the band, as in Fig. 5a and 5b, which were determined by using the marked TBs in Fig. 4a. The shear strains were distributed mainly inside the core region. Approaching the band center, the T/M lamellae were bent to the largest degree, corresponding to a maximum shear strain of \( \gamma_{\text{max}} = 0.75 \pm 0.28 \) (Fig. 5a). Much smaller shear strains are also noticed within the TRLs. It is worth noting that the dark strips bounding the core region correspond to the positions of the maximum strain gradients (8.2 \( \pm \) 5.6 and \(-7.8 \pm 5.6 \) \( \mu \text{m}^{-1} \)), suggesting that they are essentially a result of strain accommodation.

To reveal the detailed microstructural features of the dark strips, a shear band with analogous characteristics but with an even smaller shear strain (\( \gamma_{\text{max}} = 0.3 \)) is observed. As shown in Fig. 6, the bright-field image reveals a dark strip bounding the core region of the band. Inside the core region, T/M lamellae are slightly bent towards the shear direction. Some T/M lamellae within the core region are found to shrink in thickness. For example, the two lamellae indicated by black arrows are 11.9 nm and 5.9 nm thick outside the shear band, respectively, which gradually reduce to 2.6 nm and 3.4 nm within the band, respectively.

An HRTEM image (Fig. 6b) taken from the area “b” in Fig. 6a indicates that the dark strip bounding the core region consists of high density of dislocations. A misorientation angle of 4.2° across the dark strip is identified according to the deflection of \((1 1 1)_M\) atomic planes, as indicated by the white lines. To illustrate the lattice distortion clearly, inverse Fourier transformation (IFT) analysis of the rectangular area is performed. The IFT image with one-dimensional \((1 1 1)_M\) plane fringes (Fig. 6b) reveals a series of additional half atomic planes, indicating edge component of dislocations with the same sign, as marked by white \( \perp \) signs. These dislocations arrange themselves in a line roughly parallel to the shear direction, forming a tilted, low-angle dislocation boundary. The misorientation angle (\( \theta \)) of such a boundary can be calculated according to \(d_{1 1 1} = 2h_{av} \sin \theta\), where \(d_{1 1 1}\) is the spacing between neighboring \((1 1 1)_M\) atomic planes, and \(h_{av}\) is the average vertical distance (the distance projected on the \((1 1 1)_M\) plane) between the dislocations. Since \(d_{1 1 1} = 0.208 \text{ nm}\) and \(h_{av}\) was measured to be 2.45 nm, \( \theta \) is calculated to be 4.8°, which is well consistent with the measured value of 4.2°. Therefore, the misorientation across the dark strip could be mainly accounted for by these dislocations. On the other hand, the IFT image with \((1 1 1)_M\) fringes (Fig. 6b) reveals a high density of dislocations, with roughly equal numbers of opposite signs. These dislocations therefore do not contribute to the misorientation across the dark strip.

The HRTEM observation (Fig. 6c) from the area “c” in Fig. 6a shows the details of necking of a twin lamella. The twin lamella contains 15 atomic layers on the right, whereas its thickness decreases to nine atomic layers near the dark strip. The necking of the lamella is found to be associated with the existence of many TB steps on either side, which are normally one or several \((1 1 1)_M/T\) atomic layers in height. By applying the Frank circuit approach, these TB steps are identified as Shockley partial dislocations. For instance, the Frank circuit (labeled as A) enclosing a TB step indicates a Shockley partial dislocation with a Burgers vector \( b = \frac{1}{6}[1 1 2] \). In addition, an extended dislocation in the form of two Shockley partials with a stacking fault, which aligns with the \((1 1 1)_T\) slip plane and connects the TBs, is seen in the twin lamella, as indicated by a thick dashed line in Fig. 6c.

At \( \gamma_{\text{max}} > 1 \), T/M lamellae are found to break up, accompanied with disappearance of some TBs. Fig. 7a1 shows a shear band with \( \gamma_{\text{max}} = 2.0 \), in which broken and disappeared T/M lamellae are obvious. The corresponding SAED pattern (Fig. 7a3) reveals only the matrix-related elongated spots, suggesting the absence of twin lamellae and small misorientations inside the core region of shear band. Although the T/M lamellae far outside the shear band are straight with a regular twin relationship (Fig. 7a2), the TBs in the TRL adjacent to the core of shear band are obviously bent. The orientations inside the core region and the T/M lamellae in the TRLs are rotated clockwise with respect to that outside the shear band, as indicated by the SAED in Fig. 7a4 and a5.

