2402
doi:10.1017/S1431927621008606

Microsc. Microanal. 27 (Suppl 1), 2021

In-situ TEM on interfacial phase transition during shear-mediated grain boundary migration

Zhengwu Fang and Scott Mao

University of Pittsburgh, United States

Grain boundary (GB), as the most common interfacial structure in polycrystalline materials, plays a vital role in mediating the microstructural evolution of materials during plastic deformation [1]. Although the GB network evolution during plasticity of polycrystalline materials has been wildly reported in the past [2], direct experimental observations on its dynamic evolution process at the atomic scale are rare. One typical mechanism that accommodates the GB network evolution is the GB phase transformation or GB complexion transition [3], which includes GB structural transformation, facet transformation, and dissociation. However, the previous studies on GB phase transformation have mainly focused on the thermodynamics, e.g. the equilibrium GB structures under certain thermodynamic conditions, not much has been done regarding the kinetics, e.g. the dynamic transformation process. Therefore, exploring the dynamic process and underlying atomistic mechanisms of GB phase transformation would be urgently needed to advance the methodology of GB engineering.

In this contribution, we fabricated gold nano bicrystals with two kinds of < 110 > tilt faceted asymmetrical GBs, i.e., (002)/(111) + (-1-11)/(002) facets (Figure 1a) and (002)/(111) + (111)/(11-1) facets (Figure 1b), inside transmission electron microscopy via our in-situ nano-welding technique. Note that (002)/(111) GB/facet is an incommensurate GB with a theoretical misorientation angle of 54.74° and is a common facet of < 110 > tilt Σ11 ATGB in FCC metals [4]. We then investigate the atomistic mechanisms of GB phase transformation during the stress-driven GB migration at these two types of faceted GBs. We find that the (002)/(111) facets in both faceted GBs would undergo phase transformation into the Σ11 (113) symmetrical tilt GB, although the underlying atomistic mechanisms are different. This work provides the first insights into the atomistic mechanisms of GB dynamic phase transformation for the migration of high angle asymmetrical tilt GBs and its contribution to the plasticity and microstructural evolution of polycrystalline materials with complex GBs.

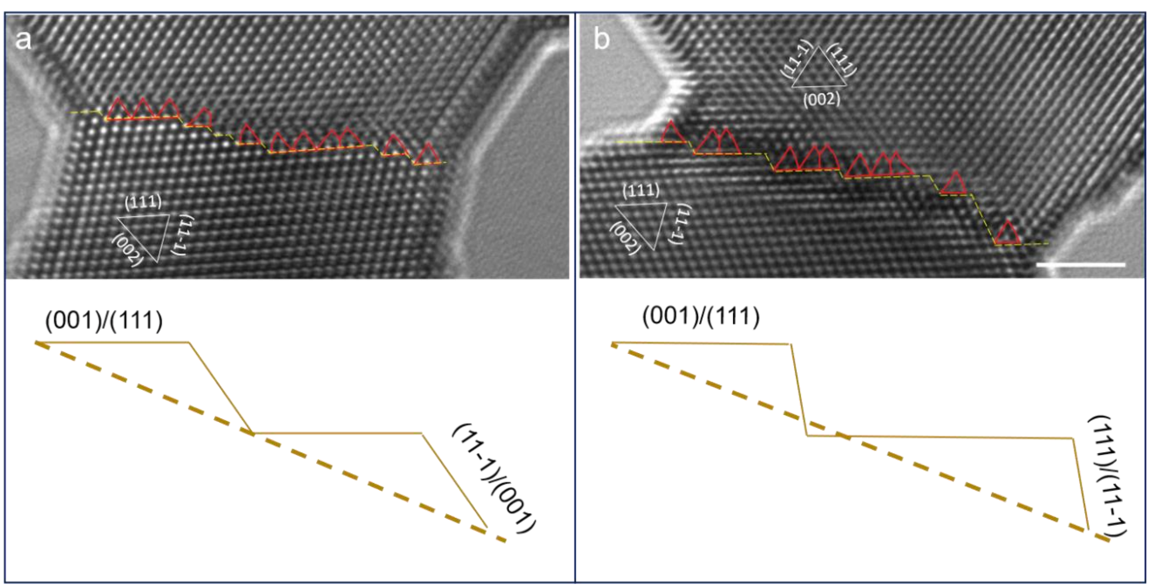

Figure 1. HRTEM images and schematic illustrations showing the two types of faceted asymmetrical GB in the fabricated bicrystals. (a) Type 1 GB consisting of (002)/(111) + (-1-11)/(002) facets, (b) type 2 GB consisting of (002)/(111) + (111)/(11-1) facets. Scale bar, 2nm.

References

[1] Shan, Z. *et al.* Grain Boundary-Mediated Plasticity in Nanocrystalline Nickel. *Science* 305, 654, (2004).
[2] Schuh, C. A., Kumar, M. & King, W. E. Analysis of grain boundary networks and their evolution during grain boundary engineering. *Acta Materialia* 51, 687-700,(2003).
[3] Cantwell, P. R. *et al.* Grain boundary complexions. *Acta Materialia* 62, 1-48,(2014).
[4] Brown, J. A. & Mishin, Y. Dissociation and faceting of asymmetrical tilt grain boundaries: Molecular dynamics simulations of copper. *Physical Review B* 76, (2007)

https://doi.org/10.1017/S1431927621008606 Published online by Cambridge University Press