Unusual Crystallographic Aspects of Microband Boundaries within {111}<110> Oriented Grains in a Cold Rolled Interstitial Free Steel

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Microbands are well-known deformation features that generate in the rolling microstructures of many metals and alloys. The boundaries across two neighbouring microbands are comprised of dense dislocation walls and they accommodate a small average crystallographic rotation in the range of 1–4°. In this study, a combination of high resolution electron backscattered diffraction (EBSD) and transmission electron microscopy (TEM) was used to observe orientation differences of up to 20° across microband boundaries in the rolling substructures of {111}<110> oriented grains in steel. Despite their high angle nature, the microband interfaces maintain their well-known crystallographic characteristics, by being closely aligned with highly stressed slip planes. Rigid body rotations are argued to take place around the interface normal between adjacent microband lattices. This results in an unusual microstructure whereby alternating microband boundaries, oriented in equal and opposite relative angles, produce an array of orientation pairs in their spatial distributions.

KEY WORDS: microbands; EBSD; deformation microstructure; crystallographic texture; steels.

1. Introduction

Microbands are generally known as low angle (≤8°) microscopic deformation features that form during the early stages of deformation in medium to high stacking fault energy alloys.1–5) Characterization of these microbands in the early years was carried out by transmission electron microscopy (TEM), whereby they were shown to be parallel arrangements of dense dislocation walls at ≤1 μm repeat distances. The misorientations between adjacent microbands were also measured by TEM diffraction techniques (e.g. selected area diffraction (SAD) and convergent beam electron diffraction (CBED)) where it was found that they almost always remain below ~6°. This characteristic (among several other key features) distinguishes microband boundaries from higher angle deformation features such as shear bands and deformation bands. Following the development of fully automated electron backscatter diffraction (EBSD) systems in the mid 1990s, the structure of microbands was carefully re-evaluated,6,7) whereby microband boundaries were always found to be low angle in nature. For example, Albou et al.6) recently reported 0.8°, 1.0° and 2.0° average misorientations across microband boundaries within deformed grains of both high purity Al and Al-0.1%Mn after 14, 40 and 80% deformation in plane strain compression. Likewise, Hurley and Humphreys7,8) observed < 2.5° mean orientation differences between adjacent microbands within deformed grains of Al–Mg alloys deformed by up to 90% reduction by cold rolling. Among the recent key TEM investigations, Chen et al.9) and Huang and Winther10,11) reconfirmed that microbands are low-angle microscopic features of the deformation microstructure.

Based on extensive research over many years, 8° appears to be the upper limit for the misorientations associated with adjacent microbands in medium to high stacking fault energy materials. In the present work, microbands with classic structural features, but exhibiting misorientations much greater than 8°, have been discovered in the deformation microstructure of cold rolled interstitial free (IF) steel. They exclusively form in some {111}<110>-orientated grains, while other γ-oriented (<111> sheet normal direction (ND)) microband-containing grains generate the typical low-angle version. This peculiar feature of the deformation microstructure was continually observed during an extensive 2D-EBSD scanning exercise needed as a prerequisite for locating suitable microband-containing regions for carrying out 3D EBSD investigations.12,13)

2. Experimental

A Ti-bearing IF steel in the form of a hot band, and containing a 30 μm average grain size, was homogenously cold rolled by successive 10% reductions in thickness to a total...
strain of ~50%. After appropriate electropolishing in a 90% acetic acid and 10% perchloric acid mixture, the rolling direction (RD)-ND sections of the sample were characterized using a FEI Tecnai TEM (operating at 200 keV) and a TRITON EBSD (attached to a JEOL 7001 field emission gun (FEG) scanning electron microscope (SEM)). Comparable TEM images were captured for each EBSD area to ensure that the features under investigation are typical microbands, and because the original microband characterizations were performed at Risø using TEM. X-ray diffraction was used for measurement of the global texture, whereby the mid-surface thickness of the rolling plane was mechanically polished and then etched in a 30% Nital solution and exposed to Co Kα radiation. <110>, <200> and <211> pole figures were generated for calculating orientation distribution functions (ODF).

