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Reliability of twin-dependent triple junction distributions measured from a section plane

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ABSTRACT

Numerous studies indicate polycrystalline triple junctions are independent microstructural features with distinct properties from their constituent grain boundaries. Despite the influence of triple junctions on material properties, it is impractical to characterize triple junctions on a large scale using current three-dimensional methods. This work demonstrates the ability to characterize twin-dependent triple junction distributions from a section plane by adopting a grain boundary plane stereology. The technique is validated through simulated distributions and simulated electron back-scatter diffraction (EBSD) data. Measures of validation and convergence are adopted to demonstrate the quantitative reliability of the technique as well as the convergence behavior of twin-dependent triple junction distributions. This technique expands the characterization power of EBSD and prepares the way for characterizing general triple junction distributions from a section plane.

1. Introduction

1.1. The need for triple junction characterization

A polycrystalline triple junction is formed by the common intersection of three grains or crystals within a polycrystal. A fully characterized triple junction consists of three crystals, three grain boundaries, and a common triple line. These features may be macroscopically defined by three crystal orientations g_A, g_B, and g_C, three grain boundary plane orientations by the boundary normals $\boldsymbol{n}_1$, $\boldsymbol{n}_2$, and $\boldsymbol{n}_3$, and a triple line orientation by the vector $\boldsymbol{t}$. Clearly these 17 parameters are not all independent and steps may be taken to reduce the number of parameters to a minimal number of independent parameters. By referencing all parameters from an internal coordinate system, or a coordinate system attached to one of the crystal lattices, the number of parameters may be reduced to 11 independent parameters of misorientations and plane parameters. To distinguish the application of an internal coordinate system, those parameters referenced from this system are appended with a subscript corresponding to the reference grain, which in Fig. 1 is grain A or g_A [1].

A microstructural distribution provides the normalized probability density as a function of character for an identified microstructural feature. As the dimensionality of a distribution feature increases, the quantity of measured data which must be collected to form the distribution increases as well. For instance, an orientation distribution contains only 3 parameters which consist of three Euler angles. A minute number of measurements would be required to form an orientation distribution as compared to a triple junction distribution containing 11 parameters. Bunge approximated that the quantity of measurements for minimal statistical reliability of a distribution is approximately 10^N, where N is the dimensionality of the desired feature [2]. Clearly, 10^{11} measurements are beyond the capabilities of any current experimental technique. This work brings the dimensionality of a triple junction to more measurable levels by focusing solely upon triple junctions containing a coherent twin boundary.

By exclusively characterizing twin-dependent triple junctions, the dimensionality of the distribution is significantly reduced. Given the mirror orientation symmetry across the grain boundary plane, the misorientation relation:

$$\Delta g_{AB} \cdot \Delta g_{BC} \cdot \Delta g_{CA} = \mathbf{I}$$

allows the two independent misorientations to be described by a single misorientation. As the incorporated twin boundary is a

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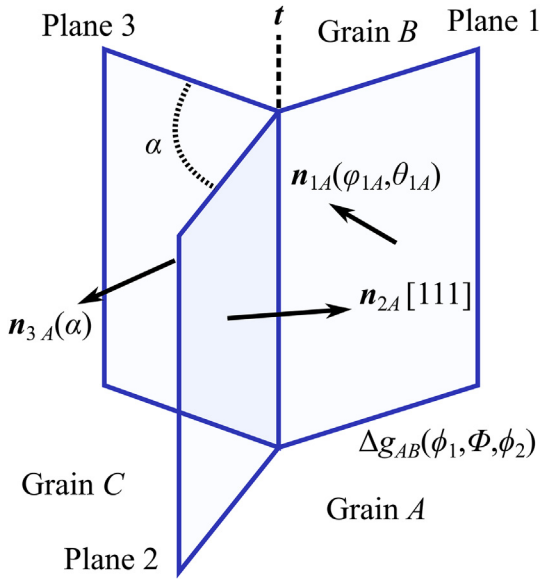

Fig. 1. The conventions and six independent parameters within the twin-dependent triple junction distribution.

coherent twin, in the considered materials or FCC materials, it always points in a ⟨111⟩ direction. By defining the reference frame such that the twin boundary or $\boldsymbol{n}_{2A}$ points in the [111] direction, this plane orientation becomes known. Given this convention, the parameters characterizing a twin-dependent triple junction are reduced to six independent parameters identified in this work as: a boundary plane normal $\boldsymbol{n}_{1A}$ given by spherical coordinates θ_{1A} and ϕ_{1A}, a dihedral angle α between $\boldsymbol{n}_{2A}$ and $\boldsymbol{n}_{3A}$, and a misorientation Δg_{AB} given by the Euler angles φ_1, Φ, and φ_2 in the Bunge convention [3]. These parameters constitute the continuous twin-dependent triple junction distribution given by $\Gamma(\theta_{1A},\phi_{1A},\alpha,\Delta g_{AB})$. The applied distribution parameters are depicted on an idealized triple junction in Fig. 1.