To explore the disappearance process of twin lamellae, dark-field images of the twin (Fig. 7b) and matrix lamellae (Fig. 7c) are taken, respectively. Three fine twin lamellae are identified according to their original thicknesses, as denoted by T 1, T 2 and T 3 in Fig. 7a-c. For clarity, a sketch of these twin lamellae is shown in Fig. 7d, where the identification of the core of shear band and the TRLs is also indicated. In the TRLs (Fig. 7b), these three lamellae are found to bend toward the shear direction, gradually decrease in thickness as they approach the core region, and finally eliminate with wedge-shaped tips. In particular, lamella T 1 terminates in the left TRL region. Moreover, tips of these broken twins are embedded in the matrix (Fig. 7c), indicating that the disappeared portions of the original twins have been replaced by the matrix orientation. It is interesting to note that a short segment of lamella T 2 is remained inside the core region (as indicated by a white arrow in Fig. 7b and c), which presents an intermediate stage of the breaking-up of twin lamellae. Based on these observations it is concluded that breaking-up of the
Fig. 6. (a) A TEM image showing the region near the boundary of a shear band with $\gamma_{\text{max}} = 0.3$. The two black arrows indicate twin lamellae whose thicknesses are obviously reduced in the shear band; (b1) An HRTEM image of the rectangular region labeled as "b1" in (a); (b2, b3) IFT images of the region marked in (b1), revealing one-dimensional $(111)_{\text{M}}$ and $(111)_{\text{T}}$ fringes, respectively; (c) An HRTEM image of the region "c" in (a). The white line segments indicate the TBs. The Frank circuit labeled as "A" encloses a TB step. The bold black dashed line indicates a stacking fault.
twin lamellae is a result of progressive thinning/necking of the lamellae from both sides. Analogously, fragmented twins have been previously investigated using TEM [17], and it was found that in most cases the fragmented twin segments exhibit no lateral displacement with respect to each other. It was suggested that the configuration of fragmented twins was caused by obstacle slip structures which evolve in the growth path of propagating twins [17]. It is worth pointing out that the case is different in the present work, since the twins are seen to be long, complete lamellae (Fig. 2) before they break up in shear bands; and shear offset is obvious between fragmented twin segments.

Disappearance of the twin relationship in shear bands developed from a T/M lamellar structure has been reported previously [4–6,11,12], and several mechanisms have been proposed to account for this phenomenon. The first involves detwinning of the existing twins induced by twin-slip interaction. The feasibility of twin-slip interaction was first demonstrated geometrically by Sleeswyk and Verbraak [18] for body-centered cubic (bcc) crystals and their analysis was later applied to fcc structures by other researchers [19,20]. The geometrical analysis showed that a slip dislocation can always penetrate into an obstacle twin but in most cases the incident slip dislocation must dissociate into a slip dislocation in the twin and a partial dislocation at the TB. Furthermore, the partial left at the TB must slip away from the reaction junction to remain the shear unchanged, giving rise to either thickening or detwinning of the obstacle twin, depending on the stress state. In fcc crystals, twin-slip interaction has been studied by

