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To cite this version:

T. Ohashi. ANALYSIS OF MULTIPLE SLIP IN COPPER TRICRYSTALS. Journal de Physique Colloques, 1990, 51 (C1), pp.C1-593-C1-598. <10.1051/jphyscol:1990193>. <jpa-00230362>

HAL Id: jpa-00230362
https://hal.archives-ouvertes.fr/jpa-00230362
Submitted on 1 Jan 1990

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ANALYSIS OF MULTIPLE SLIP IN COPPER TRICRYSTALS

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Abstract—Non-uniform multiple slip in tricrystals is analysed by a method of continuum mechanics. Analysis results show that compatibility requirements on the grain boundary planes and on the entire tricrystal specimen lead to different types of multiple slip. A mechanism for multiple slip is discussed from the viewpoint of excess stress which is generated by the slip on the primary system.

1. Introduction

Multiple slip near grain boundaries plays an important role in determination of the mechanical properties of polycrystals. So far, the multiple slip phenomenon has been studied mainly with bicrystals/1/-/4/; but, slip near junctions of grain boundaries, such as grain boundary triple lines or quadruple points, is more complicated and diversified than that in bicrystals/5/,/6/. In the present paper, slip deformation of copper tricrystals is numerically analysed to examine shear strain distribution on primary and secondary slip systems. Stress field caused by non-uniform slip is discussed, too.

2. Method of numerical analysis

The Schmid’s law is used as the activation condition for twelve slip systems [111] - <110>. If the stress components in the global coordinate system are denoted as \( \sigma \), and the critical resolved shear stress (abbreviated as CRSS) for the slip system \( n \) is written as \( \theta^{(n)} \), the Schmid condition is given by the following equations.

\[
P_{1}^{(s)} \sigma_{1} + P_{2}^{(s)} \sigma_{2} = \theta^{(s)}
\]  
(1)

\[
P_{1}^{(s)} \dot{\sigma}_{1} + P_{2}^{(s)} \dot{\sigma}_{2} = \dot{\theta}^{(s)}
\]  
(2)

where

\[
P_{i}^{(n)}(\alpha) = 1/2 \left[ \nu_{i}^{(n)}(\alpha) \dot{\nu}_{i}^{(n)}(\alpha) + \nu_{i}^{(n)}(\alpha) \dot{\nu}_{i}^{(n)}(\alpha) \right]
\]  
(3)

Subscripts and superscripts in parentheses denote the grain number and slip system, respectively. If rotation of the crystal orientation is neglected, which is acceptable while the deformation is small, the constitutive equation for each crystal grain is written as follows /4/,/7/.

\[
\dot{\sigma} = D \dot{\epsilon}
\]  
(4)

\[
D_{i,j} = \left[ S_{i,j} + \sum_{n} \left( H^{(n)} \right)^{-1} P_{i}^{(n)} P_{j}^{(n)} \right]^{-1}
\]  
(5)
Here, $S_{ij}$ denotes elastic compliance. $H^{(n)}$ is the strain hardening coefficient which defines the relation between increments of the CRSS and plastic shear strain on slip systems.

$$\dot{\theta}^{(n)} = \sum_n H^{(n)} \dot{\gamma}^{(n)}$$  

(6)

The CRSS is assumed to be a function of dislocation densities on the twelve slip systems $\rho^{(n)} (m = 1 - 12)$. 

$$\theta^{(n)} = \theta_0 + \sum_n \Omega^{(n)} G(\rho^{(n)})$$  

(7)

Here, $\theta_0$ is a constant and $\Omega^{(n)}$ is a constant matrix which is determined in accordance with the variation of reaction between dislocations on slip systems $n$ and $m$. The function $G$ is given by:

$$G(\rho^{(n)}) = a \mu \sqrt{\rho^{(n)}}$$  

(8)

Here, $\overline{b}$ is the magnitude of Burgers vector, $\mu$ is elastic shear modulus and $a$ is a numerical factor of order 0.1.

It is assumed that dislocation sources on active slip systems emit dislocation loops, and they move freely in the manner of free flight motion until they are trapped by obstacles $Z$. If it is also assumed that the shape of the trapped dislocation loops is rectangular with aspect ratio $\alpha$, then the increment of shear strain and dislocation density on the slip system are correlated as follows.

$$\dot{\gamma}^{(n)} = \frac{2\alpha}{(1+\alpha)^2} \overline{b} L \rho^{(n)}$$  

(9)

$L$ denotes the mean free flight distance of the dislocation segments. For the mean free flight distance, Seeger's model is used with a small modification.

$$L = \begin{cases} L_0, & \text{single slip region} \\ \Lambda \{ \sum_n \gamma^{(n)} - (\gamma^0 - \Lambda / L_0) \} & \text{multiple slip region} \end{cases}$$  

(10)

