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Application of chord length distributions and principal component analysis for quantification and representation of diverse polycrystalline microstructures

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ABSTRACT

Quantification of mesoscale microstructures of polycrystalline materials is important for a range of practical tasks of materials design and development. The current protocols of quantifying grain size and morphology often rely on microstructure metrics (e.g., mean grain diameter) that overlook important details of the mesostructure. In this work, we present a quantification framework based on directionally resolved chord length distribution and principal component analysis as a means of extracting additional information from 2-D microstructural maps. Towards this end, we first present in detail a method for calculating chord length distribution based on boundary segments available in modern digital datasets (e.g., from microscopy post-processing) and their low-rank representations by principal component analysis. The utility of the proposed framework for capturing grain size, morphology, and their anisotropy for efficient visualization, representation, and specification of polycrystalline microstructures is then demonstrated in case studies on datasets from synthetic generation, experiments (on Ni-base superalloys), and simulations (on steel during recrystallization).

1. Introduction

Material structure, i.e., *microstructure*, plays an essential role in guiding all materials innovation efforts aimed at improving the property combinations [1,2]. One of the central challenges in the field comes from the lack of rigorous approaches for the quantification of the microstructure. Our focus in this work is on the microstructures encountered in metallic samples, where the shape and size distributions of the individual grains (i.e., volumes of uniform crystal lattice orientation) dominate the microstructural considerations. These polycrystalline microstructures are typically studied at length scales in the range of 0.1 to 100 μm, where the grains are separated by grain boundaries. The grain structure in polycrystalline materials is naturally associated with a number of potential measures of the microstructure that can be used in the effort to capture its salient features. These measures include distributions of sizes, shapes, and orientations of grains and their interfaces [3–5]. In this work, we focus our attention on the rigorous quantification of the grain size and morphology characteristics because of their anticipated strong impact on a range of mechanical and physical properties [6–14]. One such well-known effect is in the dependence of the effective yield strength of the material on the average grain size (e.g., Hall–Petch laws [6,7]). While there is general agreement on the importance of the grain size in controlling the properties of the material, the exact definitions, measures, and characterization techniques used in the quantification of the grain size vary significantly among the practitioners. For example, given a microstructure image, protocols employed in practice include estimations of the grain size based on either intercept lengths or grain areas/volumes or grain boundary lengths/areas, which contributes to inconsistencies in the reports of the average grain size.

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Area-based estimations of the grain size are becoming the methods of choice in modern characterization efforts that yield digital pixelated datasets (e.g., digital optical micrographs, back-scattered electron images from scanning electron microscope, electron back-scattered diffraction maps). Grain areas can be readily extracted from such datasets by simply counting the number of pixels contained in each grain. Once the grain area is known, it is common practice to estimate the grain size as the diameter of an equivalent circle (henceforth referred to as the grain diameter) of the same area as the grain. The use of the grain diameter thus implicitly assumes that the grain shape is close to a circle. Similar approaches are being adopted for 3-D datasets, in which grain diameter can be obtained from the average grain volume and the consideration of an equivalent sphere [15,16]. The diameters of individual grains are typically averaged to provide for a scalar measure of the grain size of the material. As an extension of this approach, grain diameters are also often reported as distributions (i.e., histograms) that quantify the number fraction or the area fraction for each discretized bin of grain diameters [17]. Alternatively, some authors have fit the sampled grain diameters to log-normal distributions [18,19,11,12].

Despite its utility and wide adoption, the use of grain diameter leads to a loss of information regarding the distributions of grain shape and its alignment. Within the area-based approaches, some efforts have accounted for the grain shape by fitting the grain areas to equivalent ellipsoids (instead of circles/spheres) [20,3], and obtaining distributions of the major axis length, the minor axis length, and their inclination angles (e.g., [21]). The fundamental limitation of these approaches is that the grains in many samples do not really fit any specific idealized shape. This is particularly the case in microstructures of solidified [22], welded [11,12], or additively manufactured metals [16].

The approaches of estimating the grain size based on intercepts (or chords) have the potential to overcome the limitations of the area-based approaches described above. Grain size estimations based on chord lengths have a long history going back to early methods for metallographic observations [23]. Furthermore, chord length distribution (CLD), which describes the probability of finding chords of a specified length in the microstructure [24], is expected to be highly relevant to properties related to free paths in heterogeneous materials (e.g., plastic properties [4,8,9], transport properties [24,25]). Chords are defined as line segments traversing the entire grain, which originate on one grain boundary and end on the next grain boundary encountered. Chords are typically sampled by placing test lines on the microstructure, and either measuring distances between intersections of the test lines and grain boundaries or counting the number of such intersections [26]. In most reported studies, chord lengths were sampled either in randomly selected directions [26–28] or in a few specifically selected directions (e.g., along principal axes of the microstructure image [29,11,12]). For example, Lehto et al. [11,12] developed an image processing algorithm to obtain chord lengths in four directions of the microstructure (0°, 45°, 90°, and 135°, with subsequent averaging according to the standard [27]) to obtain the average grain size as well as its spatial variations in highly heterogeneous samples of welded steel.

