Viewpoint Paper

3D reconstruction of microstructure in a commercial purity aluminum

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Abstract—The topic of reconstruction of polycrystalline microstructures is briefly reviewed. An example is given of using orientation maps to reconstruct digital microstructures with a representation of a polycrystal structure that includes crystallographic orientation information. The method uses packing of ellipsoids to approximate the grain structure, coupled with Voronoi tessellation. For the example of hot rolled commercial purity aluminum that was chosen, the highly elongated grain shapes required stretching of the tessellation in order to match the observed aspect ratios.

Keywords: Microstructure reconstructions; Three dimensional; Aluminum; Texture; Voronoi tessellation

1. Introduction

There are many motivations for studying microstructures in all three dimensions (3D). There remain many gaps in our fundamental understanding of the characteristics of 3D microstructure and in appreciating the behavior of materials. Although the context for this article is that of inorganic materials, many of issues in characterizing biological specimens are identical. Thus it happens that applications of the science of obtaining quantitative information about microstructure in 3D from cross-sectional (or projected) data, i.e. stereology, are as important in biology as in materials science.1 This article is concerned with a particular aspect of 3D characterization, namely reconstruction of representative digital polycrystalline microstructures. To motivate this effort, it is straightforward to point out the practical reasons relating to simulation of material properties and materials processing. Most properties and processing of interest are inherently 3D in nature. Therefore any simulation should commence with appropriate initial conditions, which ought to include as accurate a description of the internal structure of a material as is required for the problem. Naturally not all problems are sensitive to microstructure and incorporation of microstructure incurs additional computational cost. However, most materials have non-trivial anisotropy in their properties. As for computational cost, the steadily increasing computing power available per dollar expended means that it is feasible to compute problems with millions of grid points on single central processing units. Although techniques exist that characterize a specific volume, these methods need a high level of expertise, are still under development, and are very time consuming. Noteworthy are 3D X-ray diffraction based methods [1,2] and automated serial sectioning [3]. Obtaining 3D digital microstructures from serial sections is itself a form of reconstruction although the main issue is that of alignment of the sections and interpolation. It should also be noted that 3D reconstruction based on images has been of interest to the composites community [4,5] for some time.

This article describes a method for generating a 3D polycrystalline microstructure that is representative of an experimentally characterized sample. It follows previous work in terms of ellipsoid packing [6] but describes the application of the Voronoi tessellation method for representing the grain structure. The input is from two...
orthogonal observations in the form of orientation maps of cross-sections of the polycrystalline sample. By approximating the grains as a set of optimally packed ellipsoids and transferring the grain structure to a Voronoi tessellation, a 3D microstructure was generated. Using the orientation distribution and misorientation distribution between nearest neighbor grains, the generated microstructure was overlaid with texture.

2. Experimental input

The input to the microstructure builder was in the form of electron back scatter diffraction (EBSD) maps [7]. An EBSD map is a list of pixels containing information about location in the form of \((x, y)\) coordinates and the crystallographic orientation at each point, typically in the form of three Euler angles [8]. The pixels can be aggregated into grains using a burn algorithm and a predetermined threshold misorientation between neighboring pixels. The EBSD maps provide information not only about the geometry, size and shape, of the experimental microstructure, but also of the crystallographic orientation (texture).

The experimental input to the microstructure builder consists of EBSD scans on two orthogonal planes, one perpendicular to the sample normal direction (ND) and the other perpendicular to the sample rolling direction (RD), Figure 1. The two scans must be on orthogonal planes to get the full form of distribution on the ellipsoid shape distribution function. The sample axis 1, \(X\), \(e_1\) is \(\parallel\) to the RD, sample axis 2, \(Y\), \(e_2\) is \(\parallel\) to the transverse direction (TD), and sample axis 3, \(Z\), \(e_3\) is \(\parallel\) to the ND. A third section would provide information that could be used to check the size distribution. The ellipsoids used here are assumed to have their semi-axes aligned with the specimen axes although the method allows for the ellipsoid orientations to vary (an as yet untested option).

