Measuring twin dependent triple junctions from a single section plane

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Abstract. Given that polycrystalline triple junctions are significant contributors to material properties, they are frequently becoming the focus of emerging research. Despite this interest, the tools to quickly and quantitatively analyze triple junction textures remain severely limited. To enable characterization of triple junctions on a large scale, the parameters, space, and conventions of twin dependent triple junction distributions have been developed. In addition, by adopting grain boundary stereological techniques, triple junction distributions have been generated from a single section plane for triple junctions containing a coherent twin boundary. This methodology has been validated using simulated microstructures and, with further experimental development, will provide insight into actual triple junction structures. This technique also establishes the foundation for a generalized non-twin dependent approach in the future.

1. Introduction

A triple junction is a polycrystalline microstructural feature formed by the common intersection of three grains. As defined in this work, a fully characterized triple junction consists of three crystal lattices, three grain boundaries, and a triple line. Numerous studies indicate that triple junctions possess a host of junction-specific properties. These properties include exerting a drag effect on grain boundaries during grain growth [1], serving as prime locations for heterogeneous solute segregation [2], providing locations of rapid diffusion [3], and acting as favorable sites for heterogeneous nucleation [4]. This list is not all encompassing but provides a glimpse of the influence of triple junctions on material properties. These properties also appear to be character dependent, though in most cases the relationship is not well quantified. Triple junction distributions also demonstrate unique traits from grain boundary character distributions. It has been shown that the triple junction distribution is capable of describing properties of the grain boundary network, whereas the more common grain boundary character distribution is not [5]. It has been further shown that the triple junction distribution accounts for approximately 75% of the correlations within the grain boundary network [6]. The importance of these network descriptive properties is underscored by the consideration that many material properties are likely the result of the grain boundary network as opposed to isolated grain boundaries.

Triple junctions are three-dimensional structures, which complicates experimental characterization. Triple junctions are also composed of several geometrical features which requires a preponderance of measurements for minimal statistical reliability of distribution results [7]. Currently, this
dimensionality requires a quantity of measurements beyond what is experimentally practical from three dimensional characterization methods. Many times a simplifying model is utilized to reduce the junction dimensionality. While these models have at times been beneficial, they lack resolution and frequently rely heavily on poor assumptions such as the coincident site lattice model [8]. Clearly, if integrated materials engineering is to be performed, there is a distinct need for a relatively rapid and inexpensive method for fully characterizing triple junctions on a large scale.

2. Triple junction parameters and space

2.1. Reducing the triple junction parameters

As explained, a fundamental difficulty of characterizing triple junction distributions is their high number of parameters. These parameters require too many measurements for practicality. A triple junction may be parameterized by the following macroscopic parameters: the three crystal lattices by the orientations $g_A$, $g_B$, and $g_C$, the three grain boundaries by the normal vectors $n_1$, $n_2$, and $n_3$, and the triple line by the vector $t$. The crystal orientations are given by the Euler angles $\varphi_1$, $\Phi$, and $\varphi_2$ in the Bunge convention [9]. The vectors are given in spherical coordinates by the polar and azimuthal angles $\theta$ and $\varphi$. This results in 17 macroscopic parameters, 11 of which are independent. In order to reduce the number of parameters to a more measurable number, a coherent twin boundary may be introduced into the measured junction as demonstrated in Fig. 1. This distribution will be measured in FCC materials. As a coherent twin within FCC materials always points in a $\langle111\rangle$ direction, a reduction in parameters is made by rotating the coherent twin to the $\langle111\rangle$ direction. The twin boundary then becomes known. In addition, the symmetry across the twin boundary allows the three orientations to be determined by a single misorientation $g_{AB}$. The plane parameters are referenced from the internal coordinate system within Grain A, and consist of the $n_{1A}(\varphi_1, \theta_{1A})$ Plane 1 normal and the dihedral angle $\alpha$, between Planes 2 and 3. This reduces the number of independent junction parameters from 11 to six, which is within the capabilities of two-dimensional electron backscatter diffraction (EBSD) measurements.

