A TECHNIQUE TO DETERMINE THE RELATIVE STRENGTHS OF DEFORMATION MECHANISMS IN HEXAGONAL MATERIALS

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A new technique is presented which permits to obtain the relative critical strengths of the slip and twinning systems in polycrystalline materials. It consists in an experimental and a simulation part. In the experience, slip line analysis and grain orientation measurements are carried out and the operating slip and twinning systems are identified in each selected grain. In the subsequent simulations, a crystal plasticity code is used to modelise the plastic behaviour, especially, the slip activity of the grains. The relative crss values of the slip systems are then varied and the simulations are repeated iteratively until the experimental slip activity is reproduced with the very same combination of crss for all the grains. 

An application is presented for a Titanium alloy (Ti40).

KEY WORDS: Deformation mechanisms, critical resolved shear stresses, EBSP measurements, crystal plasticity, Taylor modelling, rate dependent slip, slip systems in hexagonal structure, slip line analysis, Titanium.

INTRODUCTION

The plastic deformation of metals with hexagonal crystal structure is achieved by the activation of different slip and/or twinning systems. The available slip system families are: basal, prismatic (both of them with <a> glide) as well as the pyramidal ones (with <a> or <c+a> glide). The strengths of these slip system families (critical resolved shear stresses: «crss ») depend on the c/a ratio and on the alloying elements. Twinning is frequently observed (on pyramidal type crystallographic planes), which can also be characterised by different crss values.

The great variety of the possible deformation modes represents a significant difficulty in the determination of the nature and the physical characteristics of the deformation mechanism(s) in a given hexagonal alloy. The first problem is the identification of the operating slip and twinning system-families. Another problem arises when the activity of more than one deformation mode (i.e. more than one slip system-family, or twinning-family) is detected. Namely, the relative strengths of these deformation modes, that is their relative crss values. The knowledge of the crss values is indispensable in the calculation of any mechanical parameter related to plastic deformation (Lankford parameter, yield surface, texture development, etc.).

The identification of the active deformation modes is readily possible with electron microscopy, by determining the Burgers vectors of the dislocations (Hirsch et al (1965)).
The analysis of traces of slip lines and twin boundaries on the surface of deformed single crystals is also a good experimental technique (Cheneau-Spáth and Driver (1994)). These investigations cannot reveal, however, the relative mechanical strengths of the different deformation modes. It is only possible if, by changing the orientation of loading, single slip is realised on the crystal which corresponds to one of another family of the available slip systems. Evidently, it is very difficult to realise such experiments.

Because of the complications in the experiments, most of the times the relative crss values are obtained from theoretical simulations. This technique can be applied for the interpretation of the observed slip and twinning activities in single crystals (Akhtar (1975), Cheneau-Spáth and Driver (1994)), or for the behaviour of polycrystals (for example, by reproducing the deformation texture development (Lebensohn and Tomé (1993), Serghat (1994), Philippe et. al (1995)).

The present work introduces a new technique which consists in a combination of some experimental work and subsequent theoretical simulations. It includes a metalurgical slip line analysis, a local grain orientation measurement (by the application of the technique EBSP: electron back scattering pattern) and a theoretical simulation by a rate dependent crystal plasticity code. The technique is applicable for polycrystalline specimens. The present technique was first presented at a workshop (Tóth and Serghat (1994)).

DESCRIPTION OF THE TECHNIQUE

The sequence of the manipulations of the present technique is displayed in form of a flow diagram in Figure 1. It begins with the preparation of the sample which has to be well surface polished and recrystallised. Then the specimen is plastically deformed by tensile deformation or by rolling to a maximum of 5% strain. In case of rolling, a suitable protection of the sample surface is necessary (by a Teflon layer, for example) in order to preserve the visibility of the slip lines. These latter are then analysed in an optical microscope in a number of selected grains. The metallographic picture of a sample of a commercial Titanium alloy (Ti40) deformed in tension up to 5% is shown in Figure 2. One can clearly see the slip lines on the surface, one, too or sometimes three types of them in a grain.