3. Representation of grains by ellipsoids

The basic assumption, as stated earlier, is that the grains can be approximated as ellipsoids. Each ellipsoid can be completely described by its semi-axes

\[
\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} \leq 1
\]  

Assuming that there is no gradient in grain size through the sample and that the ellipsoids have the same orientation, then a homogeneous distribution of ellipsoids \(f(a, b, c)\) is sufficient to represent the grain size and shape distribution. Even though the full form of \(f(a, b, c)\) is impossible to calculate, one can approximate or estimate it by

\[
f(a, b, c) = f(a, b) \cdot f(c|b)
\]

Both \(f(a, b)\) and \(f(c|b)\) can be obtained from the set of orthogonal orientation scans. The procedure to obtain these is described in detail elsewhere [6].

The simulation domain is in the form of a cubical box whose dimensions are \(1 \times 1 \times 1\). This box is populated with a sampling of ellipsoids drawn from the distribution \(f(a, b, c)\). For this purpose the distribution function \(f(a, b, c)\) must be scaled appropriately. The values of the semi-axes \(a, b\) and \(c\) must be expressed in terms of fractions of the box size, in this case 1. The scaling factor is determined by the total number of grains desired in the final microstructure. For example, consider a microstructure with 1000 mono-dispersed equixed grains, that is \(a = b = c\) and \(f(a, b, c)\) is the delta function. The values of \(a\), hence \(b\) and \(c\), are picked such that

\[
1000 \times (\text{volume of a ellipsoid}) = 1
\]

\[
(\text{volume of a ellipsoid}) = \frac{4}{3} \pi \times a^3
\]

giving \(a \sim 0.05\).

For each ellipsoid generated the semi-axes are chosen from the given distribution function. This can be done by generating values for \(a', b'\) and \(c'\) such that, \(0 > a' \geq a_{\text{max}}, 0 > b' \geq b_{\text{max}}\) and \(0 > c' \geq c_{\text{max}}\), respectively. Next a random number, say \(r_1\), is generated. The choice of \(a', b'\) and \(c'\) is accepted if \(f(a', b', c') \leq r_1\).

4. Packing of ellipsoids

Out of this set of ellipsoids only a minimal subset is retained such that it optimally fills the simulation box. An optimal filling is defined as a system having minimal overlap and maximum space filling. This could be achieved by solving a many-body dynamics problem, q.v. Ref. [9]. Since there is no theory to indicate a unique solution to this problem, however, the approach discussed here uses Monte Carlo integration to approximate the packing.

A simulated annealing algorithm was used to choose a subset of the ellipsoids by minimizing the system energy. The algorithm proceeds in the following manner. A random subset of the ellipsoids is chosen from the
original set such that the total volume contained in the subset is about the same as the box volume. The total energy of the system is evaluated where the energy is calculated in terms of overlap and gaps between the ellipsoids contained in the simulation domain [6]. This energy is then minimized by a series of add, subtract, swap and jog transactions. Any transaction that reduces the energy is accepted. If a transaction increases the energy then it is accepted with a certain probability depending on the amount of increase (which is a user input). The transactions allowed are addition where a randomly chosen ellipsoid is added to the existing set; subtraction is where a randomly chosen ellipsoid is taken out of the set; swap is where a randomly chosen ellipsoid in the set is replaced by another randomly chosen ellipsoid not in the set; and jog is where a randomly chosen ellipsoid is replaced by another ellipsoid contained in it.

The procedure discussed above generates an optimal set of ellipsoids which forms the grain structure in the final microstructure. There may be regions within the simulation box that are contained in more than one ellipsoid and others that are not contained in any. To overcome this difficulty, the cellular automaton (CA) approach [6] can be used. In the CA the centroids of the ellipses are used as nucleation sites and the grains are allowed to grow until they impinge and the total space is filled. Even though this automatically eliminates overlaps and empty space in the box, the output is not a periodic structure but it can easily be made to be so. The approach discussed in the next few sections uses a Voronoi tessellation based approach to generate a non-overlapping and space filling microstructure.

