Application Note

Grain Boundary Wetting Correlated to the Grain Boundary Properties: *A laboratory-based multimodal X-ray tomography investigation*

Grain Boundary Wetting

Grain boundary wetting refers to the phenomenon that a liquid metal penetrates along the grain boundaries of a polycrystalline solid metal. Replacement of the original grain boundaries in the solid metal matrix with the liquid layer generally causes intergranular brittle fracture in otherwise ductile metals and alloys, also known as liquid metal embrittlement (LME). LME can be a serious problem for certain material processing senarios such as welding and galvanizing, as well as in nuclear reactors with a spallation target of liquid metal.

Multimodal X-ray Imaging

The combination of diffraction contrast tomography and other imaging modalities such as absorption contrast tomography available on the lab-based X-ray microscope provides complimentary information on the structure of materials, enabling direct correlation of the 3D grain map with various strutural features such as cracks, porosities or secondary phase particles.

In this application, the penetration behavior of liquid gallium in aluminum (***Fig. 1***) is characterized using absorption contrast tomography, and related to grain boundary properties obtained from the 3D grain map (***Fig. 2***) reconstructed from laboratory diffraction contrast tomography (LabDCT).

Characterizing Grain Boundary with LabDCT

The grain boundary characters are essential information to analyze grain boundary related behavior. Accessing the necessary parameters to fully describe a grain boundary in a polycrystalline structure is beyond the reach of 2D characterization techniques and only achievable through a 3D approach.

The 3D grain map reconstructed from LabDCT enables full 5D grain boundary characterization (misorientations + grain boundary plane normals) required for analysis of the wetting behavior of gallium in the aluminum matrix.

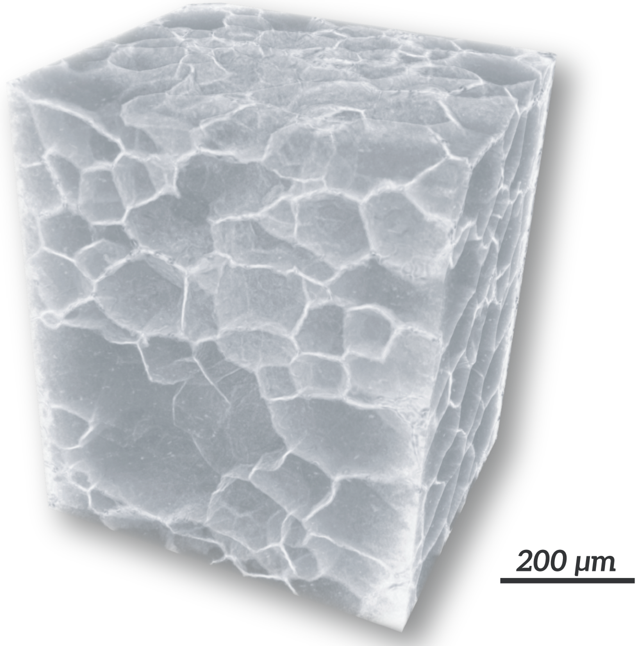

Fig. 1 *3D rendering of the network of gallium-wetted grain boundaries in an aluminum matrix visualized with absorption contrast tomography.*

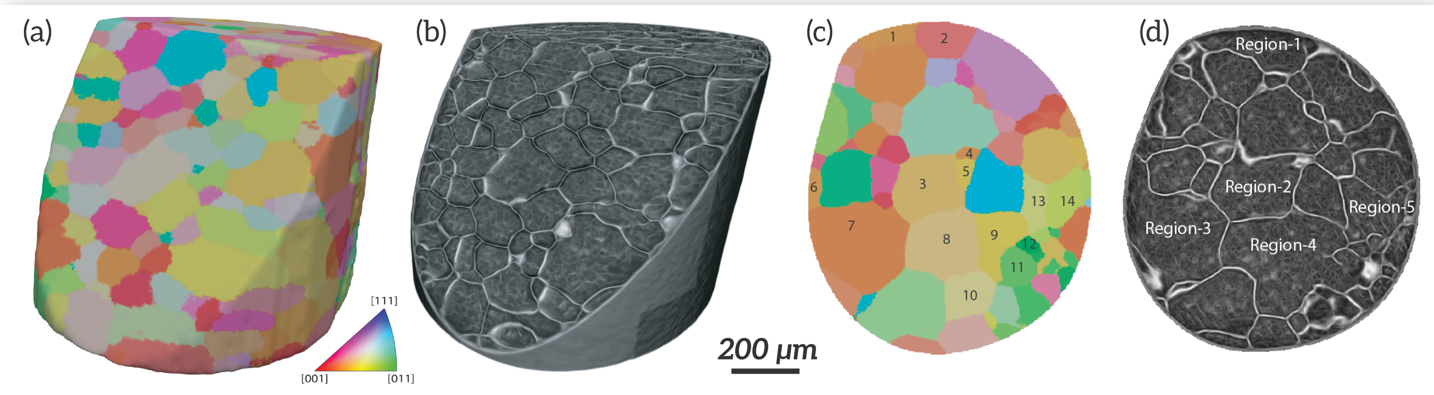

Fig. 2 *Comparison of the reconstructions from diffraction (a, c) and absorption (b, d) contrast tomography reveals that not all grain boudaries in the aluminum sample are wetted by gallium.*

Grain Boundary Wetting related to Grain Boundary Properties

Investigation of the variations of the extents of gallium wetting for more than 100 grain boundaries by correlating with the grain boundary characters suggested that it is the grain boundary energy which determines the preferential penetration path of gallium in the aluminum sample: Low energy boundaries are much more resistant to liquid gallium compared to higher energy ones.