The orientation of the slip lines with respect to a reference system fixed to the sample has to be measured. Their position can be specified by one single angle \( \alpha \), see Figure 3. An operating slip system is represented by a family of slip lines. The corresponding slip system can be identified if the angle \( \alpha \) as well as the orientation of the crystal with respect to the sample system \((x, y, z,\) see Figure 3) is known. This latter can be measured readily by the EBSP technique. An orientation is then represented by a transformation matrix \( T \) (the passage from the sample to the crystal reference system) which is constructed from the measured Euler angles. As a slip line is the intersection of the slip plane with the sample surface, the slip plane normal \( n \) in the sample reference system can be obtained by using the transformation

\[
n = T^{-1} n^c,
\]

where \( n^c \) is the slip plane normal known in the crystal reference system. Finally, the angle \( \alpha \) is related to \( n \) by the formula...
recrystallized and surface polished sample

plastic deformation ~5%

measurement of slip line orientations by optical microscopy

measurement of crystallographic orientations by EBSP

identification of the active slip plane(s)

crystal plasticity simulations to reproduce the experimental slip system activity

Result: relative c.r.s.s. of the slip and twinning systems

Figure 1 Flow diagram of the technique.
Figure 2 Metallographic picture of a Titanium alloy (T40) deformed in tension up to 5% strain at room temperature. The mark represents 10 \( \mu \)m.

Figure 3 The geometric position of a slip line on the sample.
This latter equation can be used to identify the operating slip plane by calculating all angles corresponding to each of the possible slip systems and comparing these values to the experimental measurement. Evidently, only the operating slip plane can be identified by the above procedure. Usually there is more than one slip direction possible in a slip plane, consequently, no distinction can be done between them. This becomes possible, however, with the help of the crystal plasticity simulations as it is explained below.

An important part of the present technique is the modelling of plastic deformation of individual grains. For this purpose a rate sensitive crystal plasticity code has been employed (Tóth et al. 1988, 1993). It permits to obtain the slip distribution for any prescribed deformation mode. The inputs are: the orientation of the grain, the available (assumed) families of slip and twinning systems, finally the deformation mode in the experiment. As surface grains are examined, certain deformation components can be left free, depending on the applied deformation mode. In the present work, the conditions of fully constrained deformation as well as relaxed constraints were applied in the simulations. In the following, the technique is explained for the case of a tensile deformation of a flat specimen. If the extension is applied in the y direction with a strain rate of 1.0 s⁻¹, the prescribed strain rate can be taken as:

\[
\begin{bmatrix}
D_{xx} & 0 & 0 \\
0 & 1 s^{-1} & 0 \\
0 & 0 & D_{zz}
\end{bmatrix}
\]

In case of relaxed constraints, all shear components of the prescribed strain rate are relaxed. As the sample is flat and the material is anisotropic (textured), the deformation is not axisymmetric with respect to the loading axis, as a consequence, the components \( D_{xx} \) and \( D_{zz} \) of the strain rate are not known beforehand. Therefore, a series of simulations has to be carried out with varying \( D_{zz} \) values. This is the same as varying the R value (\( D_{xy}/D_{zz} \)) of the specimen. The R value can be measured experimentally on the sample but its value is not necessarily the same in each grain. This is the reason why the experimental R value is not prescribed for the deformation of the grains. In the simulations \( D_{zz} \) was varied from -0.1 to -0.9 in steps of 0.1 which corresponds to a variation of the R parameter between \( R = 9 \) and \( R = 1/9 \), respectively.

Several simulations are necessary to carry out for each grain by varying the following parameters: the relative values of the crss of the slip and twinning families and the R value. For each combination of these parameters and for each grain, the most active slip systems have to be compared to the experimental observation. As the relative crss values are physical parameters of the material, accordance has to be achieved for each grain for the very same crss combination. As for the R parameter, it can vary from grain to grain, depending on the local neighbouring configuration of the grains.

In order to avoid the slip system selection ambiguity problem, the crystal plasticity model has to be such which guarantees a unique solution for the slip system activity. This is the reason why a rate dependent crystal plasticity code has been chosen for the simulation purposes (Tóth et. al 1988, 1993)). In that approach, the slip system strength is strain rate dependent according to the usual constitutive law:
In this relation \( sgn (\dot{\gamma}^s) \) means the sign of the slip rate \( \dot{\gamma}^s \) in the slip system identified by \( s \), \( \tau_0^s \) is the strength of the slip system corresponding to the reference slip \( \dot{\gamma}_0 \), \( m \) is the strain rate sensitivity index. It is evident from Eqn (3) that \( \tau_0^s \) is equal to the \( crss \) of the slip system when \( m \rightarrow 0 \). For the case \( m > 0 \), by changing the reference strain rate from \( \dot{\gamma}_0 \) to \( \dot{\gamma}_1 \), the reference stress \( \tau_0^s \) changes to \( \tau_1^s \) according to the formula:

\[
\tau_1^s = \tau_0^s \left( \frac{\dot{\gamma}_1}{\dot{\gamma}_0} \right)^m.
\]

Eqn (4) expresses the fact that there is no a unique value for the strength of a slip system for rate dependent slip. A given strength corresponds to a given reference strain rate. This peculiarity of rate dependent slip is only important when absolute values of the slip system strengths are sought for. In the present work, relative strengths of the different slip systems are of interest, in which case the chosen value of \( \dot{\gamma}_0 \) is not relevant.