5. Voronoi diagrams

As stated previously we are interested in generating a non-overlapping space filling structure. This is accomplished by utilizing the properties of the Voronoi diagram $V(P)$. The Voronoi diagram divides the space into Voronoi regions, which by definition is a non-overlapping set. The method used to compute the Voronoi diagram utilizes Delaunay triangulation, which is a straight line dual of $V(P)$. Computation of Voronoi diagrams was carried out with the qvoronoi program from http://www.qhull.org/. To generate the Voronoi regions the space is sampled randomly with points, so call this set $S$. For each of the sampled points in $S$, the number of ellipsoids, from the set $E$ (as defined above), that it is contained in can be calculated. Out of these sampled points, only those contained in one and only one ellipsoid are retained. That is, if a point is contained by more than one ellipsoid, or is contained in neither, it is eliminated from $S$. Using this set $S$ we construct the Voronoi diagram $V(P)$. All the Voronoi regions associated with the points in the input set $S$ which do not lie on the convex-hull of $S$ are bounded. This implies, however, that the points on the convex-hull of $S$ are unbounded. To overcome this problem and also to generate a periodic structure the input set $S$ is modified as described below. As described earlier to generate the set $S$ we sample the space, which we will call $R$. $R$ is a bounded box as defined by user. For purpose of outlining the method say it is a box bounded by the $x = 0; x = X; y = 0; y = Y; z = 0$ and $z = Z$ planes. Hence the points in $S$ are bounded by (0,0,0) and (X,Y,Z). For every point $p_i$ in $S$, 26 copies are generated by adding or subtracting $X$ or $Y$ or $Z$ to the coordinates of $p_i$. That is, if the coordinates of $p_i$ are $(x_i,y_i,z_i)$ then the copies of $p_i$ are $(x_i - X,y_i - Y,z_i - Z)$, $(x_i - X,y_i + Y,z_i)$, $(x_i + X,y_i - Y,z_i + Z)$, $(x_i + X,y_i + Y,z_i)$, $(x_i - X,y_i,z_i - Z)$, $(x_i - X,y_i + Y,z_i - Z)$, $(x_i + X,y_i - Y,z_i), (x_i + X,y_i + Y,z_i - Z)$, $(x_i - X,y_i,z_i), (x_i + X,y_i,z_i)$, $(x_i - X,y_i + Y,z_i)$, $(x_i + X,y_i - Y,z_i)$, $(x_i + X,y_i + Y,z_i)$. As a result the points which were on the convex hull of $V(P)$ are now interior points and hence the Voronoi regions associated with them are all bounded.

Figure 2 illustrates this in two dimensions. The original space from which 20 points were chosen randomly is the central highlighted square. This square is padded from all the sides with its eight nearest, first and second, neighbors. These are populated by making copies of the points, already selected, displaced in one or both the orthogonal directions by the size of the box. To demonstrate the effect on the points on the convex hull and the periodicity, consider the point, $p$, bounded by the box and contained in the central square. The box around it is the Voronoi region associated with it, obtained by drawing the perpendicular bisectors between $p$ and its nearest neighbors. This would have been unbounded if $p$ were on the convex hull. Now corresponding to $p$ there are eight more copies. The one of the most interest, however, is the one contained in square directly above it, that is in square “1”, label it “$p’$”. The Voronoi region associated with $p’$ is clearly not contained in the bounding box, square “0”. At the same time the Voronoi region $V(p’)$ is not contained entirely in “1” and some of it “leaks” into “0”. This is an exact replica of the part of $V(p)$ which lies outside the box “0” but is displaced by the box height. Thus it appears as if the Voronoi

\[ \begin{array}{cccc}
0 & 1 & 2 & 3 \\
4 & 5 & 6 & 7 \\
8 & & & \\
\end{array} \]

Figure 2. Illustration of a periodic structure applied to a Voronoi tessellation.
region associated with \( p \) is continued at the top of the box. It is easy to see that the same would hold true for any other point on the convex hull. Now if only the original square, “0”, is retained (after constructing \( V(P) \) on the extended space) then we obtain a network of Voronoi cells (regions) which are periodic in the box length.

