Review of: "Faceting–roughening transition of a Cu grain boundary under electron-beam irradiation at 300 keV"

Syo Matsumura[1]

1 Kyushu University

Potential competing interests: The author(s) declared that no potential competing interests exist.

This paper reports *in-situ* atomic resolution TEM observation of structural evolution of the grain boundary (GB) between (020) and (220) in a Cu bicrystal lamella with [100] and [110] normal under irradiation with 300 keV electrons. This can be regarded as following a preceding paper in *Scripta Materialia*, Vol. **194**, 113630 (2021) (referred as [14] in the present one), where well-defined GBs in Au bicrystals were irradiated with 1.25 MeV electrons in a high voltage TEM. Both experiments were performed in common under a condition of electron irradiation with the kinetic energy just below the atom displacement threshold in the perfect crystalline state.

It is apparent that the experiment was well-organized and was performed carefully. It has been revealed that the GB overhangs the [110] Cu domain under focused electron illumination, which is discussed in terms of various viewpoints, such as electron beam heating, surface spattering, collisional displacements of Cu atoms by swift electrons, faceting-roughening transition of boundaries predicted for driven systems and inelastic electron scattering exiting phonons. The authors have finally ascribed the GB evolution to the phonon exciting inelastic scattering. But the referee cannot be convinced with the last conclusion simply, as the discussion has been done only shortly. How can be the phonon excitation distinguished with the beam-heating effect which has been evaluated as negligible at the beginning of discussion? The beam-heating maybe includes thermalization of both electron and phonon excitations.

The results shown here are quite high quality and bring us several hints and/or speculations on the fundamental mechanism which should be discussed further.

The referee has been impressed very much with Fig. 3a. A symmetric GB structure has been formed in the encircled irradiation area, which may suggest sequential and systematic atom motions involved in the GB evolution. A specific extended GB region is recognized with remarkably clear [110] atom configuration contrast, which is only few atom layer thick in the upper and lower original GB parts but extended in a round shape in front of the overhanging tip part. The image contrast becomes blurred next to the clear GB region in the [110] grain, indicating localized lattice strain or misorientation. Furthermore, (111) planer defect like contrast is recognized in the right hand edge just outside the circle for the illumination area and below the indicator “[110]”. On the other hand, in the upper left corner just below the letter “a”, contrast line mismatching arises on (002) planes along the periphery of the illuminated area. A coarse wavy contrast appears overlayed on the lattice fringes in the bottom part of the [100] domain side. Furthermore, an extra half plane has been inserted in the right hand [110] region, forming an edge dislocation like configuration on the GB front above the two facing arrows in enlarged Fig. 3b, the formation of which cannot be explained in terms of phonon excitation.

The characteristic features of the GB structure mentioned above may suggest that a significant number of atom displacements have taken place in the irradiated area, even though the kinetic energy of incident electrons was lower than the threshold in the perfect crystal. It would be possible as less bonded atoms and wider free space exist at lattice defects such as GBs and dislocations, facilitating atom displacements and movements at a sub-threshold energy. It is known that aggregation of displaced interstitials into dislocation loops or defect clusters is enhanced around the skirt of electron beam with a Gaussian-like intensity profile, or at the periphery of the focused electron beam [*e.g*. K. Yasuda, *et al*, *Philos. Mag. A*, **78**, 583-598 (1998)], which may explain the formation of defects at just outside the illuminated area.

The further examination and discussion must be necessary to reach the exact mechanism of the interesting GB evolution under electron illumination revealed in the present paper, as the comments mentioned above are no better than speculations. I hope that this review will be of help to promote the scientific understanding.