2.2. The distribution space

The twin dependent triple junction distribution space is formed by the domains of the parameters and is depicted in Fig. 2. The six dimensional space has been broken into two three-dimensional spaces to enable visual inspection. It also conveniently separates the misorientation parameters from the grain boundary plane parameters. Each parameter is divided into equal discrete units forming unit volume cells within the distribution
space. As apparent in the figure, some of the parameters are implemented with a cosine function which forms equal volume cells within the space. This has been the common practice for discrete grain boundary distributions [10]. For the simulations presented here, a resolution of approximately 10 degrees is utilized and the parameters are divided accordingly.

Unlike grain boundary distributions, the triple junction distribution does not fill the plane parameter space. There are many variations of $n_1A(\phi_1A, \cos(\theta_1A))$ and $\cos(\alpha)$ which correspond to triple junctions with dihedral angles greater than 180 degrees. These are thermodynamically unfavorable and will not exist in actual microstructures. They are therefore treated as an empty region within the space. Inversion symmetries are removed from the plane parameters by always selecting the normal vectors such that they point in the same direction about the triple line. Grain $A$ is identified as the grain between the twin and the boundary with the minimum misorientation angle or $g_{AB}$. The coherent twin boundary, or $n_{2A}$, is selected such that it always points into Grain $A$. The other normal vectors then point in the same direction about the triple line as $n_{2A}$. A fundamental zone is a region of the parameter space where each unique triple junction is represented only once. Given crystal symmetries within Grains $A$ and $B$, there are many fundamental zones with equivalent triple junctions within the parameter space. A single fundamental zone must be designated in order to select a single set of parameters to represent each unique junction. A single fundamental zone is chosen by selecting the symmetrically equivalent misorientation with minimum misorientation angle and misorientation axis lying in an identified zone within the standard [111] stereographic projection. This is an adaptation of the method of selecting a fundamental zone for grain boundary planes [11].

### 3. Plotting triple junction distributions

A triple junction distribution formed from 500,000 simulated twin dependent junctions at a fixed misorientation is shown in Fig. 3a. The figure consists of slices through the plane parameter space at $\cos(\alpha)$ values moving into the page. Each stereographic projection is a projection of the $n_1A(\phi_1A, \cos(\theta_1A))$ parameter values. These figures are the southern hemispheres of the stereographic projections. The empty region within the parameter space is apparent in the projections. The raw distribution is plotted and the visible cells result in a pixelated appearance. $\cos(\alpha)$ values were selected at both ends of the distribution, at the approximate distribution center, and at the distribution peak which is located at $n_1A = [\bar{1}2\bar{1}]$ and $\cos(\alpha) = -0.73$ or $n_{3A} = [\bar{3}0\bar{1}]$. After generating a triple junction distribution it must be weighted by the inverse of a uniform random distribution (due to a sampling bias). This weights all values to their representative values in terms of multiples of a random distribution (MRD).

![Fig 3](image-url)
4. Measuring the distribution

In the section plane, the triple junction parameter $\cos(\theta_{1})$ is immeasurable. Given this value, all other values may be determined from EBSD measurements. By adopting Saylor’s stereological method for measuring five-parameter grain boundary distributions from a single section plane, $\cos(\theta_{1})$ may be determined and the twin dependent distribution generated [12]. To validate this application, a simulated distribution was developed as shown in Fig. 3a. 500,000 simulated triple junction measurements, as generated from EBSD on a section plane, were then produced from this known simulated distribution and the stereological method applied. The distribution as appears in Fig. 3b was that generated from the simulated section plane data at a fixed misorientation. While the peak shows some mild broadening, otherwise the technique produced a similar distribution. 500,000 measurements for a fixed misorientation are an order of magnitude larger than what may be practically measured experimentally, but this number clearly demonstrates the success of the technique. Successful results are obtained with less data but the distributions do not reach this same level of convergence.

5. Conclusion

The developed method will allow twin dependent triple junction distributions to be generated from EBSD measurements on a single section plane. No serial sectioning will be required. This work also establishes necessary foundational work for developing triple junction distributions. Not only will this work further efforts in integrated materials engineering but it prepares the way for a non-twin dependent approach in the future.

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