Concerning twinning, its mechanical behaviour is also considered to be viscoplastic according to Eqn (3), which is obviously only a working hypothesis to handle twinning.

Hardening effects are neglected in the present work, partly because the material shows little hardening during 5% strain and because an instantaneous situation is examined. The technique could certainly be improved if hardening and orientation development are tracked from the initial state up to the deformed configuration.

**APPLICATION OF THE TECHNIQUE TO THE TI40 TITANIUM ALLOY**

The first application of the present technique has been carried on a commercially pure titanium alloy; the Ti40 material. It has a hexagonal crystallographic structure at room temperature and deforms by slip as well as by \{1122\} type twinning. The activity of twinning could be scarcely observed on the surface grains in tension, possibly because of the relaxed constraints conditions of the surface grains. The case is opposite in rolling, where the deformation is more constrained on the surface and many twins can be seen.

In the present simulations, the prismatic, pyramidal \(< a > \) and \(< c + a > \) slip systems as well as the \{1122\} twinning systems were introduced. The analysis of slip lines showed no traces of the basal slip systems, so they were omitted from the list. Several hundred grains have been examined with the present technique, a population which is representative of the polycrystal (Serghat(1994)). In order to well demonstrate the technique, here we present detailed results for 8 grains. The Euler angles of these grains measured by EBSP are given in Table 1. The experimentally identified operative systems as well as the inclination of the slip traces (angle \( \alpha \)) are listed in Table 2. The results obtained by the simulations are also displayed in Table 2, for both the relaxed constraints and full constraints cases. The value of the applied slip strain rate sensitivity exponent in the simulations was \( m = 0.01 \).

The simulation results in Table 2 correspond to the following relative \( crss \) values: prismatic = 1, pyramidal \(< a > = 3 \), pyramidal \(< c + a > = 4 \), twinning \{1122\} = 4.

Among the eight grains there were two which displayed two types of slip lines (grain 3 and 6) and there was one which showed the activity of twinning together with prismatic
**Table 1** The Euler angles of the selected 8 grains

| grain | $\phi_1$ | $\phi$ | $\phi_2$ |
|-------|---------|-------|--------|
| 1     | 352,2   | 154,5 | 328,2  |
| 2     | 245,4   | 130,0 | 83,8   |
| 3     | 156,3   | 169,4 | 224,8  |
| 4     | 304,5   | 42,2  | 320,6  |
| 5     | 289,0   | 51,8  | 130,8  |
| 6     | 70,8    | 55,3  | 102,7  |
| 7     | 71,4    | 142,8 | 351,1  |
| 8     | 76,0    | 129,8 | 169,6  |

**Table 2** The experimental slip activity of the 8 grains and the results of the simulation

| grain system | $\alpha$ angle | prediction: relaxed constraints deformation | prediction: full constraints deformation |
|--------------|----------------|---------------------------------------------|----------------------------------------|
| 1 prismatic  | 57 prism 56,1  | $(-0.7, -0.2, 0.15)$ $(-0.2, 1, -0.4)$ $0.15, -0.4, -0.3)$ | prism. 144,1 $(-0.7, 0, 0)$ $0, 1, 0$ $0, 0, -0.3)$ |
| 2 prismatic  | 147 prism 144,1| $(-0.25, 0.63)$ $(-0.25, 1, 0.77)$ $0.63, 0.77, -0.3)$ | prism. 144,1 $(-0.7, 0, 0)$ $0, 1, 0$ $0, 0, -0.3)$ |
| 3 prismatic  | 145 prism 141,6| $(-0.12, -0.06)$ $(-0.12, 1, 0.07)$ $-0.06, 0.07, -0.3)$ | prism. 141,6 $(-0.7, 0, 0)$ $0, 1, 0$ $0, 0, -0.3)$ |
| 4 prismatic  | twinning 175   | $(-0.8, -1.24, -0.78)$ $(-1.24, 1, -0.41)$ $-0.78, -0.41, -0.2)$ | prism. 176,6 $(-0.7, 0, 0)$ $0, 1, 0$ $0, 0, -0.3)$ |
| 5 prismatic  | 106 prism 103,8| $(-0.51, -0.62)$ $(-0.51, 1, 1.03)$ $-0.62, 1.03, -0.3)$ | prism. 103,8 $(-0.6, 0, 0)$ $0, 1, 0$ $0, 0, -0.4)$ |
| 6 prismatic  | 155 prism 161,1| $(-0.46, 0.66)$ $(-0.56, 1, 1.28)$ $0.66, 1.28, -0.3)$ | prism. 161,1 $(-0.7, 0, 0)$ $0, 1, 0$ $0, 0, -0.3)$ |
| 7 pyramidal  | 168 pyramidal 172,5| $<c + a>$ | pyramidal 172,5 $(-0.6, 0, 0)$ $0, 1, 0$ $0, 0, -0.4)$ |
| 8 pyramidal  | 126 pyramidal 132,2| $<a>$ | pyramidal 132,2 $(-0.2, 0, 0)$ $0, 1, 0$ $0, 0, -0.8)$ |
Table 3 The predicted relative activity of the slip and twinning systems.

