Atomic Structure Characterization of ZnO Σ13 (13$\dot{4}$0) Symmetric Tilt Grain Boundaries

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Grain boundaries (GBs) in ceramic materials play key roles for various properties. A good example to be observed would be zinc oxide (ZnO) ceramics and thin films for electrical and optical applications. It is important to understand the GB structure in atomic scale because GBs can drastically change the electrical and optical properties. However, an understanding of atomic scale details for ZnO GBs is still limited for large variation of geometry. In this study, atomic arrangement of ZnO GBs has been investigated by electron microscopy imaging and computational modeling in detail.

A pristine ZnO GB was fabricated by joining two ZnO single crystals. The bicrystal has a [0001] symmetric tilt GB with the precisely aimed rotation angle of ~ 32.2^0, which corresponds to Σ13 coincidence site lattice (CSL) orientation relationship with the GB planes of (13$\dot{4}$0). The ZnO GB was observed by high resolution transmission electron microscopy (HRTEM), annular dark-field (ADF), and annular bright-field (ABF) scanning transmission electron microscopy (STEM) in order to understand its detailed structures in atomic level. In addition, the stable GB structure has been obtained by using first-principles calculations and it was compared with the experimental results.

Figure 1 shows low-magnification TEM image and diffraction pattern taken from the GB region for the ZnO bicrystal. The GB has a rotation angle of 32.4^o, which corresponds to near exact Σ13 orientation relationship, and the GB plane is flat and parallel to (13$\dot{4}$0) for both crystals. Figure 2 shows the STEM images and calculated structure model for the ZnO Σ13 GB. Both results agree well with each other, indicating the validity of the structure model. A structural period of the GB consists of particular structure units (SUs) as reported previously [1], and those SUs are connected with bulk-like units. As shown in Fig. 2(c), the ZnOΣ13 GB can be explained as repeating SUs C-D and the bulk unit, where the SUs C-D shares 6-membered atomic ring and forms zig-zag array.

In this presentation, results on praseodymium (Pr)-doped ZnO Σ13 GB will be presented. Further discussion on SU arrangements and structural stability will be made, comparing the result with our previous studies.[2-3]

References

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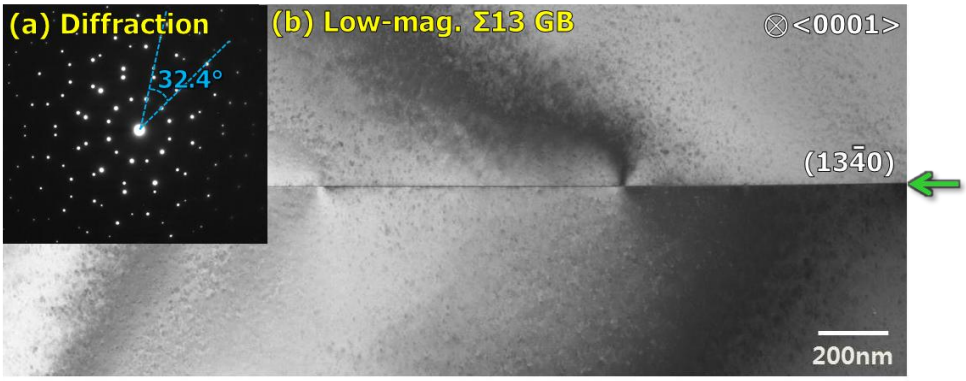

FIG. 1. (a) Diffraction pattern taken from the region including both crystals and (b) low magnification TEM image of ZnO Σ13GB.

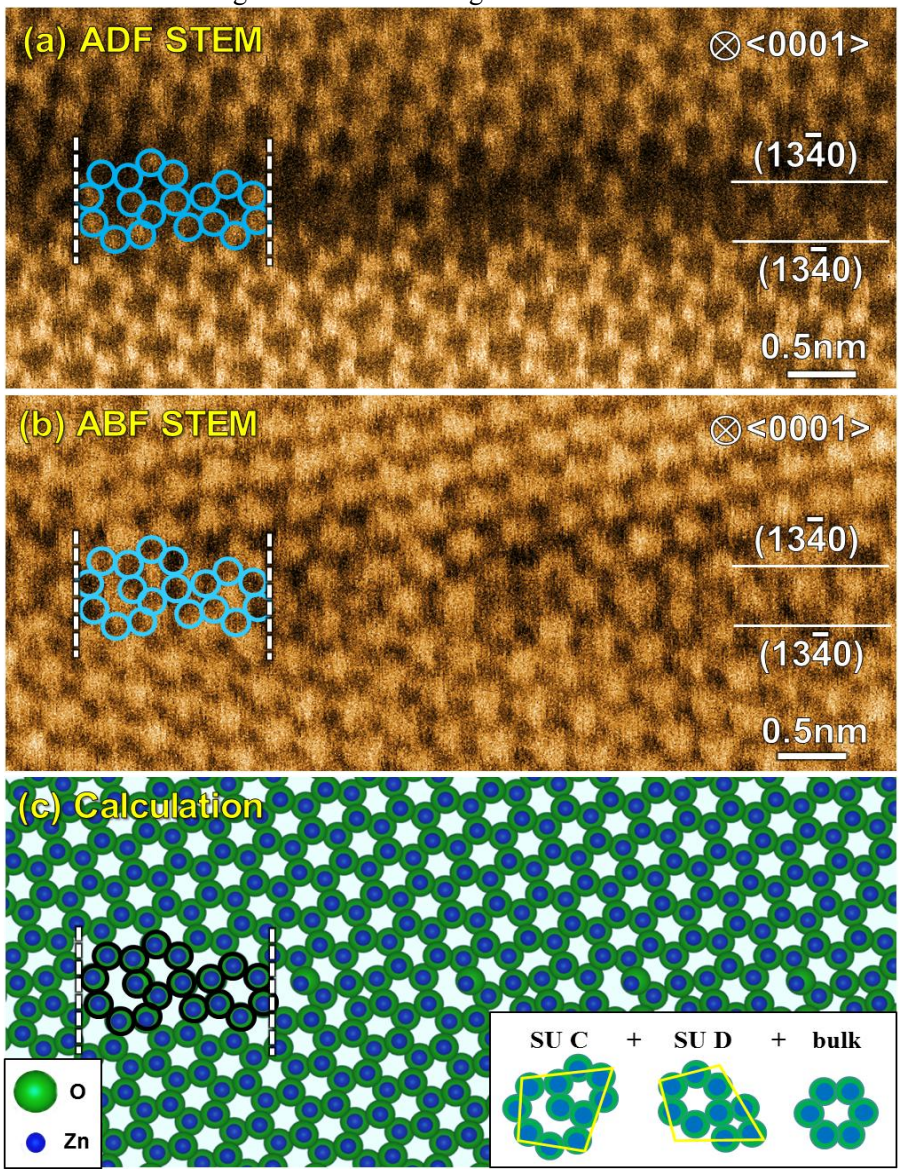

FIG. 2. (a)Annular dark-field and (b) annular bright-field STEM image of ZnO GB. (c) Calculated GB structure model with an inset showing the combination of SUs at the GB. Here, SUs (C+D+bulk) forms a single structural period at the GB.