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Integral mean curvature analysis of 3D grain growth: Linearity of dV/dt and grain volume

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Abstract The volumetric growth rate of individual grains has been found to be directly proportional to the individual grain volume V as $dV/dt = \beta(V_0\text{-}V)$. This simple result is explained through the DeHoff relationship $dV/dt = -kM_S$ between growth rate and the integral mean curvature of individual grains, M_S, combined with the experimentally observed relationship between M_S and grain volume, $M_S = \alpha(V_0\text{-}V)$. These relationships have now been observed consistently in both 3D grain growth simulations and experiments. This paper describes the relationships among these kinetic and geometric grain characteristics that provide this simple description of 3D grain growth.

1. Introduction

Grain growth models have historically focused on the change in the average linear grain size $\bar{D}$, perhaps because that was essentially the only parameter previously available for describing the process, i.e., through the line intercept count. Unfortunately, this viewpoint of studying the average behavior of growing and shrinking grains masks the important geometric details of what drives and controls the processes that occur. Recent experimental and theoretical developments have led to a new and surprisingly simple picture of grain growth. The advent of 3D methods such as DCT and computer modelling enable imaging and following the change in volume of grains that describes their growth and shrinkage rates, not previously possible. New theoretical developments have particularly involved the application of integral mean curvature of grains, M_S, to describe these volume changes resulting from curvature driven boundary motion. This descriptor, which was previously unattainable for 3D grains, can now be easily computed from the images produced by the above 3D experimental methods.

1.1 Integral mean curvature, M_S

The integral mean curvature M_S [1-3] of a grain boundary is the integral of its mean local curvature H over the surface area of a grain boundary, i.e., the product of the average mean curvature of the boundary $\bar{H}$ and the total surface area,

$$M_S = \iint H\, dS = \bar{H}S \quad (1)$$

and is defined through the sign of H as negative for concave faces, typical of relatively large, many-faced grains, and positive for smaller convex few-faced grains. Large grains with relatively large surface and sharply concave faces have large negative values of M_S, while intermediate sized grains have relatively flat faces with $M_S \cong 0$ and small concave grains have smaller, positive values of M_S.

2. Experimental methods

The examples throughout this paper of the relationships that have been experimentally found between growth rate, grain volume and M_S, have been obtained through both 3D computer simulations and LabDCT studies [4, 5]. These methods are described below.

2.1 3D Monte Carlo grain growth studies

3D kinetic Monte Carlo simulations were performed on the SPPARKS [6] platform using a simulation temperature of $kT = 0.5$ and periodic boundary conditions. Large 500^3 voxel arrays were used to produce large numbers of grains for good statistical averaging of the measured grain characteristics. These large initial numbers are necessary to allow for the large fraction of grains that are lost in the early transient stage of grain growth preceding the stable self-similar stage in which the analyses are performed.

The starting simulation grain structures were synthesized using DREAM3D [7] with initial grain volume distribution widths of $ln\sigma = 0.3$. This width, typical of grain structures in the self-similar state, enabled achieving stable grain growth early in the process while many grains were still present. Simulations typically ran for approximately 100 Monte Carlo equivalent seconds since this amount of time captured the necessary information during stable grain growth, starting at 10-20 seconds.

2.2 Laboratory DCT studies

Laboratory grain growth studies were also performed employing DCT imaging of grains in a real material, Armco iron, to test the validity of the relationships found in the prior simulations. These studies proved exciting in that they confirmed the exact trends and relationships found previously. The excellent comparison of such disparate methods validates both techniques for detailed geometric and kinetic studies such as these.

2.2.1 Material preparation. Low carbon Armco iron with a single-phase ferrite grain structure was employed as the experimental material for these studies. The grain sizes of the as-obtained hot-rolled strips were refined by cold working either 50 or 75%, for different portions of the study, respectively, and giving recrystallization and grain growth anneals for several hours at 880°C to produce an initial mean grain intercept of approximately 75μm, the minimum allowable for the following laboratory X-ray Diffraction Contrast Tomography (LabDCT [5]) analysis. Strips of the prepared Armco iron were electro-discharge machined to form cylinders with a 1mm diameter without surface damage.