3. Results

The texture of the cold-rolled steel is shown by the typical φ2 = 45° section of Euler space in Fig. 1(a). A comparison with the orientation map in Fig. 1(b) indicates that the intensities at {111}<110> are higher than the other orientations in both the γ- (<111>//ND) and α- (<110>//RD) fibres. A reasonably strong rotated cube (001)<110> component is also evident. It is well established from numerous studies that, in the α- and γ-fibre grains, the microstructures have distinctively smooth and fragmented appearances when viewed in the RD-ND section.5) The smooth grains belong to the γ-fibre and contain coarse cell structures, whereby the cell boundaries accommodate small orientation differences (<1°). Therefore, a continuation of cell structures creates a gradual change in orientation profile over a large distance along the length of the original grains. In contrast, the γ-fibre grains have a fragmented appearance, with frequent change in contrast, due to the sharp boundaries associated with microbands, shear bands and deformation bands. These features are found to accommodate relatively larger and sharper orientation differences compared with cell boundaries in α grains.

Figure 2(a) highlights the change in the orientation of transverse direction (TD), which is normal to the image, across microband boundaries in a so called inverse pole figure map i.e. TD IPF map, of an RD-ND section containing an array of classical microbands inclined at ~25° to the RD. Here, the black lines represent boundaries between adjacent microbands with >12° misorientation. A >20° misorientation plot detects shorter boundary segments, but they still appear in acceptable lengths of more than five continuous data pairs. In this area, there are adjacent microbands exhibiting very large misorientations, as compared to the usual <8° values. An orientation profile across many boundaries reveals the frequency of occurrence of such high-angle boundaries. An example is shown in Fig. 2(b), in which the black and grey lines represent the ‘point-to-origin’ and ‘point-to-point’ misorientations along X–Y in Fig. 2(a). Here, the misorientations across microband boundaries vary up to an unusually high value of 20°. There is also a cyclic trend in the orientation changes, which is realized from the increment in the point-to-origin profile in one boundary and a reduction (by the same amount) in the other boundary of a given microband. This is highlighted by the encircled region of the TD IPF map and the corresponding orientation profile. Across this boundary pair the point-to-point misorientation is almost equal. Thus, in a given microband array an orientation pair appears in an alternating sequence.

The significant grey-scale contrast between the lower-left and upper-right corners of Fig. 2(a) is a typical indicator of the large variation in orientation within the grain containing microband structures. Therefore, an orientation plot of the entire dataset shows a large spread, in which the average orientation is centred at (1 1 1)[0 1 -1]. In order to be precise at the local-scale, the orientation dataset along X–Y in Fig. 2(a) (covering ~20 microbands) is plotted as a <110> pole figure in Fig. 2(d). The encircled [110] pole shows minimum spread, as compared to the other five <110> poles. This indicates that the rotation axes across the microband boundaries lie close to this pole. To be more specific, the orientation data across the A/B boundary segment in Fig. 2(a) is plotted in a <110> pole figure (Fig. 2(c)) showing a precise coincidence at the [110] pole. Many of these orientation pairs were tested within Fig. 2(a), whereby perfect coincidence, like that shown in Fig. 2(c), was not always found, but nevertheless remain within 5° angular distances. Similarly, <002> and <112> pole figures were plotted (not shown), but no such convincing coincidence was found. The bright field TEM image in Fig. 3 (ND-RD section) shows that the microbands shown in Fig. 2(a) have typical

![Figure 1](https://example.com/figure1.png)

![Figure 2](https://example.com/figure2.png)
microband features similar to that observed by the Risø group, i.e., they: (i) consist of dense dislocation walls (parallel dark lines) separated by an average distance of ~0.75 μm; (ii) are inclined ~28° with the RD, and (iii) are relatively dislocation-free.