| grain | prismatic | pyramidal $<a>$ | pyramidal $<c+a>$ | (1122) twinning |
|-------|-----------|-----------------|------------------|----------------|
| 1     | 0.622     | 0.001           | 0.339            | 0.038          |
| 2     | 0.659     | 0.202           | 0.107            | 0.032          |
| 3     | 0.662     | 0.061           | 0.126            | 0.151          |
| 4     | 0.999     | 0.001           | 0.000            | 0.000          |
| 5     | 0.688     | 0.129           | 0.145            | 0.038          |
| 6     | 0.655     | 0.153           | 0.161            | 0.031          |
| 7     | 0.488     | 0.056           | 0.431            | 0.025          |
| 8     | 0.373     | 0.264           | 0.320            | 0.043          |
| average | 0.644   | 0.108           | 0.204            | 0.044          |

slip (grain 6). Generally, however, there was only one slip plane active in all the other grains. One can see from Table 2 that the experimental slip activity can be reproduced either by the relaxed constraints or by the full constraints conditions, or by both approaches. In two grains, however, the event of twinning (grain 4) and the pyramidal slip activity (grain 6) is not reproduced by the simulations using the above combination of the crss values (for another set of crss, it is possible). The agreement between the measured and predicted slip line inclination is limited to about 1 to 6 degrees, which can be accepted considering the fact that the result of the lattice orientation measurement by the EBSP technique depends on the position of the beam within the grain by about the same amount. This effect is caused by the heterogeneity in the deformation of the grains.

It is interesting to note that the experimental technique does not permit to distinguish between $<a>$ or $<c+a>$ type pyramidal slip but the simulation reveals the difference (grains 7 and 8). Another peculiarity is that in spite of the apparent inactivity of the twinning according to the simulation results in Table 2, this twinning possibility is not excluded and a well defined crss value corresponds to it. The reason is that Table 2 displays only the most active slip planes but the simulation allows the activity of some other slip systems simultaneously. In Table 2 only the most active slip planes are listed in the simulations. The relative slip system activity is displayed in Table 3 for each grain. This Table is made from the average of the results when both the full and relaxed constraints simulations reproduced the experimental observation. It is interesting to note from Table 3 that in spite of the higher crss value of the pyramidal $<c+a>$ slip, its activity in average is about twice as big as that of the pyramidal $<a>$ type slip system.

Close inspection of the predicted deformation modes in Table 2 reveals that the most likely deformation mode corresponds to $D_{xx} = -0.7$ and $D_{zz} = -0.3$ which represents a predicted R value of 2.33. The agreement of this value with the experimental one is very good as the latter one is $R = 2.3$ (Tóth and Van Houtte (1992)).
Finally, it has to be noted that there exist some restrictive conditions which the predicted relative crss values have to obey. As it has been pointed out by Cheneau-Späth and Driver (1993), not any combination of the crss values can lead to physically acceptable results. They examined the case of channel die compression of single crystals of the same alloy both experimentally and theoretically. They showed that some combination of the crss values can correspond to a positive (!) compression stress which is physically not possible. For this reason we have examined theoretically the case of plane strain rolling of our set of grains using the predicted crss values. It has been found that for each grain the obtained compression stress is negative so the above physical condition identified by Cheneau-Späth and Driver is satisfied.

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