Fig. 7. (a1) A bright-field TEM image of a shear band with $\gamma_{\text{max}} = 2.0$. Three pairs of black arrows (labeled as “T 1”, “T 2”, and “T 3”) indicate three fine twin lamellae that are broken within the band; (a2–a4) SAED patterns corresponding to the circled areas labeled as “a2”, “a3”, and “a4” in (a1), respectively; (a5) Schematic illustration of relative rotation from (a2) to (a4). The black spots correspond to the diffraction spots in (a2), and the gray arrow-headed arcs to the diffraction spots in (a4). (b, c) Dark-field images revealing the twin and matrix lamellae, respectively. The white arrow indicates a surviving segment of twin lamella T 2. (d) Schematic illustration of the morphology of the three broken twins.
experimental observations [20,21] and recently by molecular dynamic (MD) simulations [22,23]. The fragmentation of twins observed in deformed nitrogen bearing steels was attributed to twin-slip interaction [24]. The second plausible mechanism involves secondary twinning within the existing twin (or matrix) lamellae, which can transform the original twin (or matrix) orientation into different orientations, resulting in disappearance of the twin (or matrix) component. In previous investigations [5,6], the disappearance of matrix orientation in shear bands was attributed to the observed mechanical twinning within reoriented matrix lamellae. The third mechanism proposed previously involves the consideration that opposite crystal rotations in the twin and in the matrix may lead to annihilation of TBs [11,12].

Several characteristic features could be expected in the shear band if the detwinning mechanism plays a role. Firstly, partial dislocations, which are products of twin-slip interaction, should be left on the TBs where the twin lamellae are locally thinned or fragmented. Secondly, the lateral movement of a TB toward the twin side due to glide of partials on the TB should simply transform the region swept across by the TB from twin orientation to matrix orientation, and meanwhile remain regular twin relationship between the two sides of the TB. These features are indeed observed in the present work, in particular in Figs. 6c and 7b and c, suggesting that the disappearance of the twin relationship is governed by the detwinning mechanism.

Furthermore, based on the dislocation configurations observed in Fig. 6c, specific dislocation reactions can be proposed to demonstrate the detwinning process of a pre-existing twin lamella. Fig. 8a gives the geometric relationship to be considered in the Thompson notation. For convenience, the line sense of all dislocations is CB. A perfect dislocation CB, gliding on the z plane in the twin lamellae, is dissociated into two partials, Cx and zB (Fig. 8b1), according to

$$\text{CB} \rightarrow \text{Cx} + \text{zB} \quad (1)$$

producing a stacking fault between these two partials. The dislocation CB could have been nucleated from TBs near stress concentrations, as suggested previously by TEM observations in Cu with nano-scale twins [25]. Given the small thickness of the twin, the splitting distance between Cx and zB is large enough for them to encounter the bottom and top TBs, respectively. Upon encountering the top TB, zB splits into a Shockley partial δB, and a stair-rod dislocation zδ (Fig. 8b2), i.e.,

$$\text{zB} \rightarrow \text{zδ} + \delta B \quad (2)$$

The partial δB glides to the left on the TB under the applied stress, reducing one atomic layer in thickness of the twin. Reaction (2) has been previously proposed to rationalize the twin fragmentation in deformed nitrogen bearing steel [24]. However, dislocation zδ is obviously sessile; therefore, under stress it is most likely to further dissociate to enable shear compatibility or stress relaxation. The zδ could further split into two partials, zB and Bδ (Fig. 8b3), according to

$$\text{zδ} \rightarrow \text{zB} + \text{Bδ} \quad (3)$$

The partial Bδ slips away to the right on the twin plane, detwinning one layer of the twin lamella. The remained partial zB is still on the original slip plane, but has glided downward one atomic layer. Reactions (2) and (3) would be energetically unfavorable in the absence of stress, but can become favorable under the characteristically high stress

Fig. 8. (a) The double Thompson tetrahedron for the twin–matrix orientation relationship. The δ plane is the coherent twin boundary plane. (b1–b4) Schematics of twin-slip interactions between a perfect dislocation CB (split into Cx and zB) and a twin, which lead to detwinning of the twin. The viewing direction is CB and therefore the z plane and the δ plane are edge on, and the projection of δ plane is horizontal.
in the localized region of shear band. Note that reactions (2) and (3) provide a full reaction cycle that can be repeated to simultaneously reduce the thickness of the twin lamella from the top side (Fig. 8b4), without the need of nucleation or emission of additional Shockley partial dislocations. This reaction cycle is analogous to the self partial-multiplication twinning mechanisms proposed recently [26]. Analogously, due to the crystal symmetry, dislocation Cxz will repeat the reaction with the bottom TB according to

\[ Cxz \rightarrow C\delta + \delta x \]  

(4)

and

\[ \delta x \rightarrow \delta C + Cxz \]  