2.2.2 DCT analysis. The DCT scans of the Armco iron specimens were performed using a ZEISS Xradia 520 Versa with LabDCT. 3D grain reconstruction was performed using GrainMapper3D and volume and face measurements were performed. Multiple scans, each covering an area of 0.3mm length, 0.3mm width, and 1mm height were taken at adjacent positions and stitched together, to increase the number of grains included in each analysis [8]. For both the 50 and 75% cold worked specimens a total of 14 volumes were scanned covering five different annealing states. Figure 1 shows a typical scanned image of the specimen.

Subsequent 880°C anneals of ~8hr were given to produce incremental growth steps, after which DCT scans were performed to image individual grains and obtain their volumes, *dV/dt*, and M_S.

2.3 Determination of M_S

Several methods have been developed in recent years for determining M_S of individual grains and grain size or face classes from 3D images. Although the methods vary greatly in application, they show surprisingly good comparison. These methods are described below.

2.3.1 Rowenhorst method. Rowenhorst, et al. [9] performed the first measure of M_S of individual grains using a serial sectioned titanium alloy. After reconstruction, meshing and smoothing values of M_S were computed from the triangulated structure using equation (2a),

$$M_S = 1/2 \sum \chi \, dl \tag{2a}$$

$$= \frac{\pi}{4}(O - I) \tag{2b}$$

in which χ is the angle between face normals of pairs of contacting triangles and *dl* is the length of their shared edge. Equations (1) and (2) are equivalent except that in (1) M_S is computed for a smooth face while (2) sums the integral mean curvature contributions of the edges making up a non-smooth face.

2.3.2 DeHoff and I-O methods. Other methods for computing M_S have since been developed, including (a) the stereological method of DeHoff [10], employing measures of the areas and numbers of edges on 2D grain sections for grains identified by their 3D volume or face class, and (b) the Innie-Outtie *(I/O)* method [11], applicable to voxelated structures and with M_S computed from Eq.(2b). This latter technique is based on the same principles as Rowenhorst's, treating a surface as a network of flat facets bounded by edges, but requires no smoothing or meshing of the surfaces.

Here, Innies *(I)* are the numbers of edges between pairs of inward angled (concave) voxel faces and Outties *(O)* are the numbers of voxel edges between outward angled (convex) faces. These numbers can be computed via computer code on either an individual grain face or over an entire grain. Convex faces have a majority of *O*-edges, giving positive M_S, concave faces have a majority of *I*-edges and negative M_S and flat faces have similar *I* and *O* values with $M_S \cong 0$. Equation (2b) derives from (2a) for the special case of all edges having a length of unity and all edges having dihedral angles χ of either $+\pi/2$ for *O*-edges or $-\pi/2$ for *I*-edges, as occurs with voxelated structures from simulations or reconstructed DCT images.

The current studies have employed both the DeHoff and *I-O* methods. Figure 2 shows the close comparison between the Rowenhorst and the I-O methods after normalizing M_S by size to make it unitless, which enables comparison of grains of different relative scales such as these. Note that the plot shows $M_S = 0$ for grains with ~15 faces, which are often assumed to be fairly flat-faced and is essentially linear as will be discussed later.

$$M_S\,norm = M_S / V^{-2/3} \tag{3}$$

3. Integral mean curvature driven growth rate of individual grains

3.1 DeHoff model of dV/dt vs. M_S

The recent DeHoff model [10] of integral mean curvature driven grain growth has provided a simple assumption-free description of the rate of volumetric growth or shrinkage of individual grains or grain classes of similar size or number of faces:

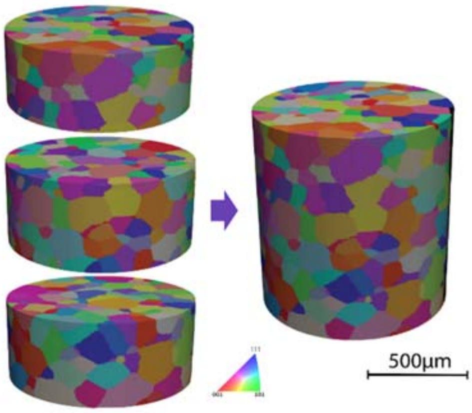

Figure 1. Image of LabDCT scanned Armco iron specimen reconstructed from stitching several individual scans to maximize the analysis volume [7,8].