The large area TD IPF map presented in Fig. 4(a) reveals numerous micro-shear bands (arrowed) within a microband-containing grain, as well as evidence of a deformation band that divides the upper (A) and lower (B) regions by a high-angle interface (represented by the black superimposed line). It is generally reported that deformation bands break up large initial grains into segments, each of which later adopt a unique deformation mode and, hence, develop microstructures as independent grains. In regions A and B of Fig. 4(a), the microbands appear in alternating light and dark grey contrast, and in opposite inclinations with the RD. The overall orientations of the upper and lower regions are shown in the <200> pole figure in Fig. 4(b) to be centred at (1 1 1) [1 0 -1] and (1 0 1) [1 0 -1], respectively. While the latter orientation is not part of the γ-fibre (see Fig. 1(a)), it is generally found to be present with fairly strong intensities (i.e. 4-5× random for a maximum intensity of 8× random) in the rolling texture of micro-alloyed and ultra-low carbon steels. In the upper left-hand corner of region A (encircled
area X) there is clear evidence of the classic kink-like structures associated with so-called S-bands. These S-bands appear in opposite inclination angles to the microband matrix. In the areas close to the deformation band (encircled area Y) they become enclosed by a pair of >8° boundaries. Their chronological transitions from that in area X to Y are described in detail in Ref. 18). These bands remain restricted within original hot-band grains and carry large shear strains and, therefore, are frequently called by ‘micro-shear bands’. The average width of these bands (~0.5 μm) is about half of that of microbands. In region B of Fig. 4(a), the microbands are crossed by the thicker version of micro-shear bands and their thickening mechanism is also described in Ref. 18). Although shear banding and deformation banding are not the principal focus of this paper, the area shown in Figs. 3 and 4 is important to study for representing another classical scenario of microband structures containing S- and micro-shear banding.12–18) Earlier, Chen et al.9) argued that the microband structure is a precursor for S- and micro-shear band formation in the γ-oriented grains of the rolling microstructures of micro-alloyed and ultra-low carbon steels.

Figure 5(a) is a high resolution TD IPF map of the rectangular area shown in Fig. 4(a). An orientation profile along A–B (Fig. 5(b)) shows that the misorientations across the microband boundaries vary from 8 to 20° (see the point-to-point profile, grey line). Similar to Fig. 2, a cyclic orientation profile is also present in the point-to-origin plot. Likewise, the curves in Fig. 5(c) represent the same characteristics for the line C–D. The orientation data associated with the A–B and C–D lines are plotted as <1 1 0> pole figures in Figs. 6(a) and 6(c), where it is clear that the rotation axes lie close to the encircled <1 1 0> poles. A more precise orientation plot across X/X’ and Y/Y’ microband boundaries are given in Figs. 6(b) and 6(d), respectively, showing that the rotation axes are consistently close to a <1 1 0> pole.

Finally, two bright field TEM images given in Figs. 7(a) and 7(b) compare the S-band and micro-shear band structures between TEM and EBSD observations.18) Figure 7(a) is consistent with region A in Fig. 4 containing S-bands within a region of microbands. The overall orientation of this area is centered at (116 148 -120) [13 -11 1], i.e. close to (1 1 -1)[1 -1 0], as determined by CBED (see inset in Fig. 7(a)). The kinked segment in the S-band is misoriented by 7–10° from the straight microband segments. The microband and S-band boundary traces were found to align with [5 -16 5] and [-16 5 5] directions and, hence, they coincide with the (1 0 -1) and (0 1 -1) plane traces. In this image there is a grey-scale contrast between neighbouring microbands, which evolve from orientation dependent electron channelling. An alternating arrangement of this feature in the microband array is therefore significant. Figure 7(b) is consistent with the microband structures in region B of Fig. 4(a), whereby a microband array is intercepted by wider (~1.5 μm) micro-shear bands. The microband boundary segments inside the shear band deviate from that in their matrix, the overall orientation of which is centered at (20 -27 21)[-34 -21 4], i.e. close to (1 -1 1)[-1 -1 0]. The traces along the microband ([1 -39 6] = [-1 0 0]) and shear band ([1 -16 32] = [-1 0 0]) respective to the microband matrix and shear band, respectively.
4. Discussion

In this investigation, unusual features have been found in typical microband structures in cold rolled IF steel. The typical characteristics of these microbands include the presence of dense dislocation walls at \(<1 \mu m\) repeat distances, 25–35° inclinations with the RD and the crystallographic alignment with the highly-stressed slip planes. The unusual microband features are discovered from their boundary crystallography, including: (i) high misorientations up to \(\sim 20^\circ\) between adjacent microbands, and (ii) equal and opposite rotations with neighbouring microbands around a \(<110>\) pole. These characteristics are exclusive to \{111\}<110> orientations in cold rolled IF steel.