(5)

leading to detwinning of the twin lamella from the bottom side (Fig. 8b2–b4). Finally, the twin lamella would fragment due to the crystal symmetry, dislocation C, which can cross-slip into the matrix lattice. Since the passage of a Shockley partial exposes one $\{111\}$ layer (~0.2 nm thick), to fragment a twin with an average thickness of 10 nm, about 25 cycles of the full reaction (2)–(5) are required from either side – this can be reasonably fulfilled, providing the extensive deformation in shear bands. Besides the dislocation reactions proposed here, we do not exclude the possibility of other reactions proposed previously for twin-slip interactions [20,21,24] to account for the detwinning mechanism.

According to the second plausible mechanism, twin nuclei in the pre-existing twin/matrix lamellae should be observed in early-stage shear bands. However, such a scenario is scarcely observed in the present work, suggesting that the role of secondary twinning is minor. It is generally accepted that formation of a stable twin comprises formation of a twin nucleus and its subsequent growth [27]. The growth of a matrix nucleus within a pre-existing twin lamella could be considered to be equivalent to detwinning of the twin, whereas formation of matrix nucleus requires additional energy. According to Ref. [22], the energy barrier to create an intrinsic stable stacking fault from a perfect lattice is larger than that to create a twin fault from a pre-existing twin plane. Therefore, the secondary-twinning mechanism is energetically unfavorable compared with detwinning mechanism. Moreover, it is usually assumed that formation of deformation twins requires formation of specific slip bands as precursors [27]. The small thickness of the T/M lamellae should hinder the formation of slip bands within a single T/M lamella, which therefore hinders the secondary twinning. In other words, secondary twinning is more likely to happen within coarser T/M lamellae. Indeed, the matrix lamella within which mechanical twinning happens in Ref. [6] has a thickness of ~60 nm, much larger than the average T/M lamellar thickness (10 nm) in the present work.

According to the third plausible mechanism [11,12], both the twin and matrix related orientation components should coexist in shear band, whereas these two orientation components deviate from regular twin relationship due to lattice rotation in opposite directions in the twin and matrix lamellae, respectively. However, such a hypothesis is not borne out by the present observations that one of the two T/M orientation components promptly disappears in early-stage shear bands, and that both the twin and matrix lamellae rotate in the clockwise direction. It is therefore inferred that the small thickness of the twin lamellae investigated in the present work allows the twin lamellae to promptly detwin at relatively low shear strains before the third mechanism might be initiated.

It is therefore concluded that the disappearance of twin relationship in shear bands is dominated by detwinning induced by twin-slip interactions, whereas the other plausible mechanisms are of minor importance.

3.2.2. Formation of DDS ($2 < \gamma_{\text{max}} < 4$)

Inside shear bands with even higher shear strains, elongated dislocation structures are formed. A typical shear band, with a core region of about 100–200 nm thick and with a shear strain of $\gamma_{\text{max}} = 3.8$, is shown in Fig. 9a1. Inside the shear band, the microstructure can not be clearly revealed when the T/M lamellae outside the band are clearly seen. The microstructure within the shear band was revealed by carefully tilting the sample in TEM, as shown in Fig. 9b1. Elongated boundaries are observed and they are roughly parallel to the shear direction. Dislocation arrays forming the boundaries could be identified, as arrowed in Fig. 9b1, and diffraction analysis showed that these boundaries are low-angle dislocation boundaries.

Two types of dislocation boundaries could be identified inside the core of shear band based on their origins. One is the boundaries that are newly generated to accommodate shear strain and cross obliquely the original T/M lamellae, such as those denoted as H–I–J–K and I’–J’–K’ in Fig. 9c. These boundaries are roughly parallel to the shear direction and are inclined at large angles ($>20^\circ$) to the original TBs. The second type consists of low-angle dislocation boundaries that cross the shear bands, such as those marked I–I’–J–J’ and K–K’ in Fig. 9c. Closer observations, e.g. Fig. 9d for J–J’, revealed that these boundaries are connected with a single twin lamella (I–I’ and J–J’) or a narrow bundle of T/M lamellae (K–K’) outside the shear bands (see Fig. 9c). The spatial and morphological correspondence between these dislocation boundaries and the twin lamellae suggests that these boundaries result from the accumulation of dislocations during the detwinning process.

