Extraction of grain boundary curvature from voxel-based representations of polycrystalline microstructures

Mingyan Wang, Shuang Wu and Carl E. Krill III
Institute of Functional Nanosystems, Ulm University, Albert-Einstein-Allee 47, 89081 Ulm, Germany
E-mail: mingyan.wang@uni-ulm.de

Abstract. Extracting the curvature of grain boundaries from 3D voxel-based representations of microstructure is challenging. Previous investigations have concluded that the accuracy of curvature estimation depends strongly on the degree of smoothing after a microstructure has been meshed. We find that best results are obtained when the degree of smoothing is determined on a boundary-by-boundary basis. Evaluating a voxelized representation of a Reuleaux tetrahedron of known boundary curvature, we establish that, for a given boundary, the optimal smoothing power minimizes the coefficient of variation (CV) of local curvature. We apply the minimum-CV criterion to the extraction of grain boundary curvatures from a measurement of polycrystalline Al-5 wt% Cu performed by 3D x-ray diffraction (3DXRD) microscopy. The results show that grain boundaries in this sample are surprisingly flat. Moreover, boundaries of larger area manifest lower curvature, while higher curvature values are observed solely for boundaries of smaller area.

1. Introduction
Grain boundary (GB) curvature is one of the most important morphological properties of any given microstructure. The product of GB energy and curvature serves as the driving force for grain growth [1], but it is the curvature alone that determines the direction in which a GB migrates. Now that polycrystalline microstructures can readily be characterized in 3D using techniques like focused ion beam nanotomography or 3D x-ray diffraction (3DXRD) microscopy [2–5], increased attention is being devoted to the extraction of accurate boundary curvature values from experimental data. The output of such characterization techniques is a voxel-based representation of microstructure, which presents difficulties for accurate curvature estimation. On the one hand, the boundaries themselves are specified in an implicit manner—as interfaces between 3D grain volumes—and, on the other hand, these interfaces exhibit roughness at the length scale of the underlying grid; the latter propagates, in turn, as errors in curvature estimation. Both issues must be addressed before any attempt can be made to relate extracted boundary curvature values to the properties of a given specimen.

In this regard, the software package DREAM.3D [6] is a promising tool, offering built-in functions for meshing grain interfaces and smoothing the mesh. It is necessary, however, for the user to tune various parameters in these functions, such as the smoothing power. The optimization of smoothing parameters was investigated by Zhong et al. [7], who applied
A Reuleaux tetrahedron has four spherical surfaces, each with a curvature of \(-1/R\), where \(R\) denotes the distance between vertices. (right) A Reuleaux tetrahedron embedded in a cubic box, with planar boundaries forming triple lines along edges of the tetrahedron.

DREAM.3D to simulated spherical grains having known boundary curvatures. These authors concluded that smaller test grains were better processed using lower smoothing powers, whereas larger spheres required higher smoothing powers. However, in real microstructures, the optimal smoothing power for a given boundary was not found to be correlated to the size of the grains meeting at that boundary \([7]\). Apparently, the optimal smoothing power is a property of individual boundaries rather than entire grains. Nevertheless, the authors of Ref. \([7]\) obtained satisfactory results using a set of smoothing parameters that worked well for the majority of GBs in an experimental dataset.

In this work, we propose a method for determining the optimal smoothing power on a boundary-by-boundary basis, based on findings derived from a voxel-based test structure similar in shape to a typical grain \([8]\). Then we apply the method to a polycrystalline Al-5 wt\% Cu specimen that was characterized by 3DXRD microscopy to determine the curvature of the sample’s boundaries and evaluate its dependence on boundary area.

2. Methods

To analyze voxel-based representations of microstructure, we employ DREAM.3D’s built-in function “Quick Surface Mesh” to generate a surface mesh of the imported data, after which all GBs are represented as surfaces composed of triangles. Vestiges of the voxelized nature of the input data can be seen in the “stepped” morphology of the GBs. Therefore, some form of smoothing must be carried out to recover the intrinsic shape of each boundary. Smoothing is implemented in DREAM.3D following the method described in Ref. \([9]\). The principal curvatures \(\kappa_1\) and \(\kappa_2\) are the eigenvalues of the Weingarten matrix \([10]\). The mean curvature \(H\) is defined as \((\kappa_1 + \kappa_2)/2\). In the DREAM.3D smoothing algorithm, the smoothing power is determined by the number of smoothing iterations, \(N\), as well as by the smoothing factor \(\lambda\), which governs how far a vertex is permitted to move from its original location during a single smoothing iteration. The final smoothing power is quantified by the product \(N\lambda\).

