Mapping 3D crystallographic orientation and strain fields in deformed polycrystalline aluminum alloy by diffraction-amalgamated grain boundary tracking

A comprehensive description of the structure of polycrystalline materials is the basis for understanding their physical and mechanical characteristics. Conventional scientific principles concerning polycrystalline materials have, however, been developed on the basis of two-dimensional (2D) observations of surfaces or thin films. A series of surface microscopic observations provides a certain amount of information on the time evolution behaviors of deformation, damage, and fracture in polycrystalline materials. Such information, however, may be considered unrepresentative of the bulk of a given material in the sense that surface-specific phenomena are often observed. To investigate actual phenomena in the bulk of a polycrystalline material, a sectioned surface can be examined, for example, by electron backscattering diffraction technique. This, however, is a fundamentally destructive and nonsequential mode of observation, and any results should therefore be interpreted with caution due to the three-dimensional (3D) complexity of microstructural features in practical materials. It has been vital, therefore, for other procedures to be developed to obtain accurate 3D *in situ* representations of polycrystalline materials.

The 3D grain structure and orientation map of polycrystalline materials can be obtained by using 3D X-ray diffraction, diffraction contrast tomography, and differential-aperture X-ray microscopy regardless of the material. All these techniques, however, require X-ray diffraction to map grain boundaries, and this means that, owing to the resulting occurrence of intensity reduction, spot blurring, and spot overlap during plastic deformation, the techniques are vulnerable to plastic deformation [1]. Spot overlap is mainly attributable to the orientation spread of individual grains.

In this study, we proposed a new technique, named diffraction-amalgamated grain boundary tracking (DAGT), which can be applied to large tensile deformation of a polycrystalline aluminum alloy. This technique is composed of an X-ray diffraction technique and a grain boundary tracking (GBT) technique, and proposed by the authors for imaging 3D polycrystalline structures and local strain distributions [2]. The GBT technique enables the accurate reconstruction of 3D grain morphologies during deformation, even close to fracture. Precise image registration is then performed for the X-ray microtomography images captured before and after gallium application to identify particles located along the gallium-enhanced grain boundaries the 3D marker-based registration is performed to calculate the necessary image shifts in all the translational and rotational directions. Each grain is then reconstructed as a polygonal mesh by connecting particles located along the grain boundaries as plane-triangle components. This triangulation of the surface of individual grains is repeated at each loading step by employing the microstructural tracking technique [3], enabling visualization of the deformation behavior of each polygonal grain by tracking all the grain boundary particles throughout deformation. A 'pencil-beam' X-ray diffraction technique is coupled with the GBT technique. Diffraction spots are obtained from all the grains during the DAGT experiment and then back-projected to a sample position to calculate the crystallographic orientation of all the grains visualized with the GBT technique [4].

Figure 1 is a schematic representation of the setup used in the pencil-beam XRD experiment, as part of the DAGT technique. Monochromatic radiation from a monochromator is collimated with a Fresnel zone plate or slit collimator to form an X-ray pencil beam to facilitate data analysis by limiting the number of diffraction spots obtained for each X-ray path. By rotating the sample through 180°, the pencil beam can scan in both the lateral and horizontal directions, thereby illuminating every location in the region of interest, from all possible directions with respect to the rotation axis of the sample, at a typical scanning step of 10 μm.

A DAGT experiment was performed using the X-ray imaging beamline **BL20XU** in SPring-8. Figure 2, in which the color of individual grains and plots is dependent on the crystallographic orientation, shows individual grains over the entire region of interest before and after plastic deformation of 27.0%. To examine