In summary, as twin lamellae disappear, the microstructures inside shear bands get softened. Hence, subsequent shear strain may prefer to concentrate on the inner part of shear bands, resulting in the formation of dislocation structures. Dislocation boundaries are mainly formed from two approaches. One is that for initial shear banding, extended dislocation walls are formed between the sheared and the un-sheared region, intersecting the original T/M lamellae (as in Figs. 4a and 6a). These dislocation walls are aligned with the shearing direction, for accommodating large shear strains and strain gradients. As shear strain...
increases, these dislocation walls evolve into dislocation boundaries for energy minimization [28]. On the other hand, the different diffraction contrast between the two matrix lamellae separated by the shrinking twin J–J‘ (Fig. 9d) suggests a difference in orientation between them. This orientation difference could be caused by the different slip activities in the lamellae due to local stress state variations. As a result, a dislocation boundary forms to accommodate the orientation difference.

3.2.3. Formation of NGS (4 < γ \text{max} < 7)

The subsequent shear deformation continues to localize within the shear bands. A shear band with γ \text{max} = 4.2 is shown in Fig. 10a. The T/M lamellae are abruptly broken by intensive shear within a core region of about 100 nm thick. Moreover, obvious deformation of the T/M lamellae is also noticed in the TRLs of about 600 nm thick on both sides of the core. The morphology accords well with the measured distribution of shear strain (Fig. 10b) and shear strain gradient (Fig. 10c). In the core region, shear strain increases dramatically from 1 to 4.2, with strain gradients as large as 63 \mu m^{-1} at the boundaries. In the TRLs, shear strain is within 0–1 associated with shear strain gradient.

The intensive shear in the core region of shear bands results in the evolution of a DDS into a NGS that is equiaxed or elongated along the shear direction. Fig. 11
shows a shear band with $\gamma_{\text{max}} \sim 4.7$. At the left portion of the band, the morphology is analogous to that of the shear band in Fig. 9a; moreover, tilting revealed an elongated dislocation structure similar to that in Fig. 9b. At the right portion of the band, elongated and equiaxed (sub)grains are seen. The different contrast between these (sub)grains suggests obvious misorientation among them.

The above sequence of events, involving the formation of extended dislocation walls, elongated dislocation boundaries, and roughly equiaxed grains or subgrains, resembles the general pattern of microstructural evolution well established for plastic deformation of coarse-grained metals and alloys [29–31]. A similar process of microstructural evolution has been demonstrated for macroscopic shear bands by applying a hat-shaped technique [32,33]. Note that the microstructural evolution in shear bands after the twin lamellae disappear is dominated by dislocation glide rather than mechanical twinning, probably because the crystalline orientations in the shear bands after the twin lamellae disappear are not favorable for twinning which is strongly dependent on grain orientations [27,34,35].

3.3. Shear band thickening ($\gamma_{\text{max}} > 7$)

As an NGS is developed in the core region of shear bands of 100–200 nm thick, subsequent shear straining leads to thickening of the bands. A well-developed shear band of about 1 µm thick is shown in Fig. 12a, in which elongated or roughly equiaxed grains are observed. In contrast with the regular T/M relationship outside the band (Fig. 12b), the corresponding SAED pattern within the band (Fig. 12c) shows diffraction rings, indicating large variations in the crystallographic orientations of grains. Dark-field imaging, Fig. 12d, shows that many of the grains are still linked to their neighboring ones along the shearing direction (Fig. 12d), suggesting that they are broken down from their parent elongated (sub)grains. The statistical measurements of transverse size of the grains, $D_T$, inside the shear band are shown in Fig. 12e. A peak value of 53 nm is seen. The distribution of the thicknesses of the T/M lamellae outside the shear band is shown in Fig. 12f. The peak value corresponds to about 10 nm, which is five times smaller than the transverse size of the grains within the band.

