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Abstract. While the classic KJMA model is frequently used to fit experimental recrystallization kinetics data, the fitted values in most cases are inconsistent with the observed microstructural evolution. In this paper, we review the much more powerful microstructural path modeling (MPM) methodology. A basic assumption in this next generation of recrystallization models is related to the spatial distribution of nucleation sites, which may be uniform in the mathematical sense, i.e. randomly distributed in the sample volume, or clustered either along lines or on planes. For example nuclei are often observed to be linearly aligned because they have formed along original grain boundaries or stringers of second phase particles in the deformed matrix. In this paper, we present a new MPM, which is extending the former idealized linear MPM, allowing the recrystallizing grains to grow with different speeds in different directions, thus becoming prolate spheroid shaped. Finally issues concerning experimental determination and analysis of growth rates, are discussed.

1. Introduction

The kinetics of primary recrystallization, occurring within a deformed matrix, have been frequently followed experimentally by quantitative microscopy (stereology). Until very recently, in standard recrystallization studies of opaque solids like metals and alloys, the frozen-in states of partially reacted test specimens would be examined microscopically on plane sections through three dimensional specimens. Unbiased global microstructural parameters (descriptors of a statistical nature) would be estimated on these sections using stereological principles. To that end, when a series of specimens is studied for a range of reaction times, the deployment of a modeling approach could be adopted to study the path and the dynamics (kinetics) of the microstructural change. DeHoff [1] has described in detail the various measurable microstructural properties necessary for the scientific study of the path of such transformations.

The concept that the path of microstructural evolution can be represented by a mathematical state function involving unbiased global, statistical variables was first enunciated by DeHoff [2] and later summarized by Vandermeer [3]. Initially the most important variable to be studied was V_v, the volume fraction recrystallized. Later, S_v, the grain boundary area density separating recrystallized grains from the still-deformed volumes, and either $\langle\lambda\rangle$ or $\langle\lambda\rangle_{max}$, or both, where $\langle\lambda\rangle$ is the mean intercept-free chord length in the recrystallizing grains and $\langle\lambda\rangle_{max}$ is the maximum measured chord length, were recognized for their importance. A further discussion of the methodology for model development may be found in [3].

Parallel with the evolution of recrystallization modeling were the important advances that have been made in the measurement tools, e.g. data collection using electron backscattering diffraction (EBSD) [4,5], necessary to determine the stereological properties describing the microstructural state and path. From the early light microscope, to EBSD and now the powerful 3D X-Ray microscope [6,7] along with automated computer measurements, much tedium has been removed from the data collection process and new possibilities including simultaneous characterization of microstructure and crystallographic orientations as well as non-destructive 3D mapping have been achieved.

Historically, the genesis of recrystallization modeling in terms of nucleation and growth began just short of a century ago. But not until Kolmogorov [8], Johnson and Mehl [9] and Avrami [10] (KJMA) took serious account of impingement, which occurs when the boundary movement between a growing grain and an abutting grain ceases, did the first substantive progress in the development of analytical kinetic models begin. The KJMA approach was based on the abstract conceptualization of the nucleation and growth processes in which the new grains are imagined not only to grow unimpeded through one another but nucleation continues in already recrystallized regions as well as in unrecrystallized volumes (phantom grain concept). The totality of the volume recrystallized in such an abstraction is called the "extended" volume fraction recrystallized, V_{vex}. In this imagined view some regions will be counted as recrystallized more than once. Thus, V_{vex} can reach values greater than one. Similarly, S_v can be described in "extended" space as well and becomes S_{vex} [1]. The extended space concept is important because it can easily be visualized geometrically for modeling purposes. Furthermore, if the recrystallizing grains can be regarded in a statistical sense as being in a uniform distribution throughout the volume, i.e. impingements will take place uniformly throughout, then there exists a simple mathematical relationship in differential form between V_{vex} and V_v namely

$$\frac{dV_v}{dV_{vex}} = 1\text{-}V_v \tag{1}$$

The term ‘uniform distribution of the nuclei’ in the statistical sense is equivalent to what many call ‘random distribution of the nuclei in the volume’. Equation 1 which has been in vogue for over 80 years, provides the starting point for modeling recrystallization geometrically. Avrami [10] was led to propose a general kinetic equation for isothermal transformation processes including recrystallization. It has the form

$$V_v = 1\text{-}\exp(-Bt^k) \tag{2}$$

where B and k are experimentally determined constants related to the nucleation rate, growth rate, grain shape and dimensionality of growth and t is the isothermal annealing time. Much use has been made of equation 2 in recrystallization studies over the decades, but simple geometric models, i.e many recrystallization situations, were often times woefully inadequate to be explained by equation 2 [3], e.g. the k was not a constant and its values were deemed inconsistent with the proposed models.

