Slip Behavior and Local Stress near Grain Boundary in High-Cycle Fatigue of Copper Polycrystal

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Recent development of OIM (Orientation Imaging Microscope) makes the measurement of crystal orientation easy and advanced computer technology allows us to conduct a detailed stress analysis of component with microstructure. In this study, a high-cycle fatigue test was carried out for a copper polycrystal, where the shape and orientation of each grain is measured by the OIM. Thirteen PSBs are found along the grain boundaries, and the location and slip system are different from those expected by the Schmid factor. FEM analysis is conducted for the copper polycrystal with the same orientation and shape. It reveals that the increase of resolved shear stress, $\tau_{rss}$, of specific slip system due to the constraint of deformation between grains causes the unique slip behavior near the grain boundary.

Key Words: Fatigue, Stress Concentration, Numerical Analysis, Finite Element Method, Slip Behavior, Persistent Slip Band, Grain Boundary, Copper Polycrystal

1. Introduction

In a high-cycle fatigue of metal, crystallographic slip takes place on a specific system, and the localized deformation brings about persistent slip band (PSB) with increasing number of cycles. The interface between the PSB and the matrix is a preferential initiation site for fatigue crack(1). Moreover, the slips govern the early propagation stage of crack, whose length is about a grain diameter or less(2). The slip behavior in the fatigue of a single crystal is dependent on the loading direction and the crystal orientation. However, in a polycrystal, it is not so easy to describe the slip behavior because the deformation of neighboring grains affects the local stress. The influence of the neighboring grain through the grain boundary is often investigated by using a bicrystal specimen(3)–(9). The experimental observation revealed that the unique slip occurs near the grain boundary in the high-cycle fatigue of bicrystals(9). In a previous paper(10), we carried out a high-cycle fatigue test of bicrystal of an $\alpha/\gamma$ two-phase stainless steel, and observed the unique slip behavior near the interface. A detailed stress analysis clarified that the unique slip behavior was attributed to the increase of resolved shear stress due to the constraint of deformation by the neighboring crystal. However, the bicrystal is adjoining to the free surface while a grain in a polycrystalline is surrounded by other ones. Thus, the influence of the deformation constraint on the slip behavior in the polycrystalline might be greater than that in the bicrystal. However, it was extremely difficult to measure precisely the shape and orientation of all constituent grains. Moreover, computers did not have ability for a stress analysis taking into account the micro-structural inhomogeneity. Therefore, the relationship between the slip and the local stress in polycrystalline has not been investigated yet in spite of the practical importance. In recent years, the development of orientation imaging microscope (OIM)(11) makes the measurement of shape and orientation of each grain easy, and the improvement of computer ability allows us to conduct a large-scale numerical analysis.

In this study, a polycrystalline specimen, which consists of several tens of large-sized grains, is subjected to a high-cycle fatigue after the shape and crystal orientation in each grain is evaluated by means of the OIM. The focus is put on the slip behavior near the grain boundaries. In addition, a numerical analysis by a finite element method (FEM) is conducted for the polycrystal with the
same shape and crystal orientation in each grain on the surface, and the local stress condition for the crystallographic slip is examined.

2. Experimental Procedure

2.1 Specimen

A specimen, of which shape and size are shown in Fig. 1, is extracted from a plate of 99.9999% mass copper polycrystal using an electric discharge cutting machine. The gage length is 5 mm, and the cross section is 2.75 mm × 0.89 mm. After wet mechanical polishing, the specimen is annealed cyclically (973 K 0.5 h + 1073 K 0.5 h) for 48 h in a vacuum. The surface layer is removed by chemical polishing using nitric acid, and the orientation of each grain on the surface is measured by means of the OIM. In addition, it is polished as mirror by buffing and by electro-polishing in a phosphoric acid-ethanol mixture before the fatigue test.

2.2 Crystallographic structure of specimen

Figure 2 shows the crystal orientations evaluated by the OIM, where the two surfaces are designated by “obverse surface” and “reverse surface”, respectively. The color of each grain represents the crystal orientation along the normal direction to the specimen surface, which corresponds to the one indicated in the standard stereo-triangle in the figure. Consecutive numbers are assigned to each grain for identification. Considering the thickness of the specimen (0.89 mm), same number is assigned to the grains, which are regarded as one grain from the orientation and the location on the both surfaces. There are several tens of large-sized grains with the diameter of about 1.0 mm in the gauge of specimen.