While triple junctions are composed of three constituent grain boundaries, they are distinct microstructural features. This is evidenced by their independent properties and microstructural effects, which are detailed in numerous studies [4–11]. Some of these properties are noted in a previous publication which lays the foundation for this work [12]. Despite understanding the independent nature of triple junctions, junction properties are not well linked to character. This is in part the result of the lack of an experimental method for characterizing triple junctions on a large scale. This deficiency in an experimental method is the result of the inherent difficulty of measuring the junction's many parameters within three-dimensions.

By developing a method for experimentally characterizing triple junction distributions, junction character could be better linked to microscopic as well as macroscopic material properties. In addition, triple junctions provide grain boundary network information which is unavailable from grain boundary distributions alone [13–16]. A method of characterizing triple junction distributions would also allow grain boundary energy distributions to be easily approximated on a large scale. Grain boundary energy distributions have been extracted over the full range of grain boundary parameters in a few significant studies, but always with great experimental effort [17–22]. By enabling triple junction distributions to be generated from measurements on a section plane, the grain boundary character and energy distributions could be extracted from these data [23,24]. In short, in order to perform integrated materials engineering, triple junctions must first be characterized on a large scale.

1.2. Shortcomings of current three-dimensional characterization techniques for characterizing triple junction distributions

Three-dimensional characterization techniques have seen great advances over the past decade and will continue to increase in efficiency and efficacy [25,26]. The techniques mentioned here are those capable of characterizing polycrystalline microstructures on the grain and grain boundary scale. These techniques include methods of high-energy X-ray tomography and diffraction and serial sectioning methods such as three-dimensional electron backscatter diffraction (EBSD) by mechanical sectioning, focused ion beam milling, or laser ablation [27–39]. These techniques have advantages over traditional two-dimensional techniques in that they can reveal information which cannot be extracted from two-dimensional planes [40,41]. Despite these advantages and advances in automated techniques [42,43], the three-dimensional techniques are typically expensive and tend to require substantial time and effort to carry out.

Given the time and effort required to collect data, current three dimensional approaches are incapable of providing the quantity of data necessary for practically forming statistically reliable triple junction distributions. For grain boundary distributions, Morawiec recently showed that despite the great advances in the ability to collect three dimensional datasets, these datasets are still relatively small compared to the quantity of measurements required for reasonable resolution and statistical reliability [44]. He estimated that for the largest dataset measured at the time, the relative error of the grain boundary distribution at 1 MRD was approximately 53% at best. The relative error for the distribution at its peak was approximately 34%. These error estimates were made for a 5-dimensional grain boundary distribution which included both the boundary misorientation and plane orientation. Smaller datasets would likely result in higher estimates of relative error over the full boundary distributions. While the generated grain boundary distributions will require more measurements to reduce the approximate relative errors, triple junction distributions would require substantially more data. Despite the reduction in parameters of a twin-dependent triple junction, the data required for generation of a triple junction distribution is still approximately an order of magnitude greater than that for a grain boundary distribution. It may be concluded that if it is challenging for the three dimensional techniques to generate grain boundary plane distributions with an acceptable relative error, then they would be ineffective or impractical when the quantity of data must be increased an order of magnitude for twin-dependent triple junction distributions.

1.3. Advantages of a stereological approach

Despite the inability of current three-dimensional techniques to generate reliable triple junction distributions, the technology exists to generate these distributions through stereology. As defined by Russ, “stereology is the science of the geometrical relationships between a structure that exists in three dimensions and the images of that structure that are fundamentally two-dimensional”, [45]. In this instance, the two-dimensional images would be EBSD maps from a section plane through the triple junctions.

There are several advantages to characterizing a triple junction distribution by a stereological technique. Primarily, a stereological technique could supply the quantity of data necessary for statistical reliability. The nature of a three dimensional technique requires characterizing each microstructural feature from many progressive planes in order to measure the feature with a reasonable resolution. A stereological technique will typically require less time since each individual feature requires a single measurement. From a single measurement applied to many similar features, the three