2. Methodology - Microstructural Path Modeling

Over time improved models of recrystallization have been developed to account for some of the earlier discrepancies. This has led to the Microstructural Path Modeling (MPM) method of model development. Table I has been prepared to summarize the evolution over time of model development by the MPM method as it has been applied to recrystallization studies in a variety of metallic materials. In this table, the models are also roughly sorted in order of increasing complexity (increasing number of microstructural variables and solutions). This provides the researcher with a "menu" of models, from which to choose to study recrystallization and the microstructural properties that need to be involved.

Table I: Overview of the MPM models.

Model id	Micro property	Nuclei distribution	Grain shape	Preexisting nuclei	Nucleation rate	Growth rate	Model	Key references
KJMA	V_v	Volume uniform	sphere	yes	zero	constant	1A	[8-10]
KJMA	V_v	Volume uniform	sphere	no	constant	constant	1B	[8-10]
"relaxed" KJMA	V_v,S_v	Volume uniform	sphere	yes	zero	power law	2A	[3,11]
"relaxed" KJMA	V_v, S_v	Volume uniform	sphere	no	power law	power law	2B	[3,11]
VR	V_v, S_v, e	Volume uniform	spheroid	yes	power law	power law	3A	[14]
VR	V_v, S_v, e	Volume uniform	spheroid	no	power law	power law	3B	[14]
VMC planar	V_v, S_v, s	Planar array	spheroid	yes	constant	constant	4 (*)	[18]
VMC linear	V_v, S_v, L	Linear array	cylinder	yes	constant	constant	5 (*)	[18]
V linear	V_v, S_v, e, L	Linear array	prolate spheroid	yes	constant	variable	5M(*)	This paper

* refers to the possibility to include p subsets

In the simplest KJMA models, Model 1A/B in table I, the nucleation and growth rates of the "transformation", i.e. recrystallization, are assumed to be constants. The KJMA Models 1 A/B require an Avrami k of 3 or 4. Rarely have values this high been observed for moderate to heavily rolled metals. Thus, in those cases they can usually be disqualified immediately from consideration. The "relaxed" KJMA models offer some consolation. They require, however, an additional microstructural property to be measured, giving rise to a companion equation to the Avrami equation. That is the DeHoff equation [1] for the extended interfacial area density,

$$S_v = (1-V_v)\cdot S_{vex} \tag{3}$$

where the extended interfacial area, $S_{vex} = K\, t^{\,m}$ and *K* and *m* are experimentally determined constants. In addition, a microstructural path function relating S_v and V_v may be considered. This function can be helpful in the modeling process and contains information important as to the nucleation character and shape of the recrystallizing grains. It is given by [11]

$$S_v = (1-V_v)\cdot C\cdot[-\ln(1-V_v)]^q \tag{4}$$

where C and q are constants. When experimental data are described by these three equations, nucleation and growth rate parameters for either Model l, 2, or 3 may be estimated. Of the three equations 2 - 4, only two are independent, however.

There have been a number of successful recrystallization modeling efforts that have taken advantage of the "relaxed" MPM approach (Model 2A/B in Table I). Vandermeer et al. [11] have detailed the methodology. In the "relaxed" KJMA models the nucleation and growth rates are assumed to be power-law functions of time and so the model exponents can be directly related to the experimental k, m, and q parameters. These model rates may be written as

$$\dot{N} = N_1\cdot t^{\delta-1} \tag{5}$$

$$G = r\,P{\cdot}t^{r-1} \tag{6}$$

where $\dot{N}$ and G are the nucleation and growth rates respectively and δ, r, N_1 and P are model constants. The time exponents in equations 5 and 6 can be equated to the experimental k and m to yield

$$r = k\text{-}m \tag{7}$$

$$\delta = 3m\text{-}2k. \tag{8}$$

In Model 2A the nucleation rate is assumed to be zero (and therefore δ should be 0), while a fixed number of preexisting nuclei, $N°_v$ would be expected in that model. The development of the "relaxed" KJMA models requires replacement of the Avrami and DeHoff equations, i.e. equations 1 and 2, with solutions obtained using the mathematics of LaPlace transforms. The following equations result [11]:

$$V_{vex} = K_v P^3 N_1 \Gamma(B) t^k \tag{9}$$

$$S_{vex} = K_s P^2 N_1 \Gamma(K) t^m \tag{10}$$

where K_v and K_s are shape factors and Γ(B) and Γ(K) are gamma functions given in terms of the measured exponents:

$$\Gamma(B) = \Gamma(k+1-\delta)\Gamma(\delta)/\Gamma(k+1) \text{ and } \Gamma(K) = \Gamma(m+1-\delta)\Gamma(\delta)/\Gamma(m+1)$$

The Gamma function values may be obtained from Math Handbooks or from standard software like Matlab or Python.

It may be observed from the above experimental and model equations that the preexponential coefficients B and K can be expressed in terms of the model parameters as

$$B = K_v P^3 N_1 \Gamma(B) \text{ and } K = K_s P^2 N_1 \Gamma(K) \tag{11 a\&b}$$

Making the further assumption that the recrystallizing grains in Model 2 may be idealized as shape preserved spheres ($K_v=4\pi/3$ and $K_s=4\pi$) allows the above equations to be solved for P and N_1. The calculation of the nucleation and growth rates can then be accomplished using equations 5 and 6.

It is sometimes worthwhile to determine the number of recrystallized grains per unit volume, N_v. To do this for Model 2A/B requires the integrations:

$$N_{vex} = \int_{t_i}^{t_f} \dot{N}\, d\tau \text{ and } \Delta N_v = \int_{t_i}^{t_f} (1\text{-}V_v) B\tau^k N_1 \tau^{\delta-1}\, d\tau \tag{12 a\&b}$$

where $N_v = N_{vex}(t_i) + \Delta N_v$, and t_i and t_f are the times of the initial and final data points. Here it is assumed that at the earliest annealing time $N_v = N_{vex}$. The $_{vex}$ in these equations refers to nucleation in "extended" space.

While the MPM Model 2B nucleation-wise can be quite compelling, its assumption that the recrystallized grains can be idealized as growing shape preserved spheres may have shortcomings. The MPM model and experimental microstructures of rolled and recrystallized aluminum AA5182 [12,13], for example, suggested that the new grains may be better regarded as spheroids. The average experimental chord length in the rolling direction differed from that in the normal direction giving rise to an aspect ratio (AR) for the <λ>'s greater than 1. It was deemed essential, therefore, to include spheroidicity in the MPM equations. This is what models 3A/B do differently from models 2A/B. The MPM models allowing the recrystallized grains to be spheroids are described in more detail in [14].

Up to this point in the evolution of MPM modeling, a uniform distribution of recrystallized grains was assumed. Early metallographic serial sectioning however revealed linearly dispositioned nucleation to be operative in the recrystallization studies of dilute high purity aluminum alloys rolled 40% [15,16].

The nuclei were associated with the original grain boundary edges in the deformed matrix creating the linearity feature. The experimental V_v obeyed an Avrami equation with k=2 in agreement with the theoretical estimates of Cahn [17]. Cahn had developed a nucleation and growth phase transformation model for nucleation at matrix grain boundaries{planar arrays}, grain edges{linear arrays} and grain corners{points}. He did not however include S_v in the calculations. Later, Vandermeer and Masumura [18] extended the Cahn model to include S_v and the S_v/V_v relationship for the various grain nuclei dispositions (Models 4 and 5 in Table I).

To calculate the time dependence of V_v and S_v for a linear disposition nuclei model (Model 4), the formalism from the transformation modeling study had to be adopted and modified [18]. It was supposed, that the nuclei are positioned in approximately linear arrays such that the preferential first impingement of the new grains occurs with adjacent new grains *in the same array* (cluster). Impingements with grains from other adjacent arrays remain operative and later will occur in a uniform (random) manner in the two dimensions perpendicular to the studied array. Under these circumstances the recrystallized grains tend to be cylindrical in shape and to cluster in approximately linear arrays in the fashion of shish kebabs, or strings of beads, for example. For the linear model example detailed here, additional model parameters are required. One is L, the *total* length of nucleation array length per unit volume of material. Others are G, the growth rate of the grains, N_e^O the number of preexisting nuclei per unit length, and $\dot{N}_e$, the continuing rate of nucleation per unit length, all of which are constants in the model. There is an additional model parameter, *p*, (chosen by the modeler) which allows one to assign the relative importance of continuing nucleation as opposed to preexisting nucleation. Both aspects of nucleation are allowed in the model. A high *p* favors preexisting nucleation while a low p favors continuing nucleation.