2.3 Pull-push fatigue test

A pull-push fatigue test is carried out by a servo-hydraulic fatigue-testing machine in an air at room temperature. In order to prevent the introduction of initial strain to the specimen during the set-up to the machine, the bottom of the specimen is soaked in a pot filled with the wood metal after the top is clamped to the upper jig, and the bottom is fixed by cooling. The test is carried out under a triangular waveform of tension-compression load with the frequency of 2.5 Hz. The stress amplitude is increased gradually with checking the sufficient hardening on the hysteresis loop. Both side surfaces are observed in situ by means of a Nomarski differential interferophrometer. The test is terminated when a PSB is recognized in the gauge section. After the fatigue test, the specimen surface is observed in detail by means of a Nomarski differential interferophrometer and a scanning electron microscope (SEM).

3. Analytical Procedure

Focusing on the analysis of stress distribution on the obverse surface, a model is constructed on the basis of the shape and crystal orientation in each grain of the experimental specimen. The mesh division is illustrated in Fig. 3. It consists of 69,480 elements, and the region near the grain boundary where the stress concentration is expected is divided into fine mesh. The width of the smallest mesh is about 4 µm. The ratios of height, depth and width in the gauge section of the model are 5 : 0.89 : 2.75, which are same as the ones of the experimental specimen. Strictly speaking, it is required for the model to simulate three-dimensionally same shape and same crystal orien-
tation of grains in the specimen. However, a previous paper\(^{12}\) revealed that the elastic stress due to the deformation constraint of the neighboring crystal concentrated on the region near the junction between the free surface and the grain boundary. Moreover, it is impossible to evaluate the shape and crystal orientation of the grain inside the specimen by means of the OIM. Then, we conduct the analysis using a two-dimensional polycrystalline model; in which each grain has columnar shape on the obverse surface. MSC/NASTRAN for Windows (Version 4.6) is used for the FEM analysis. On the basis of the elastic orthotropism of the fcc metal, the elastic constants in each grain are determined by the crystal orientation and the standard elastic constants of copper single crystal, \(C_{11} = 168.4\) GPa, \(C_{12} = 75.4\) GPa and \(C_{44} = 121.4\) GPa\(^{13}\). The uniform stress, \(\sigma_0\), is applied to the top and bottom, and the perfect bonding condition is imposed to the interface between grains.

4. Results and Discussion

4.1 Slip behavior in high-cycle fatigue

A fcc metal has 12 independent crystallographic slip systems, and the Schmid factors \(\tau/\sigma_0 = \cos\phi \cdot \cos\lambda\), \(\tau\): the resolved shear stress to the slip direction, \(\phi\): the angle between the loading axis and the normal to the slip plane, and \(\lambda\): the angle between the loading axis and the slip direction) are evaluated for each slip system. The largest Schmid factor in a grain is designated as \((SF)_{\text{max}}\), and its magnitude in the gauge section is in the range of 0.32 – 0.49. The plastic strain begins to appear on the hysteresis loop at the stress amplitude of 4.1 MPa (350 cycles). The maximum resolved shear stress in each grain is in the range of 1.3 – 1.2 MPa. After hardening in the continuous load cycle, the applied stress amplitude is gradually increased. Although the slight steps are formed along the specific grain boundaries at the stress amplitude of about 12 MPa (170 000 cycles), the crystallographic slips are not identified. The PSBs are recognized near the grain boundary between the grains, Nos. 6 and 11, on the obverse surface at stress amplitude of about 53 MPa (700 000 cycles), and the test is interrupted. Figure 4 shows the change of the hysteresis loop during the test.