Microbands are commonly observed in the microstructures of \(\gamma\)-fibre grains of many types of cold rolled steel. The \(\gamma\)-fibre consists of \(2\times\) \{111\}<110>, \{111\}<112> and \(3\times\) \{111\}<123> texture components. A connection between these variants constitutes the complete \(\gamma\)-fibre skeleton, as shown in the \(\phi_2=45^\circ\) section of Euler space (Fig. 1(a)). The rolling texture of the steel investigated in this study (Fig. 1(b)) has the \{111\}<110> orientation as the peak intensity, thereby indicating the high orientation stability of this component. It is important to note that \{111\}<110> is a common texture component of both the \(\alpha\)- and \(\gamma\)-fibres. Consequent-

ly, grains of this orientation comprise both smooth ‘\(\alpha\)-type’ and fragmented ‘\(\gamma\)-type’ microstructures. It has been explained from a rotation trajectory that, if a grain rotates to \{111\}<110> through the \(\alpha\)-fibre components, it generates an \(\alpha\)-type smooth substructure. Conversely, if it rotates through the \(\gamma\)-fibre orientations then complex \(\gamma\)-type substructures are generated. Therefore, the coexistence of both microstructures in a given grain is rare after medium to high levels of rolling (>50% reduction). Although the \{111\}<110> orientations are easy to locate in the deformation microstructure due to their high intensity and wide variations in structures, the unusually high-angle microband boundaries highlighted in the present investigation have not been reported.

There are two main theories for addressing the evolution of microband boundaries. In the earlier theory, dislocation cross-slip was described as an essential event.\(^{19,20}\) Briefly on this theory, at the growth head of a microband channel one set of dislocations experiences cross-slip and gets separated from the remaining dislocations and, thus, they form a pair of dislocation walls. Therefore, freshly-formed microbands generate dislocations in their walls with identical configurations. Across the walls, rotations by an equal and opposite angle have been observed, i.e. the rotation generated by the first wall is balanced by an opposite rotation across the second wall. In this theory, the axis of the rotation was also predicted as the normal of the most highly stressed slip system. Experimental evidence of this theory is provided in Refs.\(^{21,22}\) According to the later theory, a dense dislocation boundary tends to split after generating a considerable misorientation (>1.5°) and, thus, a pair of microband boundaries evolves.\(^{3,4,23}\) The resultant misorientations of the newly-formed pair remain equal to the original boundary and, therefore, they are related by opposite rotations to each other. Evidence of boundary splitting has been observed in a wide range of metals and alloys.\(^{7,4,23}\) In the present work, there is also evidence of boundary splitting in several locations of the deformation microstructure (see Figs. 2–5), with recent 3D-EBSD investigations revealing that splitting is a major source of convoluted microband interfaces.\(^{24,25}\) In both theories described herein, the alternating rotation phenomenon with neighbouring microbands can be explained, although only a few degrees of misorientation is possible for the double cross-slip mechanism.\(^{19,20}\) The slightly larger misorientations can be explained by the boundary splitting mechanism.\(^{23}\) Overall, while the current theories are capable of explaining the origin of reasonably small misorientations between adjacent microbands, they cannot account for the large microband boundary misorientations observed in the present investigation.

The large microband boundary misorientations (up to 20°) observed herein have an important ramification on the question of their crystallographic alignment, i.e. a boundary interface separating two widely misoriented lattices cannot be in mutual crystallographic alignment with both, except for two situations. The first situation may arise due to the presence of a coincident site lattice (CSL) interface. However, CSLs are specific in misorientation and boundary interface parameters, which are not found in the current dataset. In the second situation, if the rotation axis between adjacent microband orientations coincides with their bound-

Fig. 7. Bright field TEM micrographs of RD-ND sections showing (a) S- and (b) micro-shear-bands in microband matrix structures. The CBED measured Kikuchi patterns (insets) represent matrix orientations.

\[16] = [\text{-1 -2 1}]\) boundaries coincide with the traces of (011) and (101) planes.
ary surface normal then the formation of a high-angle crystallographic interface is possible. Therefore, this is a three-dimensional problem. In recent 3D-EBSD investigations, microband boundaries were found to be irregular and curved but crystallographically aligned. In these investigations, typical low-misoriented (~5°) microbands were studied and, hence, the misorientation axis was not a major concern. Using a combination of conventional 2D-EBSD and TEM techniques, it is also possible to approximately deduce microband surface alignments through conventional trace analyses. For example, direction ‘p’ in Fig. 2(a) lies on a microband boundary trace. From the angular relationships with RD and ND, (p and its trace) can be plotted in the pole figure (Fig. 2(c)), whereby the pole of the microband interface should lie on the ‘trace of p’. The precise location can be worked out from the boundary alignments in the other orthogonal cross sections, RD-TD or TD-ND. It is inspiring to find that the common <110> pole falls on this trace at a distance of 14° from the RD-ND axis (which is the trace of the TD). This indicates that if the microband boundary trace has ~14° inclinations with the TD in the TD-ND cross section (an angle which is within the range of commonly reported inclinations), then the interface normal coincides with the common <110> pole. Similarly, the common <110> poles observed in Fig. 6 possibly coincide with the corresponding boundary interface normal. Therefore, it can be concluded that the rotation axis across a given microband interface closely coincides with its surface normal.