This conclusion is supported by the current experimental evidence:

- Most of the unwetted boundaries in ***Fig. 3*** have low misorientation angles, for which the Read-Shockley equation predicts energy to increase with misorientation, matching the observed gallium wetting fraction increase with misorientation in the range 5 to 12°.
- The high angle boundaries with low or medium gallium wetting fractions in ***Fig. 3*** and ***Table 1*** are found to be CSL boundaries with low sigma values, which are known to have lower energies.
- MD simulations have shown that for ∑3 boundaries, those with planes closer to {111} have lower energy, consistent with the results in ***Fig. 4***.

This application has documented the potential of laboratory multimodal X-ray tomography for characterization of sample volumes large enough for statistical studies of correlations between the metal microstructure and grain boundary wetting behavior.

The experimental approach promises to be a routine tool for grain boundary characterization. The complete 3D description of the grain boundary network from LabDCT, makes it readily feasible to compute the grain boundary characters, and can be used as input for and validation of grain boundary models.

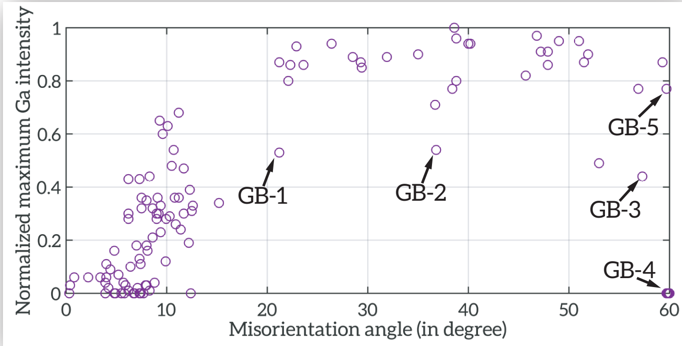

Fig. 3 *Gallium wetting fraction plotted against aluminum grain boundary misorientation angle.*

GB	Misorientation angle/axis	Brandon Criterion
GB-1	21.2°/[-0.43,-0.63,-0.65]	3.72°/3.27° (Close to ∑21a)
GB-2	36.8°/[-0.47,-0.64,-0.60]	4.84°/5.66° (∑7)
GB-3	57.3°/[0.55,0.56,0.62]	4.0°/8.66° (∑3)
GB-4	59.9°/[-0.58,0.58,0.58]	0.1°/8.66° (∑3)
GB-5	59.2°/[0.37 0.66 -0.65]	15°/8.66° (not ∑3)

Table 1. *Examination of CSL boundary type for GB-1 to GB-5 highlighted in Fig. 3, according to Brandon criterion.*

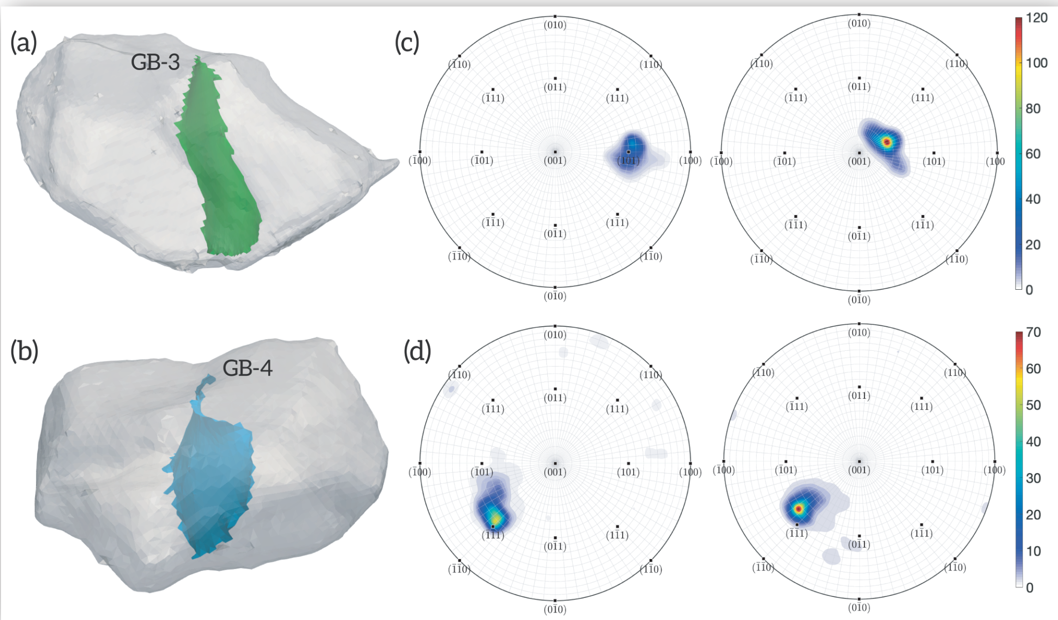

Fig. 4
For the highlighted ∑3 grain boundaries in Fig. 3: Volume renderings (a, b) and plane normal distributions in the crystal systems of both the grains forming the boundaries (c, d).
The grain boundary normal of the non-wetted GB-4 is much closer to the low energy {111}-type than that of the wetted GB-3.

References

J. Sun, et al., (2019), Scripta Mater., vol.163, pp. 77-81.

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