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In Situ Observation of Disconnection-Mediated Grain Rotation

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Grain growth kinetics is greatly influenced by stress accumulation within a grain during the grain boundary migration process in polycrystalline systems due to the coupling of grain boundary (GB) migration and shear stress across the GB [1, 2]. Therefore, the relaxation of shear stress induced by GB migration is critical for understanding dynamics of GB migration and grain growth. A few mechanisms have been proposed to explain the stress effect during a grain growth process, including plastic deformation (dislocation motion or twinning within the grain), grain rotation, and repeated switching between distinct disconnection modes that exhibit β values of opposite sign [1].

In this work, we focus on an asymmetric Σ33 GB area in a polycrystalline Pt sample as seen in Fig. 1(a), which is semi-coherent and constrained by triple junctions at the two ends. Five disconnections can be observed on the GB. As shown in Figure 1, heating of the sample leads to GB migration via propagation of disconnections. Fig. 1(b) shows that, after 37 seconds, two disconnections on the left side and one disconnection on the right side propagated and became accommodated by the triple junctions. At the same time, two disconnections in the middle of the GB propagated toward the right side for one and two interatomic distances, respectively. Since disconnections carry burger's vector, the propagation of disconnections would inevitably induce stress inside the system. Fig. 1(b) shows that the rotation of two grains takes place in opposite direction which release the shear stress built up near the GB. Fig. 1(c) demonstrates that further propagation of disconnections without any disconnection - triple junction interaction also leads to grain rotation. This observation provides unambiguous evidence that the migration of an asymmetric tilt GB takes place by the propagation of disconnection and the stress established in this process can be released by grain rotation. It also suggests that the direct driving force of grain rotation comes from the propagation of disconnections.

Further observation was conducted on another low-angle GB, as shown in Fig. 2, which demonstrates that grain rotation leads to the aggregation of grains. Fig. 2(a) shows the grain in the center was surrounded by other GBs of various types. When the sample was heated to 600 °C, as shown in Fig. 2(b), the GB of the center grain migrated approximately one interatomic distance, and the center grain rotated slightly at the same time. This decreased the misorientation between the grain at the center and the grain below it. Then Fig. 2(c) shows that, after 6s, the center grain rotated and merged into the grain below it. At the same time, the GBs of the upper grains migrate downwards. Although we didn't observe the detailed atomic process of GB migration due to insufficient time resolution, this observation, combined with that of Fig. 1, suggests that GB migration could lead to the grain rotation, which further facilitates grain growth by grain aggregation.

In summary, we studied GB migration dynamics in a Pt polycrystalline sample at 600˚C by *in situ* scanning transmission electron microscope (STEM). Grain boundary migration took place by the propagation of disconnections, and the subsequent accumulation of shear stress was released by grain rotations. We also found that grain rotation led to the aggregation of grains which were divided by low-angle GBs. Our observations suggests that GB migration leads to the grain rotation, which could further facilitate grain growth by grain aggregation [3].

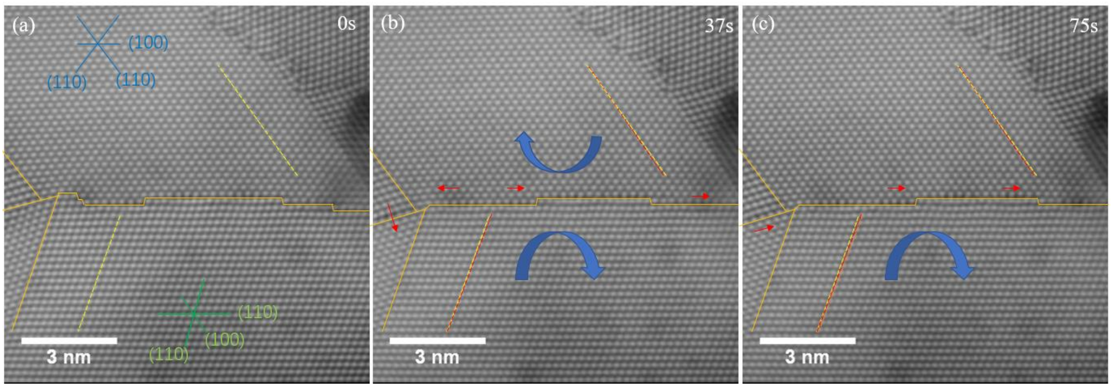

Figure 1. Sequential *in situ* HAADF images of GB migration in a Pt polycrystalline sample at 600˚C. (a) Initial state of the Σ33 GB with 5 disconnections. (b) GB migration took place via propagation of disconnections. The induced stress was released by rotation of two grains in opposite direction. (c) Further disconnection propagation induced more rotation of the bottom grain.

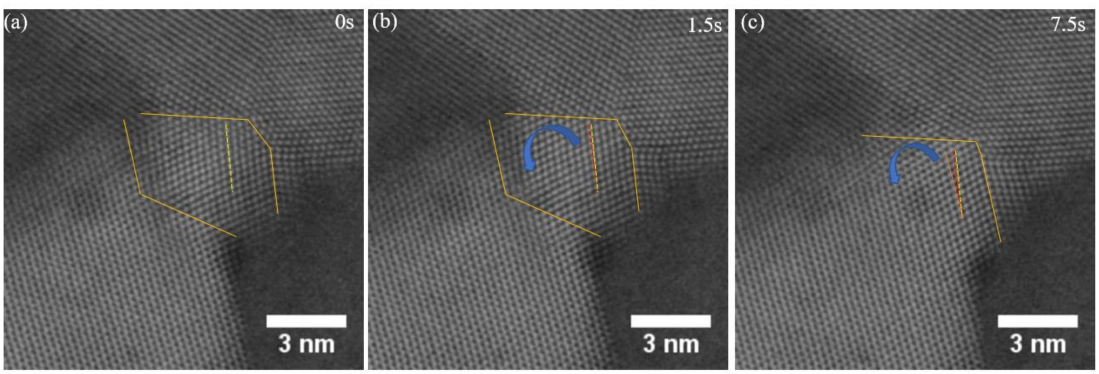

Figure 2. Sequential *in situ* HAADF images of grain aggregation by grain rotation at 600˚C. (a) Initial state of the polycrystalline sample. (b) GB migration took place, together with a slight rotation of the grain at the center. (c) The grain at the center merged into the lower grain by rotation. The upper GBs migrated downwards at the same time.

References:

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