3. Results

3.1. Determination of boundary curvatures on the test structure

Instead of the spherical grain shape used in Ref. \([7]\), we validate our curvature analysis strategy against a test grain having the shape of a Reuleaux tetrahedron. The latter is defined by the intersection of four spheres of radius \(R\) that are centered on the vertices of a regular tetrahedron of side length \(R\) (figure \([1]\)). By construction, the curvature of each surface of the Reuleaux tetrahedron is \(-1/R\). We embedded the tetrahedral grain in a cubic box, dividing the surrounding space into four regions of equal volume by placing planar boundaries along diagonals of the cube faces and extending them inwards until they intersect the Reuleaux tetrahedron along
Figure 2. Influence of smoothing power on curvature estimation for the test structure with \( R = 40 \). The smoothing parameter \( N \) takes values of 25, 100 and 800 from left to right. Images in the top row show values of local mean curvature \( H \) for one of the surfaces of the Reuleaux tetrahedron. Corresponding distributions of \( H \) are plotted below, after excluding locations adjacent to triple lines; red curves are fits of Gaussian functions to the histograms.

its edges. All dihedral angles between boundaries meeting at triple lines are 120°, resembling the dihedral angles observed in real microstructures.

This construction was then mapped onto a cubic grid and imported into DREAM.3D. The voxel side length was kept at 1 for all test structures examined in this study. After the meshing step, the triangular mesh was subjected to DREAM.3D’s smoothing algorithm, whereby \( \lambda \) was set to 0.2 for each vertex of a surface triangle but reduced to 0.1 for vertices located at a triple line or quadruple point (to suppress shrinkage of the central grain during smoothing).

We first test the influence of smoothing power on the mesh by varying the number of iterations \( N \) (holding \( \lambda \) at the values specified above). In order to cover a wide range of smoothing power, \( N \) is set to 25, 50, 100, 200, 400 and 800. The influence of \( N \) is shown in figure 2 for one of the curved surfaces of the test structure with \( R = 40 \). Here, the surface is colored such that patches with extracted curvatures close to the true value \((-1/40 = -0.025)\) are green, while white and red patches denote under- or over-estimations of the magnitude of curvature, respectively. Curvature estimation is highly inaccurate close to triple lines, as evidenced by the preponderance of red patches at the edges of each surface. This finding is not surprising, given the abrupt change in surface orientation that occurs at a triple line. After excluding the latter regions, we generate histograms of the local curvature value \( H \) for the remaining triangles of the GB mesh. The mean and standard deviation of these histograms are found to vary strongly with \( N \). When \( N = 25 \), the overall degree of smoothing is inadequate, as indicated by the presence of reddish patches in the boundary interior. Raising \( N \) to 100 improves the uniformity of the extracted curvature values, but progressing to still higher values of \( N \) results in oversmoothing, with an increasing fraction of the boundary taking on a curvature close to zero.

To quantify these observations, we fit Gaussian functions to the histograms of figure 2 yielding average boundary curvatures \( \langle H \rangle \) of \(-0.0256\), \(-0.0250\) and \(-0.0163\) for \( N = 25\), 100 and 800, respectively; the corresponding relative errors are 2.4%, 0% and 34.8%. From this we conclude that the optimal smoothing parameter \( N_{opt} \) is approximately 100 when \( R = 40 \).

Intuitively, one might expect \( N_{opt} \) to be related to the resolution with which the surface in question is voxelized \([7]\)—e.g., to the ratio between the size \( R \) and the voxel size. Higher
resolution ought to yield a more accurate representation of grain boundaries, thereby better preserving their intrinsic curvature. We test this notion by allowing $R$ to take values of 20, 40, 80, 160 and 320, varying $N$ in each case from 25 to 800. In figure 3(a), we plot the absolute value of the relative error (RE) in curvature against $N$ for each $R$. As in the previous example (figure 2), the RE is found to be large when $N$ is either too small or too large. For each $R$, the optimal choice for $N$ is marked in figure 3(a) by a filled black circle. Clearly, $N_{\text{opt}}$ varies with the size of the tetrahedron, tending toward larger values with increasing $R$. This is consistent with the conclusion drawn by Zhong et al. [7] from spherical test structures of various diameters.