6. Grain assignment

As stated in section above, the space is sampled and only points that lie inside one and only one ellipsoid are retained. Hence it is possible to assign every point in \( S \) to an ellipsoid. After constructing the Voronoi diagram on the extended set \( S' \) the resulting Voronoi regions have a one to one correspondence to the points in \( S \). That is, for every Voronoi region \( V(p_j) \) there is a unique point \( p_j \) in \( S \). Hence the Voronoi regions/cells can also be assigned to ellipsoids in \( E \). These Voronoi regions can be aggregated into grains by assigning them to an ellipsoid. For example if ellipsoid \( E_m \) in \( E \) contains points \( p_1, p_2, \ldots, p_k \) and hence the Voronoi regions \( V(p_1), V(p_2), \ldots, V(p_k) \) are aggregated to form a single grain, with grain id \( m \). Thus all the Voronoi cells can be aggregated to form a set of grains.

As the cells themselves are non-overlapping and space filling, the grains are just collections of cells, are also non-overlapping and are space filling. Also, since the grains are roughly similar to the ellipsoids in the set \( E \), they have a similar shape and size distribution as dictated by distribution function \( f(a, b, c) \). The detailed quantitative relationship between these distributions has, however, yet to be determined. The output microstructure obtained is in terms of Voronoi vertexes, edges, and patches. The volumes of each subset of Voronoi cells that represents a grain are obtained and used in the orientation assignment described below for calculating the orientation distribution. The areas between each pair of grains are also calculated and used in the orientation assignment for the calculation of the misorientation distribution. If desired one can convert it to a regular grid in the following manner:

1. Sample the box on a regular grid. For example, insert points along the \( X \) axis with a step size of 1.
2. For every point find the Voronoi region and hence the grain that it is contained within.
3. Assign each point the grain id.

7. Texture assignment

Once the microstructure has been generated, orientations are assigned to the individual grains to generate a texture using the approach discussed by Miodownik et al. and Saylor et al. \([6,10]\). The assumption made is that the crystallographic texture for the entire polycrystalline material can be sufficiently summarized in terms of the orientation distribution function (ODF) and the misorientation distribution function (MDF) across grain boundaries. Also the orientations are assumed to be uncorrelated past the first nearest neighbor; orientation correlation functions have, however, been explored and appear to be a reasonable approach for imposing such correlations on reconstructed microstructures \([11,12]\).

8. Application to aluminum alloy 1050: experimental observations

Figure 3 shows two orthogonal views of the commercial purity Aluminum sample that was to be modeled \([13]\). The planar view is of a section perpendicular to the sample ND and the transverse view is of a section perpendicular to the sample RD. The EBSD maps were obtained in a Phillips FEI XL40 field emission gun scanning electron microscope using the TSL\textsuperscript{TM} EBSD software. The first conclusion one can draw by visually inspecting the microstructure is that the grains are extremely elongated along the rolling direction. After analyzing the microstructure the grains were shown to have semi-axes ratios of approximately \( >20:4:1 \). The material also shows the expected rolling texture components, \( S \), brass and copper, along with some amount of cube component. About 32\% of the texture could not be resolved into any of the standard texture components for aluminum.\(^4\)

9. Geometrical stretching

Due to the memory constraints on a serial machine and the design of the algorithm there is a limit on how many grains can be included when generating a microstructure. Also, if the experimentally observed microstructure has elongated grains then it puts additional constraints on the microstructure builder. One could solve this problem while still working within the framework of the microstructure builder by parallelizing the code. This, however, would have been a time intensive solution. The other way is to get around it is by generating a slightly non-equiaxed structure and then subject it to an affine expansion. The microstructure builder can be broken down into four parts. These are summarized in Table 1. The first three steps are carried out the same way as described earlier. The output of step three (tessellation) gives the Voronoi cells which are then aggregated to from the grain structure in step four. We expand the Voronoi cells by scaling the vertexes forming the cell appropriately. For example let the desired stretching by \( 5 \times 2 \times 1 \) along the RD, TD and ND, respectively. To achieve this stretch each set of vertex co-ordinates of each cell are multiplied by a \( (5,2,1) \) stretch, assuming that the RD is \( \parallel X \) axis, the TD is \( \parallel Y \) axis and the ND is \( \parallel Z \) axis.

