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IOP Conf. Series: Materials Science and Engineering **82** (2015) 012023 doi:10.1088/1757-899X/82/1/012023

Shear banding and its contribution to texture evolution in rotated Goss orientations of BCC structured materials

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Abstract. Due to progressive deformation, the dislocation densities in crystals are accumulated and the resistance of grains to further deformation increases. Homogeneous deformation becomes energetically less favorable, which may result for some orientations in strain localization. In-grain shear banding, a typical kind of localized deformation in metals with BCC crystal structure, has been accounted for by the geometric softening of crystals. In this study, the occurrence of shear bands in rotated Goss ({110}<110>) orientations of Fe-Si steel is predicted by crystal plasticity simulations and validated by EBSD measurements. It was observed and confirmed by crystal plasticity modeling that such shear bands exhibit stable cube orientations The orientation evolution of crystals in shear bands and its impact on annealing texture of materials are also described.

1. Introduction

Plasticity of structural materials, in general, is induced by dislocation slip, mechanical twinning and grain boundary sliding. For BCC structured materials, which have high stacking fault energy, the plastic deformation of mechanical twinning is not energetically favored. In addition, super-plasticity by grain boundary sliding hardly occurs during conventional deformation processes of polycrystalline materials. Therefore, dislocation slip is by far the dominant way to induce plasticity in BCC structured materials.

During plastic deformation, dislocations are generated and accumulated in the grains of the polycrystal. The interactions and accumulations of dislocations result in an increase in the resolved shear stresses of the slip systems, and hence inhibit grains from further plastic deformation. In an aggregate, because of the difference in slip activities, the accumulation of dislocations in various grains is not the same. The total density of dislocations stored in a grain depends on its crystallographic orientation, the strain mode applied and the manner in which this strain mode is accommodated locally. For grains of higher slip resistance, i.e. less favorable for plastic deformation, the density of accumulated dislocations is usually higher. On the contrary, grains, which have higher susceptibility to deformation, trap fewer dislocations, and thus have lower dislocation densities.

In the first approximation of crystal plasticity, the accumulation of dislocation density in a crystal grain can be represented by the Taylor factor (M). This factor is defined by the ratio of the internally dissipated friction work (per time unit) and the plastic work (per time unit) done by the applied deformation:

$$M = \frac{\sum_s \tau_s^c \left|\dot{\gamma}_s\right|}{\tau^c \dot{\varepsilon}_{vM}} \tag{1}$$

in which τ_s^c and $\dot{\gamma}_s$ are the resolved shear stress and the slip rate of active slip system (s), τ^c and $\dot{\varepsilon}_{vM}$ are the equivalent shear stress and strain rate of external deformation. The sum in eq. (1) is taken over all active slip systems, regardless of their glide directions. To simplify, a unique value is usually assigned to τ_s^c and τ^c which accounts for the very beginning or the steady state of deformation where hardening is saturated and all slip systems have nearly the same resolved shear stress. Providing the same strain rate is applied to all grains in an aggregate, the Taylor factor is directly proportional to the total slip rates of crystallites.
For BCC structured materials, the Taylor factors of the preferred orientations in plane strain compression of conventional rolling can be observed in the φ_2 =45° section of Euler space. From this Taylor factor map, it is expected that the resistance to slip and the dislocation densities of crystallites oriented along the α-fiber (<110>//TD) are lower than for crystals along the γ-fiber (<111>//ND). These differences in behavior of α- and γ-fiber oriented grains can be well demonstrated by orientation images of the deformation microstructures. In an inverse pole figure (IPF) map of any BCC structured material after conventional rolling the grains which have <100>-axes parallel to ND mostly appear as long and continuous bands. On the contrary, grains having <110>- and <111>-axes close to ND are usually fragmented into inclined strips and contain smaller grains. The grain fragmentation in high plastic resistant crystallites (i.e. with high Taylor factors) is due to the inhomogeneous deformation at grain scale.
Another effect of in-grain inhomogeneous deformation is the occurrence of micro shear banding. Micro shear bands appear in grains as narrow and inclined strips of heavily deformed crystallites. They are not crystallographic features, since the band inclination angles are not related to any specific crystallographic orientation of the grains. However, the occurrence of micro shear bands is greatly influenced by the grain orientations. They are more frequently observed in high Taylor factor grains, rather than in those with low Taylor factor. Inside bands, crystallites are severely strained by shear, whereas outside they are hardly deformed.