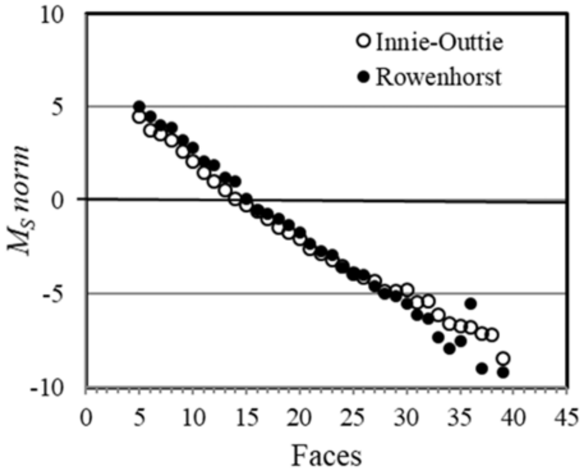

Figure 2. Comparison of the Rowenhorst and I-O methods for determining M_S. Data are for individual grains grouped by face class. The M_S values have been normalized by size to make unitless for comparing grains of different scales.

$$dV/dt = -k\, M_S \tag{4}$$

where k is the rate constant. Note that $dV/dt = 0$ when $M_S=0$, as for flat-faced grains. This linear relationship, shown in figure 3 for (a) 3DMC simulated grain growth and (b) LabDCT characterized grain growth in Armco iron, has now been confirmed in numerous simulations and experiments, and provides the basis for the later analyses in this paper. In (b) the data include an abnormal grain in the specimen that received heavy cold work prior to recrystallization. Note that this grain has an extremely high dV/dt and a high negative value of M_S but fits the same trend as the normal grains, implying that its linear growth rate v is dependent on the same proportionality to H, through k.

$$v = -k\, H \tag{5}$$

Combining equations (1) and (5) with the kinematic description of dV/dt as the product of boundary velocity and surface area shows the origin of equation (4), describing growth rate as only a function of the value and sign of M_S for a boundary or grain.

$$dV/dt = \iint v\, dS = \iint -kH\, dS = -k\, M_S \tag{6}$$

3.2 Simple relationships between dV/dt, M_S and V of individual grains

The DeHoff relationship forms the basis for the following investigations of the relationships among those grain characteristics that are known to control growth and shrinkage of individual grains, such as face class, curvature and size. The goal of this study is to find and understand the relationships of these characteristics to M_S which is the final element controlling growth kinetics.

3.2.1 Relationship between M_S and individual grain volume V. Through these studies where the properties of individual grains, M_S, V and dV/dt are now available in simulations or experiments several novel and