A limited number of prior studies [8,9,30] have targeted chord lengths in directions beyond the principal axes. Fromm et al. [8] introduced a grain size and orientation distribution function (GSODF) that was evaluated using chord lengths in specific directions in each grain related to its slip systems. The grain size estimated in this manner was incorporated into a Taylor-type polycrystal plasticity model of h.c.p. α-Ti to study the effects of crystallographic texture and grain size distribution on the macroscopic mechanical response of the material. Sun and Sundararaghavan [9] extended the above concept by accounting individually for the available slip lengths for each slip system in a selected grain and modeled its evolution during the imposed large plastic strains on the sample. Turner et al. [30] presented a scan-line approach to computationally efficient calculations of CLDs for the full range of directions in 2-D and 3-D microstructures, and demonstrated their approaches on a number of composite microstructures. Their algorithm scans over all pixels of digital microstructure images and simply counts the number of voxels inside every microstructure constituent along the scan line. While such pixel-based computations are straightforward along the principal axes of microstructure images, other directions require special treatment such as the use of Bresenham lines [31].

In this contribution, we approach the quantification of the grain structure in metallic samples using angularly resolved CLD and its low-rank representation using principal component analysis (PCA). In this effort, we will develop and utilize an approach that takes advantage of the grain boundary segments that can be identified and extracted from modern characterization techniques such as electron back-scattered diffraction (EBSD) [3]. This method of CLD calculations offers an alternative to the scan-line approach [30] mentioned earlier that identifies boundaries only indirectly by the changes in phase content (or grain orientation) between neighboring pixels. A potential advantage of explicitly representing the grain (or phase) boundary segments with continuous coordinates is that it lends itself to easier conversion to a conformal finite element mesh [32] for the analyses of mechanical response. The second contribution of this work is in the extraction of the low-dimensional representations that are likely to be highly valuable in at least two aspects: (i) classification and visualization of large and diverse ensembles of microstructures, and (ii) the formulation of data-driven process–structure–property linkages [33–36]. In this work, we will focus mainly on the viability of using PCA as an effective dimensionality-reduction strategy in the classification of a diverse set of grain morphologies in polycrystalline microstructures.

2. Angularly Resolved Chord Length Distribution

2.1. New Boundary-based Approach for CLDs

In the present study, we develop and employ an approach based on geometrical considerations of boundary segments in the microstructures being studied. Boundary segments, defined as straight segments between two adjacent points along a grain boundary, can be extracted from routine post-processing of datasets obtained from both experiments (e.g., grain boundaries established by thresholding misorientations in EBSD maps) and simulations (e.g., grain boundary contours tracked by recrystallization simulations [37]). At the core of the approach presented here is the computation of coordinates of intersection points between test lines and boundary segments.

We start by considering two arbitrary line segments, *AB* and *CD*, in 2-D space with end points $\mathbf{A}(x_A,y_A)$, $\mathbf{B}(x_B,y_B)$, $\mathbf{C}(x_C,y_C)$, and $\mathbf{D}(x_D,y_D)$, respectively. The parametric equations describing all the points on these line segments can be expressed as [38]:

$$\mathbf{P}_{AB} = \mathbf{A} + t_{AB}(\mathbf{B} - \mathbf{A}), \tag{1a}$$

$$\mathbf{P}_{CD} = \mathbf{C} + t_{CD}(\mathbf{D} - \mathbf{C}), \tag{1b}$$

with $t_{AB} \in (0,1)$ and $t_{CD} \in (0,1)$.

The coordinates of the intersection point between the two segments can be found by setting $\mathbf{P}_{AB} = \mathbf{P}_{CD}$, which yields a system of two linear equations (corresponding to two coordinates in two dimensions) with two unknowns, t_{AB} and t_{CD}. Bourke [39] provided solution for the problem as follows:

$$t_{AB} = \frac{(x_D - x_C)(y_A - y_C) - (y_D - y_C)(x_A - x_C)}{(y_D - y_C)(x_B - x_A) - (x_D - x_C)(y_B - y_A)}, \tag{2a}$$

$$t_{CD} = \frac{(x_B - x_A)(y_A - y_C) - (y_B - y_A)(x_A - x_C)}{(y_D - y_C)(x_B - x_A) - (x_D - x_C)(y_B - y_A)}, \tag{2b}$$

which gives the coordinates of the intersection point, $\mathbf{T}(x_T,y_T)$, as

$$x_T = x_A + t_{AB}(x_B - x_A), \tag{3a}$$

$$y_T = y_A + t_{AB}(y_B - y_A). \tag{3b}$$