2. Geometric softening
Strain localization in the form of shear bands can be accounted for by geometric softening [1] of heavily deformed polycrystals. According to this theory, the accumulation of dislocations in grains during progressive deformation increases the resolved shear stresses for slip activities. Thus, homogeneous deformation of the entire grain volume becomes less energetically favorable than local straining of a specific sub-volume. When the applied deformation is better accommodated in local bands, shear-banding occurs. The transition from homogeneous to local plastic flow of materials is usually marked by a plastic instability point ($d\sigma/d\varepsilon = 0$) on the stress-strain (σ-ε) curve. Beyond this point, geometric softening ($d\sigma/d\varepsilon < 0$) due to local strain accommodation is dominant, and thus grains in shear bands are deformed.
Geometric softening is not a reduction of dislocation density in crystals by thermally activated processes, like recovery or recrystallization. It is simply a change of the deformation geometry to *soften* the high hardening stage of crystals. The condition for this change of deformation configurations is proposed by Dillamore et al [1], based on crystal plasticity theory:

$$\frac{d\sigma}{d\varepsilon} \propto \frac{dM}{d\varepsilon} \leq 0 \tag{2}$$

Accordingly, shear banding will occur, if the rotation of crystals in localized bands is towards lower Taylor factor orientations.

3. Shear banding in BCC structured materials
In BCC structured materials after conventional rolling, micro shear banding is most frequently observed in {111}<112> oriented grains. Previous studies [2-4] showed that the presence of shear bands in such grains indeed exhibits the geometric softening effect. In

addition, calculation results confirmed the formation of the Goss ({110}<001>) orientation in these shear bands. These Goss oriented crystals are believed to have important effects on the nucleation of recrystallized grains during subsequent annealing.

Among all preferred orientations in BCC structured materials after conventional rolling, the {111}<112> orientation has a Taylor factor of 3.5, which is one of the highest values. However, the maximum value in the Taylor factor map of BCC structured materials in plane strain compression is 4.24 at the rotated Goss ({110}<110>) orientation. An interesting question is why geometric softening by shear banding occurs in this orientation and what is the preferred orientation in these shear bands.

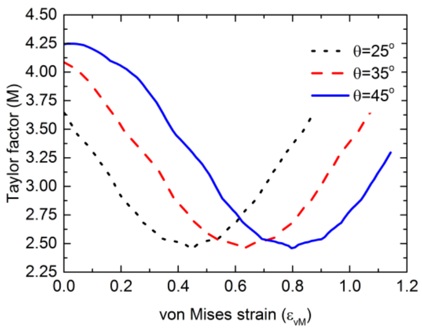

Figure 1. Strain evolution of the Taylor factor for a rotated Goss oriented crystallite in shear bands of different inclination angles (θ = 25°, 35° and 45°).

To investigate shear banding in the rotated Goss orientation, simulation and experiment have been carried out. The full constraints Taylor model was used to investigate the geometric softening effect and the orientation evolution of crystallites in shear bands. Deformation of crystallites in shear bands inclined by 25°, 35° and 45° with respect to the rolling plane were simulated. In all three simulations, a strong geometric softening effect can be observed (Figure 1). The softening effect is strongest in bands of 45° inclination. It starts at the highest Taylor factor value (4.24) and finishes after the highest strain (0.8). Furthermore, the formation of shear bands is supported by the maximum shear stress of conventional rolling, which is on the plane 45° inclined to the normal direction. Shear bands with 45° inclination angle, therefore, should have the highest potential to form in the rotated Goss oriented grains.