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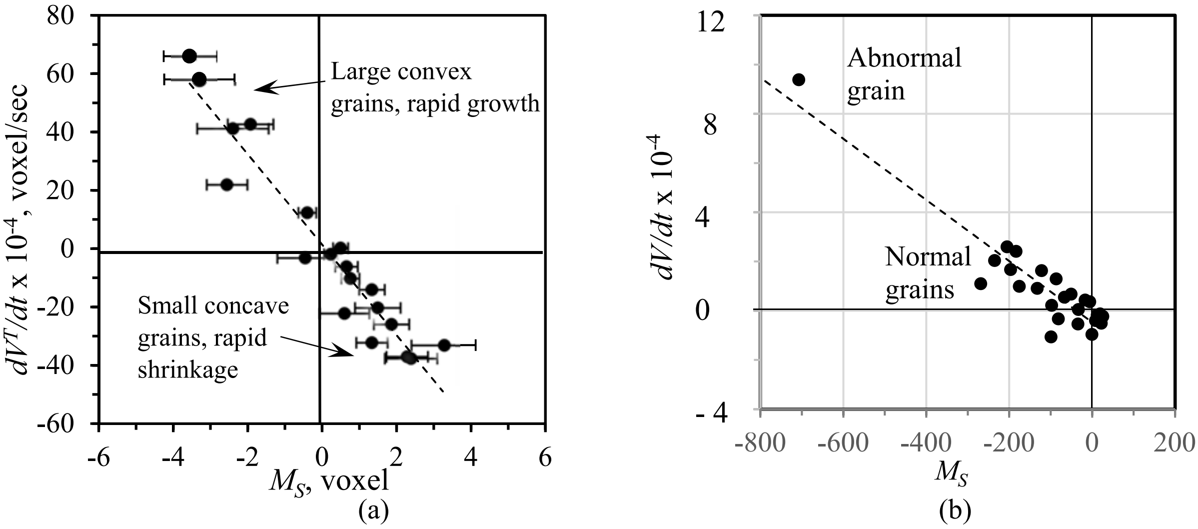

Figure 3. Linear relationship between *dV/dt* and M_S of individual grains averaged by size (a), or face class (b), passing through the origin and supporting equation (4). In (a) *dV/dt* was computed from 3DMC simulation data and M_S found by the DeHoff method. In (b) DCT analysis was used to compute *dV/dt* and the automated I-O method used for obtaining M_S.

consistent relationships have been found, including a linear relationship between M_S and V, described by equation (7) and shown in figure 4,

$$M_S = \alpha(V_0 - V) \tag{7}$$

The individual lines of data points in figure 4 represent different simulation-equivalent times of grain growth, i.e., 10, 20 and 40 seconds, and the slopes α decrease in magnitude with increasing grain growth time, i.e., with increasing scale of the system. The grain volume at the zero-growth rate x-intercept, V_0, represents the volume of the grains that at that time neither grow nor shrink. V_0 increases with time and the scale of the system and has been found to equal the mean grain volume, $\langle V \rangle$ at each time.

Since M_S has units of length, α in equation (7) and the slopes of the lines in figure 4 must have units of $V^{-2/3}$. In addition to α connecting M_S to grain size, equation (1) shows that slope must also carry information about grain shape (number of faces, through *H*), which also varies with grain size. This grain size information exists both through the overall scale of the structure, where each separate line has a different mean volume $\langle V \rangle$ and through the variation in grain volume along each line at fixed times.

Figure 5 shows the effect of *overall structural scale* on the slope, plotting *α* vs. $\langle V \rangle^{-2/3}$. This linear path throughout grain growth passes through the origin with the relationship of

$$a = \gamma\, \bar{V}^{-2/3} \tag{8}$$

In this plot of α vs. $\langle V \rangle^{-2/3}$, the slope $\gamma \cong -2.7$. Since *α* has units of $\langle V \rangle^{-2/3}$, this proportionality constant is unitless and describes a self-similar condition throughout the process. The significance of this plot is that although *a* contains both shape and size components of M_S, it still scales in a steady-state manner with *overall structural scale*, expressed as a function of mean grain volume. Thus, *α* still carries information about the variation in grain size and shape at any *single* state, expressed through the slope γ.