In well-developed shear bands, the arrangement of grains along the shearing direction reflects direction of the imposed deformation, consistent with previous results [32,36,37]. The average transverse grain size obtained inside the shear band is much larger than the average thickness of the original T/M lamellae. Obviously, in the present
case, the microstructural size within shear bands is determined by the sizes of the formed dislocation structures. The shear-banding-induced structural coarsening has been reported in cold-rolled austenitic stainless steels [11], in agreement with the present results.

To explore the thickening mechanisms of well-developed shear bands, the microstructural features were inspected in detail for the regions along the interface between a shear band and a TRL. In many cases, it was found that such regions consist of coarser (sub)grains or elongated dislocation structures, and an example is shown in Fig. 13. In the inner core region (the lower left part of Fig. 13b), elongated or equiaxed grains with an average size of 49 nm (in accordance with Fig. 12) are observed. In the core region adjacent to the TRL, the (sub)grain sizes are apparently larger. For instance, the (sub)grains denoted by numbers 1–6 have an average transverse size of 100–200 nm. The structure morphologies of this region are similar to the DDS or newly formed (sub)grains in the core region in the last stage of shear band nucleation (as in Fig. 11), clearly indicating that this region is newly developed from the contacting TRL with increasing shear strain.

These observations point to a fact that the thickening of a shear band at higher strains is a process in which TRLs transform successively into the core region via deformation of T/M lamellae and subsequent formation of DDS and nano-sized (sub)grains, and meanwhile adjoining original T/M lamellae are deformed to form new TRLs. Or in other words, during the thickening process of a shear band, the core region increases its thickness continuously by pushing the two TRLs outwards and consuming more and more original T/M lamellae. This process is schematically illustrated in Fig. 14.

It is generally accepted that shear banding is a softening process, i.e., bands become softer than their original (or surrounding) matrix. Our observations are in accord with this argument. As the dimension of the microstructure inside the shear band (core) is evidently larger than that of the original T/M lamellar thickness, the core region is expected to be softer than its surrounding matrix. Moreover, as stated above, within the core region the layers adjacent to the TRLs are structurally coarser than the inner part of the core. Hence, it is anticipated that these layers are even softer than the inner core region. Consequently, it is reasonable to suggest that the most shear strains are likely accommodated by the out-bound layers of the core region and the TRLs. The out-bound layers of the core may absorb shear strains to transform the DDS into finer (sub)grains with more random crystallographic orientations. The outward moving TRLs accommodate strains
by deforming original T/M lamellae. It means that during thickening of a shear band, the most shear strains might be concentrated (localized) in the vicinity layers of the core/TRL interfaces, corresponding to the highest strain gradients.

Fig. 15 summarizes the nucleation and thickening processes of shear bands in the T/M lamellae structure. The unique underlying mechanism of shear banding in the T/M lamellae structure might shed light on the mechanical behaviors of the nano-twinned metals and alloys, including their strength, ductility, and fracture toughness [38–40].

4. Conclusions

The development of shear bands in nano-scale T/M lamellae of a Cu–Al alloy processed by means of DPD was investigated systematically. Two characteristic stages, nucleation and thickening, were identified based on extensive TEM and HRTEM observations.

The nucleation of a shear band in the nano-scale T/M lamellae leads to the formation of a core region of shear band composed of nano-sized (sub)grains, which is accomplished through the following three steps:

1. initiation of shear banding (bending, necking and detwinning) of the T/M lamellae,
2. formation of DDS, and
3. transformation of the DDS into NGS.

In the nucleation stage, the thickness of shear bands remains almost constant, being 100–200 nm. On the two sides of a core region, two TRLs of deformed T/M lamellar structure with much lower shear strains are present. The interface boundaries separating the core region and the
TRLs are characterized by very large strain gradients accommodated by high density of dislocations.

The thickening process of shear bands at increasing shear strains is composed of thickening of the core region by transforming the TRLs into the core region with DDS and NGS, analogous to steps (2) and (3) of the nucleation process, and outward movement of the TRLs by deforming the adjoining original T/M lamellae. Grain sizes in the well-developed shear bands are obviously larger than the lamellar thickness of original T/M lamellae, and the structure in the out-bound layers of the core is coarser than that in the inner core region. During thickening of a shear band, most shear strains are anticipated to be concentrated in the vicinity layers of the core/TRL interface boundaries.

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