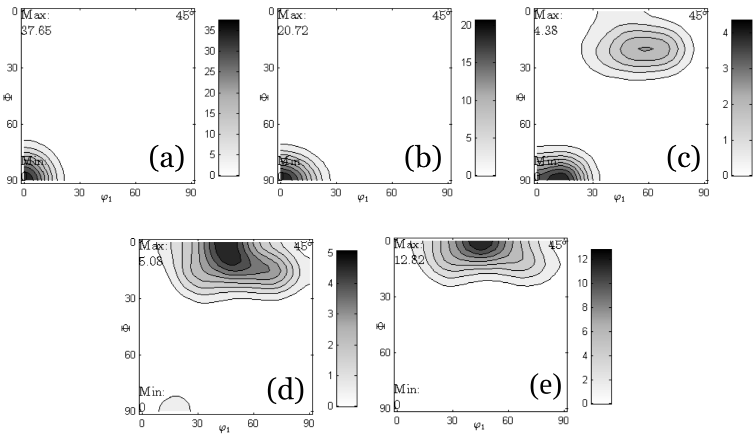

Figure 2. Texture evolution in the 45° inclined shear band of a rotated Goss grain, after straining (ε_{vM}) of (a) 0, (b) 0.2, (c) 0.4, (d) 0.6 and (e) 0.8.

The texture evolution in a shear band with 45° inclination angle was simulated after strain steps of 0.2 from 0 to 0.8. A strong rotated Goss texture discretized by a set of 2000 orientations was used as initial texture for crystal plasticity calculations. Deformations and rotations of these orientations in the shear band are calculated by the full constraints Taylor model. The interpolation of continuous ODFs from discrete orientation sets for each deformation step was then calculated by the MTEX toolbox of the MATLAB software. The φ_2

= 45° sections of these ODFs are shown in Figure 2. With increasing strain from 0 to 0.8 the intensity of the rotated Goss orientation decreases, while above a strain of 0.4 the intensity of the Cube ({001}<100>) orientation appears and strengthens. When the equivalent strain increases from 0.6 to 0.8 the intensity of the Cube orientation increases by a factor of 2.5, i.e. from 5.1 to 12.8 random. Since the geometric softening in the 45° inclined shear bands is exhausted at the equivalent strain of 0.8 (Figure 1), the in-band texture may not further evolve after this deformation. As a result, the Cube oriented crystals are the most stable in shear bands of the rotated Goss grains.

To validate simulation results, the microstructure of deformed materials has been investigated by the electron backscatter diffraction (EBSD) technique. A Fe-1.2 wt.% Si alloy after thickness reduction of 75% by conventional cold rolling was used as material. In the rolled steel sheet, the rotated Goss oriented grains are not very frequently observed, as rotated Goss only represents a minor component of the rolling texture. Although the stability of these grains in plane strain compression is very high, the {110}<110> oriented grains are virtually absent in the texture because even before deformation the volume fraction of this component is quite low. However, by chance it is possible to find some rotated Goss grains in the samples studied. In Figure 3, shear bands in a rotated Goss grain can be clearly observed. Orientations in these bands, indeed, are very close to the Cube orientation.

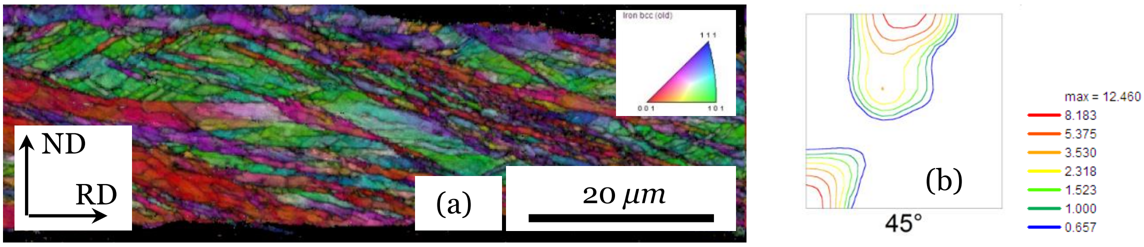

Figure 3. Microstructure (a) and texture (b) of the rotated Goss orientation

4. Summary

During plastic deformation, the accumulation and interaction of dislocations increase the hardening of crystallites. The homogeneous deformation of certain crystallites becomes energetically less favored compared to local plastic flow in micro shear-bands. Micro shear banding in heavily deformed crystals can be accounted for by geometric softening of crystal plasticity. In BCC structured materials, rotated Goss oriented grains have the highest resistance to plane strain compression, therefore they exhibit the most prominent potential for micro shear banding. The most preferred orientation in shear bands of rotated Goss oriented grains is the Cube orientation.

Acknowledgement

The authors acknowledge the financial support from the Belgium Federal Science Policy Office for the Interuniversity Attraction Poles (IAP) program via the project P7/21 INTEMATE.

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