3. New MPM development

Because, recrystallization of heavily rolled metals often involves two of the aspects discussed above – namely linearly clustered nucleation and shape preserved spherical growth, the idealized linear model (Model 5) had to be modified further. In the new model, the array lengths comprising L are all assumed to be aligned approximately with the rolling direction and the individual recrystallized grains themselves are assumed to be prolate spheroids with their major axes aligned with L. In a prolate spheroid model, the G is composed of two components, G_a and G_b, the growth rates in the spheroid's major and minor axis directions, respectively. Because the model grains are prolate spheroids and the L components are aligned in the rolling direction the growth rate, G is given by

$$G = (1-e^2)\langle v\rangle_{ch}^{max} \tag{13a}$$

where e is the eccentricity of the prolate spheroid grain and $\langle v\rangle_{ch}^{max}$ is taken to be the Cahn/Hagel growth rate at the start of recrystallization. Note:

$$\langle v\rangle_{ch}^{max} \approx G_a \text{ and } 1-e^2 = \left(\frac{G_b}{G_a}\right)^2 \tag{13 b\&c}$$

Finally, the total number of recrystallization nuclei per unit volume for the model will be N_v where at time, t

$$N_v = LN_e^O + L\dot{N}_e \cdot t\,. \tag{14}$$

Unfortunately, the time dependencies of V_v and S_v in the case of a linear dispositioned nucleation model can not be obtained in analytical forms. It is necessary, therefore, to solve them numerically and present them in tabular or graphical form. An example of one such linear model solution is shown by the master curves in figure 1 where

$$V_{vex}(n)=\left[\left(\frac{2N_e^{O^2}}{(\pi L)}\right)\right]\ln\left(\frac{1}{1-V_v}\right)\ ,\ S_{vex}(n)=\left[\left(\frac{N_e^O}{(\pi L)}\right)\right]S_v(1-V_v)\text{ and }\ a_e=\left[\left(\frac{\dot{N}_e}{L}\right)G\right]^{\frac{1}{2}}t. \qquad (15\ a,b,c)$$

a_e is a 'grain dimension' parameter.

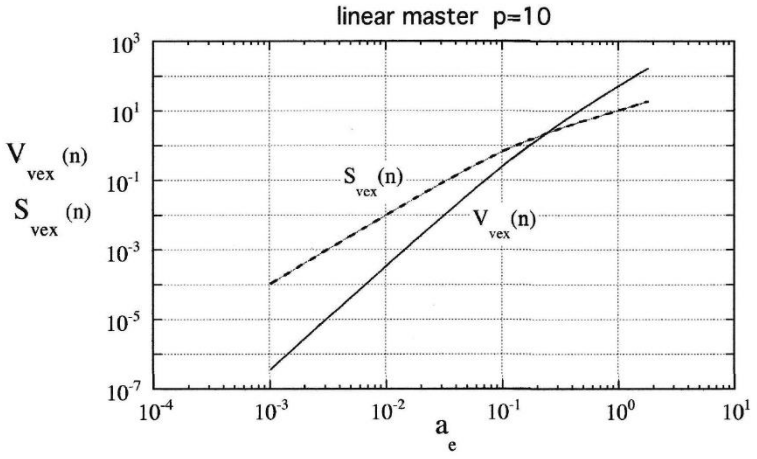

Figure 1. Recrystallization master curves of the microstructural evolution with time of the extended volume fraction and the unimpinged extended interfacial area density for a linear disposition nucleation model with p=l0.

A path master function, S_{vex} vs V_{vex}, for this case is presented in figure 2. Note the downward bending of the three path functions in figures 1 and 2. Also plotted in figure 2 is q, the derivative of the logs of the path functions. In this model q is not a constant but varies as the volume fraction increases, from a value of 2/3 down to 1/2. The change in q represents the transition to a situation, where all the lengths L are covered by recrystallizing grains which then grow two-dimensional.