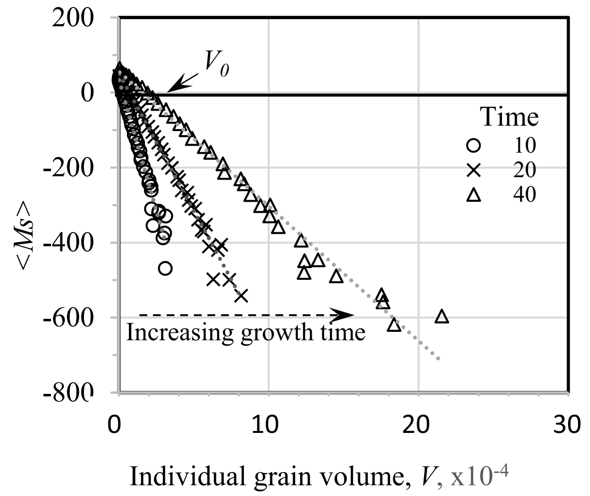

Figure 4. Linear relationship between M_S and individual grain volume, here grouped by face class, as described by equation (7). Data from 3DMC simulation.

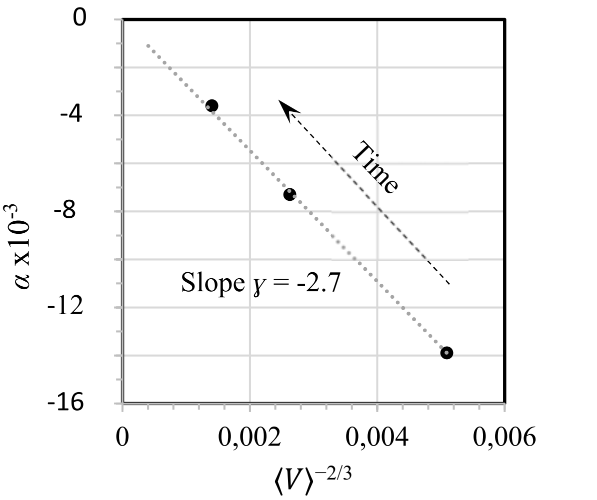

Figure 5. Unitless scaling relationship between the term α in equation (7) and overall scale of the system, expressed as $\langle V \rangle^{-2/3}$.

Combining the above relationships,

$$M_S = \alpha(V_0 - V) = \gamma \langle V \rangle^{-2/3}(V_0 - V) \tag{9}$$

it is apparent that a plot of

$$M_S / \langle V \rangle^{-2/3} \; vs. (V_0 - V) \tag{10}$$

still with slope γ, should provide a linear scaling relationship over all times and grain structure scales, as shown to occur in figure 6.

3.2.2 Relationship between dV/dt and individual grain volume V. An equally simple though fundamental relationship has also been observed for the first time between *dV/dt* and individual grain volume *V*, described by equation (11) and shown in figure 7.

$$dV/dt = \beta(V_0 - V) \tag{11}$$

The lines of data in figure 7 represent different times of grain growth, with the slopes, β, decreasing with increased growth time. The data points on each line represent the average properties for the grains grouped by face class, with the grains with larger numbers of faces showing the highest growth rate and those with the fewest faces shrinking. For the plots of each growth time, the face class on the x-axis with zero-growth rate is typically ~ 15 faces. These grains have volume V_0 in equation (11) and represent the volume the grains that at that time neither grow nor shrink. V_0 is essentially identical to the mean grain volume $\langle V \rangle$ at all times throughout grain growth, with the identity:

$$V_0 \cong \langle V \rangle \tag{12}$$

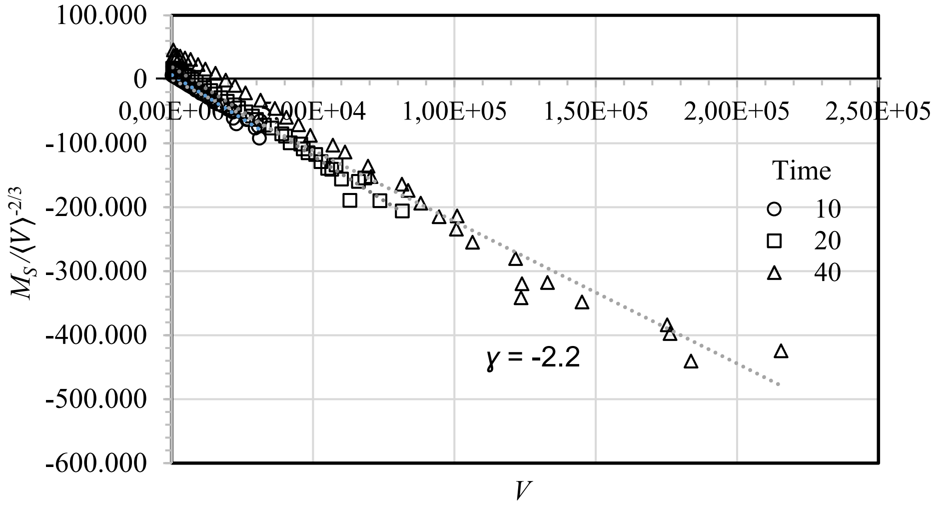

Figure 6. Unitless scaling relationship between $M_S/\langle V\rangle^{-2/3}$, i.e., M_S normalized by the *scale of the grain structure* and individual grain volumes, V, here, averaged by face class.

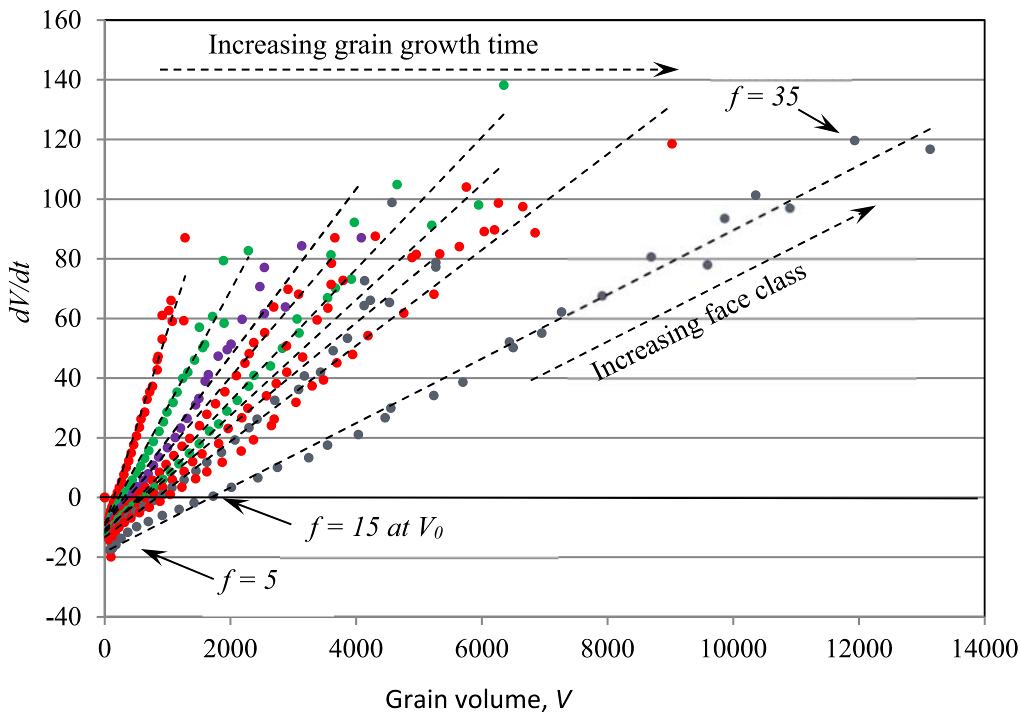

Figure 7. Plot of dV/dt vs. individual grain volume, here grouped by face class. Data obtained through 3DMC simulation.

Summary
The volumetric growth rate of individual grains in an aggregate has been consistently observed to be directly proportional to the individual grain volume V as $dV/dt = \beta(V_0\text{-}V)$. This relationship is explainable through the DeHoff relationship $dV/dt = -kM_S$ between growth rate and the integral mean curvature of individual grains, M_S, combined with the experimentally observed linear relationship between M_S and individual grain volume, $M_S = \alpha(V_0\text{-}V)$.

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