In a real microstructure, however, the effect of smoothing on a specific boundary is not directly correlated with the grain size [7]: after all, it is possible for any surface of a chosen grain to be highly curved or nearly flat. Since $N_{\text{opt}}$ cannot be chosen based on grain size, we must formulate a different strategy for optimizing the smoothing power—preferably one that can be applied to grain boundaries on an individual basis.

In all curvature histograms that we extracted from surfaces of the test structure, $N_{\text{opt}}$ was found to generate not only the smallest RE but also the narrowest distribution. To quantify the latter, we use the coefficient of variation (CV), which is defined as the ratio of the standard deviation $\sigma$ to the absolute value of the mean $|\mu|$, both extracted from a Gaussian fit. In figure 3(b) we plot CV against RE for different sizes of the Reuleaux tetrahedron. For each $R$, the point of minimum CV is marked by a filled black circle. These points coincide with the points of lowest RE in figure 3(a). We conclude that the minimum-CV criterion identifies smoothing conditions that lead to curvature estimation with a relative error below 5%.

3.2. Boundary curvatures of polycrystalline Al-5 wt% Cu

The curvature analysis procedure established in the previous section is now applied to an experimental dataset. A cylindrical sample of diameter 1.4 mm was cut by spark erosion from an Al-5 wt% Cu plate that had been cold rolled to 50% reduction in thickness, followed by heat treatment at 640°C for 20 min. The microstructure of this specimen was mapped in 3D by 3DXRD microscopy performed at the synchrotron radiation facility SPring-8. The morphology of individual grains was reconstructed from near-field diffraction patterns using the reconstruction routine described in Refs. [5,11,12]. The voxel size of the dataset is 5 $\mu$m.

Figure 4 shows a 3D mapping of the sample. The internal microstructure of the sample is visible in a cross section, in which GBs are marked in black: most of the latter are curved, but
some are nearly flat. We mapped a total of 942 grains and 5082 grain boundaries. Adopting the previous section’s method of curvature extraction, we plot the resulting curvature values as the blue histogram in figure 5. Most grain boundaries in the specimen are found to have rather small average curvatures, as the median of the curvature distribution is just $0.0016 \mu m^{-1}$.

4. Discussion
In Ref. [7], Zhong et al. held $N$ and $\lambda$ fixed while extracting the curvature of GBs from voxel-based measurements of austenitic and ferrite steel microstructures. Their choice of optimal smoothing power is equivalent to $N = 50$ in our study. In figure 5 we compare our variable-$N$ analysis of boundary curvature in polycrystalline Al-5 wt% Cu to curvatures determined using $N = 50$. The median value is nearly identical in the two cases ($0.0017 \mu m^{-1}$ for $N = 50$ vs. $0.0016 \mu m^{-1}$ for $N_{opt}$), but there is a difference for boundaries with $\langle H \rangle > 0.002 \mu m^{-1}$, which the fixed-$N$ approach systematically undersmooths, leading to an increased number of boundaries having larger curvature values compared to the distribution produced by our procedure.

The median value for $\langle H \rangle$ of $0.0016 \mu m^{-1}$ corresponds to a median radius of curvature of $\sim 630 \mu m$, which is 7.5 times larger than the specimen’s average (equivalent-sphere) grain radius of $84 \mu m$. We conclude that GBs in this sample are much flatter on average than would be expected simply by equating the average boundary curvature to the inverse average grain radius.
This finding agrees with the qualitative impression given by the cross section in figure 4, in which several nearly flat boundaries are visible.

Finally, in figure 6 we examine the relationship between GB curvature and boundary area. Although most curvature values are small, regardless of the boundary area, there is a clear trend (highlighted by the red dashed line) for boundaries of larger area to have smaller curvature. Likewise, whenever a boundary’s curvature is large, the corresponding area is small.

5. Conclusions
The software package DREAM.3D provides built-in functions for extracting grain boundary curvatures from voxel-based representations of 3D microstructure, but accurate values are obtained only as long as appropriate parameters are determined for the smoothing step that follows meshing of the input data. Using test structures based on a Reuleaux tetrahedron of various sizes, we validate a new method for choosing the best-performing smoothing conditions, finding that the most accurate curvature values are obtained when the coefficient of variation of a boundary’s curvature distribution is minimized. The method is applied to a voxel-based 3D mapping of polycrystalline Al-5 wt% Cu that was acquired using x-ray microscopy. In this sample, we find most grain boundaries to be relatively flat, with a median value of only 0.0016 μm$^{-1}$ for the overall distribution of boundary curvatures. We also discover that grain boundaries of larger area tend to manifest smaller curvature values, and highly curved boundaries are always small in area.

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