Here, $L_0$ and $\Lambda$ are constants. $\gamma^0$ denotes the shear strain at which multiple slip occurs. From equations (7)-(9) $h^{(n)}$ is given as:

$$h^{(n)} = a \frac{(1+\alpha)^2}{4\alpha} \mu \Omega^{(n)} / (L \sqrt{\rho^{(n)}})}.$$  

(11)

The finite element method is used for numerical analysis. Fundamental equations for the method are,

$$[K] \{ \dot{u} \} = \{ \dot{f} \}, \quad [K] = \sum [k],$$  

(12)

$$[k] = \int [B]^T [D] [B] dV,$$  

(13)

where, $\dot{u}$ and $\dot{f}$ denote increments of nodal displacement and nodal force. Matrix $B$ is a shape function of each element. $D$ is the matrix expression of $D_{ijkl}$ which is given by equation (5). Propagation of slip is analysed by an incremental procedure.
3. Tricrystal models

Two special tricrystals are considered. The first one is shown in figure 1(a). Crystal orientations for its grains are given in figure 2(a). The crystal orientation for grain 2 has mirror symmetry with grain 1, with respect to the yz plane. Normal vector of the slip plane and slip direction for the primary slip systems $p$ of grains 1 and 2 lie on the xy plane. Moreover,

$$\nu^{(s)}_{x, (i)} = \hat{b}^{(s)}_{x, (i)}, \quad \nu^{(s)}_{z, (i)} = \hat{b}^{(s)}_{z, (i)}, \quad (i=1,2,3).$$

(14)

Here, $\nu$ and $b$ denote unit vectors of the slip plane normal and slip direction, respectively. When only the primary slip system is active, strain component is,

$$\varepsilon_{x, (i)}^{(p)} = P_{x, (i)}^{(s)} \gamma^{(p)}. \quad (15)$$
According to equations (3) and (14) all strain components are identical for both grains when $\gamma \{ s \} = \gamma \{ t \}$. This means that the compatibility requirement is naturally satisfied and no mutual constraint of deformation between grains 1 and 2 will occur.

Crystal orientation of grain 3 is that for a $\pi/2$ rotation of grain 1 about the y axis. Slip plane normal and slip direction are parallel to the yz plane. Therefore, the primary system in grain 3 is neither continuous to that in the grain 1, nor symmetric to it with respect to the grain boundary between grains 1 and 3 (abbreviated as grain boundary 1-3, hereafter). Therefore, compatibility requirements will cause multiple slip in the vicinity of this grain boundary plane. The same will occur between grains 3 and 2. On the other hand, as a whole, the geometrical relationship of the 3 primary slip systems in each grain have a symmetric relationship with respect to yz plane. Then, this tricrystal is referred to as a symmetric type.

The second crystal orientation considered here is shown in figure 2(b). In this case, the orientation relationships between grains 1 and 2 and between 2 and 3 are symmetric with respect to the yz and zx planes, respectively. The primary system for grain 3 coincides with that for grain 1. Therefore, if the structure of tricrystal model is chosen as in figure 1 (b), compatibility condition is satisfied on all grain boundary planes. This tricrystal is referred to as a pseudo-compatible type.

The following data are used for both types of tricrystals.

<table>
<thead>
<tr>
<th>Elastic constants</th>
<th>$\Lambda = 4 , \mu m$</th>
<th>$\rho_0 = 1 \times 10^9 , / m^2$</th>
<th>$\Theta_p = 0$</th>
<th>$G^{(n)} = 1 , (n, m = 1 \ldots 12)$</th>
<th>$L_0 = 1000 , \mu m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_{11} = 5$, $S_{22} = 1.5$</td>
<td>$S_{44} = 13 \times 10^{-17} , m^2/N$</td>
<td>$b = 2.555 \times 10^{-10} , m$</td>
<td>$\alpha = 1$</td>
<td>$\alpha = 1$</td>
<td>$\alpha = 1$</td>
</tr>
</tbody>
</table>

The tricrystals are divided into 784 composite elements with eight nodes. The grain boundary planes are treated as zero thickness interfaces on which continuity of displacement and traction are maintained. External load is given to the specimens by application of uniform displacement in the y direction on their upper and bottom surfaces.

4. Results and discussion

4.1 Symmetric tricrystal

a) Early deformation

Distribution of shear strain on the primary slip system in an early stage of deformation is shown in figure 3(a). The shear strain is small in the vicinity of the triple junction and increases along the grain boundary 1-2. The minimum and maximum of the shear strain are $0.33x10^{-5}$ and $2.57x10^{-5}$, respectively. The ratio of the maximum to the minimum is about 7.8.

The process for formation of this distribution is thought to be as follows; on the grain boundaries 2-3 and 1-3, lack of compatibility causes suppression of activation of the primary slip systems near the grain boundaries and results in distribution of smaller shear strain around the triple junction. As compensation for this, a bigger shear occurs along the grain boundary 1-2.