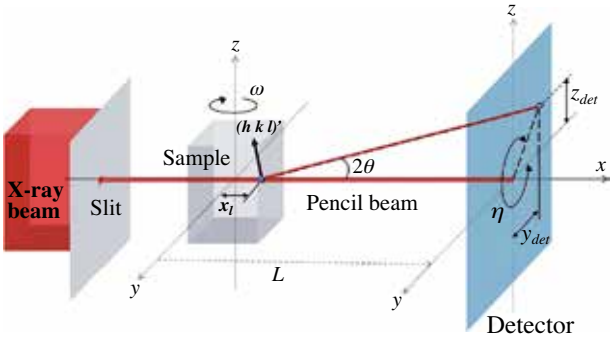
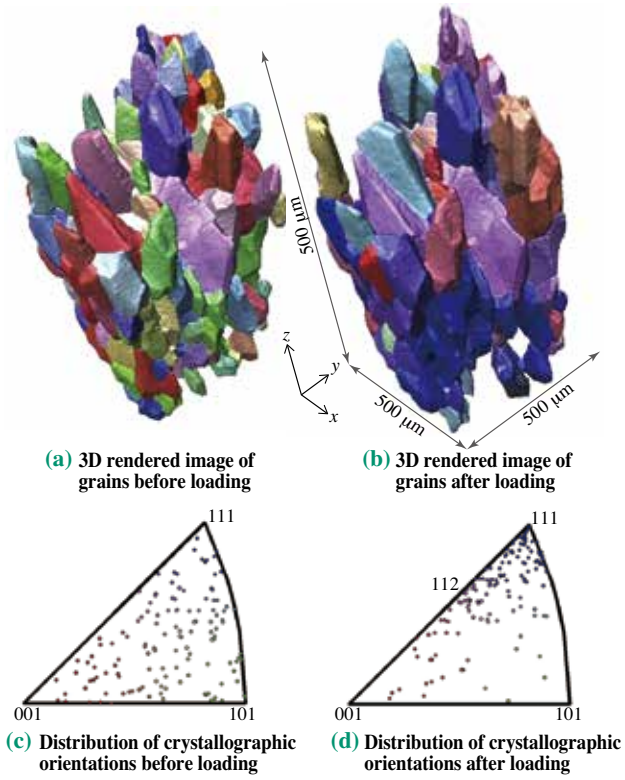


Fig. 1. Schematic diagram of the setup for the pencil-beam XRD experiments.

the texture evolution during tensile deformation, the average orientations of the grains before and after plastic deformation are represented in inverse pole figures for the loading directions in Figs. 2(c) and 2(d), respectively. Figures 2(b) and 2(d), which show the distribution of the crystallographic orientation after uniaxial tensile deformation, reveal that certain crystallographic axes are almost parallel to the tensile direction. The stereographic triangle in Fig. 2(d) clearly shows that the orientation space is subdivided into three regions, including grains with their tensile axes near the crystallographic <111> direction, along the hypotenuse, and outside these regions. The first and second groups correspond to the deformation texture characteristic to tensile deformation, which has preferential orientations of <111> and <112> in the case of aluminum alloys.

Figure 3, which illustrates such a spatially distributed orientation in a specific grain, was plotted from stacked 2D images of the orientation distribution, drawn on the corresponding *x*-*y* cross sections. Six grains are adjacent to the grain in this virtual cross section. Some of these grains share relatively wide grain-boundary areas with the grain. Some grains have average orientations close to <112>, while the others are on average close to <111>. It is interesting to note that the crystallographic orientation in the lower left side of the grain, which is adjacent to the grains having average orientations close to <112>, is different from that in the other regions; at the same time, this region exhibits intense shear strain, as shown in Fig. 3(b). The internal orientation gradient is observable in Fig. 3. The 3D observation, in which a more complex 3D grain shape is observable than in conventional 2D observation, has revealed the effects of inhomogeneous and strong interactions with selected surrounding grains.



(a) 3D rendered image of grains before loading
(b) 3D rendered image of grains after loading
(c) Distribution of crystallographic orientations before loading
(d) Distribution of crystallographic orientations after loading

Fig. 2. Results of the DAGT analysis, showing the distributions of crystallographic orientations before and after loading with a plastic strain of 27.0%. The colors of the grains and inverse pole markings represent locations in the inverse pole figures: [001] oriented grains are red, [101] green, and [111] blue.

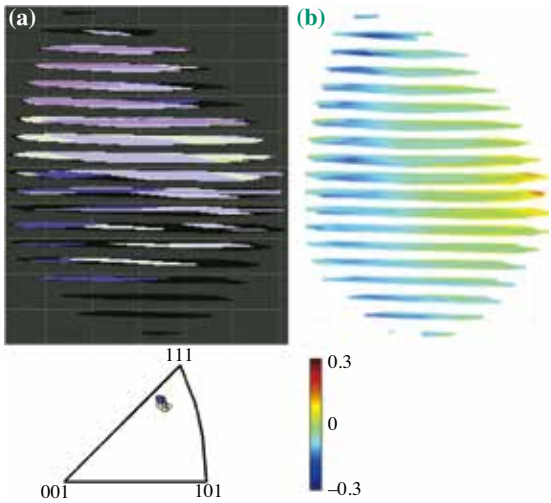


Fig. 3. Results of the DAGT analysis, showing the 3D distribution of crystallographic orientation in a grain **(a)**, and the corresponding 3D distribution of shear strain, γ_{xy} **(b)**. The colors in (a) represent the locations in the inverse pole figure.

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