Although the active PSBs are found only near the grain boundary between the grains, Nos. 6 and 11, by in situ observation, the detailed examination after the test reveals that the PSBs are formed along other boundaries as well. Thirteen PSBs observed are illustrated in Fig. 5 (thick black lines in the figure), and they are designated as (1) – (13) respectively. In a single crystal, the PSB formation is governed by the Schmid factor. If it is applicable to the PSB formation in the polycrystalline as well, uniform slip should appear in each grain. However, it is clear from the figure that all PSBs are formed only near the grain boundaries. Moreover, the slip system of some PSBs is different from that expected by the Schmid factor. Then, the focus is put on the most active PSBs on the obverse surface (PSB (6) in Fig. 5) and two PSBs which slip system is different from the prediction by the Schmid factor (PSBs (2) and (8) in Fig. 5). Figure 6 shows the SEM photographs of PSBs (2), (6) and (8), respectively. Extrusions, which are the typical feature of PSB, are observed,
and PSB (6) shows the most active behavior, which corresponds with the result obtained by in situ observation. PSBs (2), (6) and (8) are formed in the grains Nos. 6 and 13, respectively, of which the stereographic projections are shown in Fig. 7. In the figure, the slip plane and slip direction are described by Schmid and Boas notation. The four slip planes are termed as A (critical), B (primary), C (conjugate) and D (cross), and the six slip directions are designated as 1–6, respectively. For example, the primary slip system is represented as B4. Therefore, the B4 slip system should be activated in the grain, if the slip obeys the Schmid factor. Since PSB (6) is formed on the primary slip plane (B), the prediction by the Schmid factor works in this case. On the other hand, the slip plane of PSBs (2) and (8) are the critical slip plane (A), which is different from the prediction by the Schmid factor.

Here, it should be noted that all the PSBs are formed on the specific slip near the grain boundary.

4.2 Stress analysis for slip

Figure 8 shows the resolved shear stress on each slip system normalized by the applied stress, $\tau/\sigma$, in the element where PSBs (2), (6) and (8) are formed. In the figure, the Schmid factors in each grain are plotted for comparison. Schmid factor is the normalized resolved shear stress without the influence of the deformation constraint of the neighboring grain. On the other hand, $\tau/\sigma$ takes into account it. Figure 8(a) signifies that the slip system with the largest Schmid factor for PSB (2) is B4, but the slip system with the largest magnitude of $\tau/\sigma$ is A3. Since PSB (2) is formed on the critical slip plane (A) of the grain No. 6 in the experiment, the highest resolved shear stress brings about the slips in the region. At the most active PSB, (6) (Fig. 8(b)), the largest $\tau/\sigma$ is on the slip system B4, and it is larger than that of the Schmid factor. Considering that the Schmid factor represents the resolved shear stress on the center of the grain (away from the grain boundary), the analytical result points out that the resolved shear stress on B4 increases with approaching the grain boundary. In the surface observation, PSB (6) is formed only near the grain boundary by the activation of the primary slip system (B4), and
Fig. 8 Schmid factors and \( \tau/\sigma_0 \) on the slip systems

the result coincides with the stress analysis. As the grain boundary along PSB (6) is a coherent twin boundary \((\Sigma 3(111))\) boundary, the slip system of PSB (6) is parallel to the boundary, (111) plane. In addition to the high resolved shear stress, it is the reason why the remarkable PSB is formed near the twin boundary. At PSB (8) in the grain No. 13, \( \tau/\sigma_0 \) on A3 is the largest, and it corresponds with the experimental observation as well (Fig. 8 (c)).

After all, it is summarized that the specific slip near the grain boundary in high-cycle fatigue of polycrystalline is caused by the increase of the resolved shear stress due to the deformation constraint by neighboring grains.

5. Conclusions

A high-cycle fatigue test is carried out for a copper polycrystalline specimen with several tens of large-sized grains in the gauge section, and the following results are obtained.

1. The PSBs are formed near grain boundary.
2. The slip planes of PSBs do not agree with those expected by the Schmid factor.
3. The most active PSB is formed near the twin boundary.

A stress analysis for a polycrystalline model is conducted by FEM, and the following results are obtained.
4. The PSBs are formed at the locations where the magnitude of \( \tau/\sigma_0 \) is larger than that of the Schmid factor on B4 (primary slip system).
5. The active PSB is developed near the twin boundary because the slip system is parallel to the twin boundary.
6. The specific slip behavior (PSB formation) near the grain boundary in high-cycle fatigue is attributed to the deformation constraint on the grain boundary.

References