Figure 3(b) shows distribution of von Mises's equivalent stress. This stress is a measure of elastic strain energy. Figures 3 (a) and (b) indicate that the von Mises's stress reflects the extent of shear strain gradient on the primary systems.

b) Subsequent deformation

Distributions of shear strain on the primary and critical system at a later stage of deformation are given in figures 4(a) and (b). The qualitative aspect of the shear strain distribution on the primary system remains unchanged. The minimum and maximum of the strain are $1.04x10^{-5}$ and $6.86x10^{-5}$. The ratio of the maximum to the minimum is about 6.6.

Regarding the critical system which is activated along the grain boundaries 1-3 and 2-3, the magnitude of the shear strain is one order smaller than that on the primary system. Comparison of figures 3(b) and 4(b) suggests that activation of the critical system provides a release mechanism for strain energy that is accumulated through the non-uniform slip on the primary systems.
Fig. 3 (a) Shear strain on the primary slip system and (b) equivalent stress in the symmetric tricrystal at an early stage of deformation. The mean stress and the mean strain in the y direction are 1.52 MPa and $1.31 \times 10^{-5}$, respectively.

Fig. 4 (a) Shear strain on the primary slip system and (b) the critical slip system in the symmetric tricrystal at a later stage of deformation. The mean stress and the mean strain in the y direction are 1.55 MPa and $2.49 \times 10^{-5}$, respectively.

4.1 Pseudo-compatible tricrystal

Figures 5(a) and (b) show distributions of shear strain on the primary and conjugate system in the pseudo-compatible type tricrystal. As already mentioned, deformation compatibility on the grain boundary planes is assured through the symmetry or continuity of the primary slip systems in three crystal grains. The reason for the non-uniform distribution of the shear strain on the primary system and activation of the secondary one is discussed below.

Because the slip directions for the primary systems in the three grains are parallel to the xy plane, only three strain components $\varepsilon_{xx}$, $\varepsilon_{yy}$, and $\varepsilon_{xy}$ should be considered. When the shear strain on the primary slip systems in three grains are identical, magnitudes of the strain components $\varepsilon_{xx}$ and $\varepsilon_{yy}$ in each grain are identical (refer to equations (3) and (15)). But, from equation (15) and figure 2(b) $\varepsilon_{xy}$ is derived as:

$$\varepsilon_{xy, (1)} = \varepsilon_{xy, (3)} = -\varepsilon_{xy, (2)}$$

Generation of this discontinuity and the condition that the upper and lower surfaces of the specimen are kept flat brings about the non-uniform slip on the primary system. With a symmetric bicrystal, Hook and Hirth/3/ have already reported the effect of the in-plane shear strain component. Their experimental results for slip line distribution and the present results are essentially the same.

The discontinuity of the in-plane shear strain causes a mechanical interaction between the component grains, too. For discussion, assume that grain 2 is cut out of the specimen and uniform shear on the primary slip systems occurs in three grains. Because the in-plane shear strain in grain 2 occurs in the opposite direction to that in the remaining part, then the shape of grain 2 is not the same as the shape of the space it once occupied next to grains 1 and 3. This disagreement in shear deformation causes grain 2 be cramped by grain 1 and 3 when the tricrystal is deformed as one continuous body. This cramping effect produces an internal stress field.
Fig. 5 (a) Shear strain on the primary slip system and (b) the conjugate slip system in the pseudo-compatible tricrystal. The mean stress and the mean strain in the y direction are 1.74 MPa and 2.31 x 10^-5, respectively.

Fig. 6 Stress distribution in the unloaded pseudo-compatible tricrystal. (a) Tensile stress and (b) compressive stress.

To examine the internal stress, the specimen is unloaded until the total force on the loading surfaces decreases to zero. Distribution of the maximum and minimum principal stresses in the unloaded specimen is given in figure 6. Through the triple junction there are slanting bands in which tensile stress parallel to the bands occur. The direction of the internal stress in the tensile band rotates toward the x and -x axes. On the other hand, Figure 2(b) shows that in grains 1 and 3, rotation of the stress axis toward the x axis favors the activation of the conjugate system. And actually, in the vicinities of the triple line, the direction of the region of double slip coincides with the direction of the band. These facts suggest that the secondary slip system in this tricrystal is activated on account of this internal stress.

Zaoui and co-workers/5, 6/ have reported a junction type multiple slip region which is not generated along the grain boundary plane, but propagates into the grain interior from grain boundary junctions. The Region of secondary slip shown in figure 5(b) is similar to the junction type multiple slip region. Thus, not only the compatibility requirement on grain boundaries, but also the cramping effect which causes plastic multiple slip in polycrystals must be taken note of.

5. Reference