\(^3\)Even though the point \( p_j \) is contained in ellipsoid \( E_m \), the associated Voronoi region \( V(p_j) \) need not be entirely contained in \( E_m \).

\(^4\)We used a 15° disorientation from the exact location of a component as the criteria for binning.
10. Simulated microstructure

In this example, the initial input to the microstructure builder was a list of ellipsoid centers sampled from a $1 \times 1 \times 1$ box. Even though the observed semi-axes ratio was $>20:4:1$, it was not possible to generate a microstructure with a large number of grains having a distribution with an average semi-axes ratio of $>20:4:1$. Hence initially a microstructure with semi-axes with a ratio of $3 \times 2 \times 1$ was generated which was then subjected to an expansion of $5 \times 2 \times 1$.

Each ellipsoid was assigned values for the semi-axes drawn from a flat distribution centered around an average value of $(0.09, 0.06, 0.03)$. The center coordinates are chosen using the following scheme. Choose an arbitrary point in the box as the coordinates of the center of an ellipsoid. Compare the box size with the minimum of the semi-axes lengths of said ellipsoid. If the box size is greater than twice the minimal semi-axis then divide the box into eight quadrants and re-sample, that is, add another, new, ellipsoid (for each quadrant) to the list. This procedure is repeated by subdividing each of the boxes recursively until the box size is less than or equal to a user input fraction (default value set at 0.333) times the minimal semi-axis length. Figure 4 illustrates the above by means of a flow diagram.

**Table 1. Microstructure builder steps**

<table>
<thead>
<tr>
<th>Step no.</th>
<th>Description of step</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Extraction grain geometry from the EBSD maps</td>
</tr>
<tr>
<td>2</td>
<td>Generation of a optimal set of ellipsoids</td>
</tr>
<tr>
<td>3</td>
<td>Tessellation</td>
</tr>
<tr>
<td>4</td>
<td>Grain aggregation from the tessellation</td>
</tr>
</tbody>
</table>

**Figure 3.** Deformed microstructure from experimental observation on the Al-1050 sample, (a) in the rolling plane and (b) in a cross-section normal to the RD.

**Figure 4.** Flow diagram illustrating the process of population of ellipsoids.

**Figure 5.** Simulated microstructure (output of the microstructure builder).
Using the above set of ellipsoid centers as input we selected a subset which had maximal space filling and minimal overlap. The set of ellipsoids thus generated was then padded from all sides by half the box size, following the scheme as discussed above, to form an input to the tessellation. The Voronoi cells were then grouped to form the final microstructure.

Figure 5 shows the simulated microstructure after the stretching. The microstructure depicted has of order 800 grains. Using the procedure described by Saylor et al. [6] orientations were assigned to the grains in the microstructure. Figure 6(a,b) shows a comparison of the input texture and the final orientation distribution after the fitting process was complete. The fitting process decreased the relative error by a factor of 100. Figure 6(c) shows the MDF of the input.

11. Summary

The application of the microstructure builder method to a specific material has been described that produces a 3D digital microstructure. A method for producing highly elongated grain shapes has been given in terms of taking an initial tessellation that may or may not have some finite grain shape and applying an affine stretch in order to produce arbitrarily large aspect ratios. The example given contained less than 1000 grains but despite the small number, a reasonable fit to the texture was obtained. The digital microstructure thus obtained was subsequently used as input for simulation of recrystallization which will be described in a forthcoming paper.

References