The well-documented characteristic showing the close coincidence of microband boundary surfaces with the highly stressed slip planes can be checked for the current microband boundaries. The resolved shear stresses (in the form of Schmid factors) on the (12×<110><111>) and (12×<112><111>) slip systems are calculated for six microband orientation pairs. It is to be noted that, in a given microband array, there are two sets of microbands (Figs. 2 and 4). In each set there are also orientation spreads of up to 10° (primarily along the microband length). Therefore, the central orientation of each set is taken as their representative orientation data and listed in pairs in the first column of Table 1. Here, rows 1–3 display the orientation data from Figs. 2–6 and rows 4–6 show three supplementary orientation pairs having identical high-angle boundary characteristics. Of the possible {110}<111> slip systems, five of the highest stressed systems are tabulated in descending order in columns 1 to 5. Likewise, the three of the most highly stressed {112}<111> slip systems are tabulated in columns 6 to 8. It turns out that the planes representing the common poles in Figs. 2 and 6 are either the first or second (shown in bold) most highly stressed slip planes. Therefore, this finding leads to the conclusion that the microband interfaces, which are previously found to accommodate rotations around their normal, also align with the most highly stressed slip planes. Several other {112}<111> slip systems were also found to have high Schmid factors (as shown by the values in columns 6 to 8), but none of these show coincidence with microband boundary interfaces. This outcome also matches the finding of Chen et al. who showed that the {110}<111> slip systems accommodate shear processes.

Table 1. Calculated Schmid Factors on highly stressed {110}<111> and {112}<112> slip systems of the orientations shown in Figs. 2 and 6, and three supplementary examples having comparable microband features.

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<th>Fig. 2</th>
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in IF steel during low levels of deformation (~10% reduction) at room temperature.

The foregoing discussion confirms that high-angle microband features evolve in two stages. In the first stage, typical low-angle microband boundaries form on highly stressed slip planes, followed by stage two where the high-angle features develop by a relative rigid body rotation between neighbouring microbands about the normal of their boundary interface. The first stage occurs early in the deformation process and is considered to be a generic event in all microband-containing grains, while the second stage occurs in some {111}<110> grains in the latter stages of deformation. Grains with {111}<110> orientations are the most stable in the γ-fibre (peak intensity component in the rolling texture, Fig. 1(b)) and, unlike other unstable/metalastic orientations, they remain in place without experiencing rotations during further deformation. Therefore, in {111}<110> grains, the maximum shear stresses remain restricted onto the existing microband boundaries. As a result, further deformation proceeds by achieving rotations at the microband boundary interfaces and around their surface normal directions, as shown in Figs. 2, 4 and 5. The mechanism associated with this particular type of rotation is now known. There is another deformation feature, known as deformation banding structures, which also generate high angle interfaces within original grain interior. The distances between deformation band boundaries are much larger (depends on strain) than microband boundary separation, which is typically ~1 μm. It is pertinent to note that, due to the low-angle interfaces associated with classical microband boundaries, they are not expected to have a significant influence on recrystallization. However, the high-angle microband boundaries observed in this work may exhibit high mobility during recrystallization if the stored energy criterion is fulfilled. Thus, in a given microband array consisting of highly alternating orientations, it is possible that any one of these microbands may expand laterally during annealing, although their growth will cease when another microband of the same orientation is encountered due to ‘orientation pinning’. Hence, recrystallization in these regions of {111}<110>-oriented grains is difficult despite the high-angle microband boundaries. This may also explain why {111}<110> texture components do not dominate the recrystallization texture in cold rolled and annealed steels despite these components dominating the rolling texture.

5. Concluding Summary

High-angle microband boundaries with misorientations up to ~20° between adjacent microbands were identified in the microstructures of cold-rolled IF steel. The following is a summary of the salient features of these deformation structures:

- They form in the {111}<110>-orientated grains after moderate rolling reductions.
- They rotate with neighbouring bands by equal and opposite angles, around the axes lying along the surface normal of their interfaces. Thus, an alternating orientation pair forms for a given microband array.
- Their boundary interfaces coincide with the most highly stressed crystallographic lattice planes.

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