4. On the use of Cahn/Hagel growth rate

The growth rate, and in particular the experimental determination and analysis hereof requires further considerations. The Cahn-Hagel growth rate [19], $\langle v\rangle_{ch}$, is a stereologically-based dynamic (kinetic) microstructural characteristic. It describes the time dependence of the average rate of the recrystallized grain boundary migration during the annealing process, and can be estimated from the microstructural properties by the following:

$$\langle v\rangle_{ch}=\left(\frac{1}{S_v}\right)\cdot\left(\frac{dV_v}{dt}\right) \qquad (16)$$

Many recrystallization studies have measured $\langle v\rangle_{ch}$ using microstructural property data with equation 16. The data are then plotted as a power-law function of time and often expressed as

$$\langle v\rangle_{ch} = K_{ch}t^{-\alpha} \qquad (17)$$

where K_{ch} and α are constants. An important issue is that there can be considerable variation in that function's power-law parameters depending on the mathematical representation chosen for the derivative in equation 16.

To clearly reveal the growth rate dynamics, it is proposed, alternatively, to present the $\langle v \rangle_{ch}$ as a *kinetic* path function plotting the data as a function of V_V, instead of time. In such plots, several growth rate states are often observed. For example in AA5182, $\langle v \rangle_{ch}$ decrease rapidly with time during the first stages of recrystallization, after which the rate decreases very slowly (is nearly constant) [12]. How should this be interpreted now becomes an issue, which we will discuss in a subsequent publication.

Another way to evaluate the growth behavior is with a length parameter, *a*, which may be defined as the average migrating distance a moving grain boundary element travels while unimpinged. It may be written mathematically as

$$a = \int \langle v \rangle_{ch} \, dt \tag{18}$$

The time dependence of *a*, here, is postulated then to be a measure, on average, of the distribution of growth paths of the individual recrystallizing grains in the manner envisioned by DeHoff [1].

It has long been recognized that recrystallized grains each have their own characteristic growth patterns. Early modeling studies introduced either a growth rate distribution [15] or a grain size distribution [16] in order to achieve agreement with the KJMA equation parameters. In agreement with these ideas Lauridsen et.al. [7] using 3D X-ray diffraction microscopy demonstrated in aluminum that each recrystallizing grain followed its own growth kinetics profile. DeHoff [1] proposed that the continuum of curves describing the geometric evolution of all particles, e.g. grains, in the system, as the growth path envelope of the system. An average growth parameter, such as *a*, (see equation18), therefore, is proposed then to characterize the continuum, i.e. the path envelope.

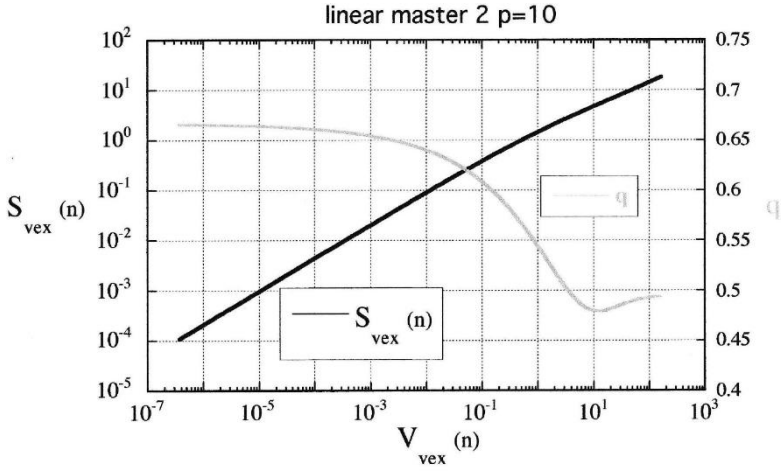

Figure 2. The evolution with V_{vex}, during recrystallization of the microstructural path master curve function, S_{vex}, and it's derivative, q, for a linear disposition nucleation model with p=10.

5. Conclusion

A new microstructural path model (MPM) for primary recrystallization is presented as an extension of previously developed MPMs. The new model can take all of the following recrystallization characteristics into account: linearly clustered nucleation, site saturation as well as continuous nucleation (both of which may occur in a given sample with a certain fraction of the nuclei pre-existing), and non-spherical growth. Tabular or graphical forms of the time dependencies of V_v and S_v are needed when fitting the experimental data to the model. We suggest that the 'menu' of MPM models is capable of analysing a very large fraction of primary recrystallization situations. When analyzing experimental data for recrystallization growth rates, we propose to visualize the data as a function of V_v instead of

time, and a growth path envelope with an average growth parameter may be the optimal choice to characterize a continuum of growth rates.

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