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ON THE CORRELATION BETWEEN DISTRIBUTION OF CSL BOUNDARIES AND GRAIN GEOMETRY

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ABSTRACT

This paper addresses the possible correlation between grain size distribution and the geometrical properties of grain boundaries. A series of functions are used to describe the grain size and the shape distribution, and considerations given to the population of grain edges and corners which result. In turn this is then correlated with the fraction of special and general (random) grain boundaries.
The concepts introduced here are then tested by looking at some microstructural and textural data from a grain growth experiment on high purity aluminum. In parallel with this a model of the distribution function of the grain boundary misorientation parameter is employed. The outcome of this series of investigations is the ability shown to establish a correlation between parameters describing the distribution of size and shape of the grains, and other parameters describing the fraction of grain edges which join boundaries having random and special character.

Key words: polycrystal, geometry and physical properties of grain boundaries, stereological description.

INTRODUCTION

Grain boundaries, and as a result the grains, differ in their physical and geometrical properties. Both physical and geometrical properties of grain boundaries have an influence on properties of polycrystals (Petch 1953; Watanabe 1988; Ralph 1988; Kurzydłowski & Przetakiewicz 1988; Bucki & Kurzydłowski 1992). The existing models for the properties of polycrystalline materials concentrate attention either on the physical or geometrical properties of grain boundaries. However, if the geometrical properties (size of grains) are correlated with their microstructure, and in turn other properties, the conclusions drawn with regard to the role of one or the other factor are likely to be incomplete or unsubstantiated. The aim of the present paper is to describe the results of a study of a possible correlation between the geometry of grains and distribution of grain boundary microstructure.

CHARACTERIZATION OF GRAINS

Grains in polycrystals can be described in terms of their distribution of grain volume, f(V), which describes the size of individual grains. This distribution of grain volume can be characterized by parameters such as the mean volume, E(V), standard deviation, SD(V), and coefficient of variation, CV(V) = SD(V)/E(V).

The process of grain growth results in a systematic increase in the mean volume of grains. Changes in the mean value, E(V), are accompanied with variation in SD(V) and frequently with CV(V):

$$\frac{d}{dt}CV(V) \neq 0 \qquad (1)$$

Two dimensional space E(V)-CV(V) can be used to discriminate the grain growth character (Łazęcki et al. 1993). If CV(V) is constant with time the process is termed "normal". If CV(V) increases with time the process can be called "abnormal" and if CV(V) decreases with time - "supernormal".

Due to the technical difficulties involved in grain volume measurements, the grain geometry is usually described by other parameters such as the grain area, A, or an equivalent grain diameter, d, (calculated as the diameter of the circle that has the same area as a given grain section). The grain growth path can then be plotted in the space E(A)-CV(A) or E(d)-CV(d) (Łazęcki et al. 1993). Stereological rules link the grain area (diameter) distribution function with the volume distribution and under some additional assumptions (Bucki & Kurzydłowski 1992), a monotonic dependence of CV(V) on CV(A) can be expected.

The geometry of grains can be described more precisely by parameters which also define their shape (Kurzydłowski et.al 1990):

a) grain perimeter, p, and shape the factor, $\beta = p/\pi \cdot d$;

b) maximum chord, d_m, and the shape factor, $\alpha = d_m/d$ (for equiax grain structures the mean value of the factor α is in the range 1.25 - 1.30).

POPULATIONS OF THE GRAIN BOUNDARIES

Grain boundaries in polycrystals form populations characterized by distributions of geometrical and physical properties. A single grain boundary is distinguished by the area of its surface, S_i, its curvature, H_i, and a set of parameters, P_{ij}, defining its structure. These parameters include:

a) misorientation angle, Θ, (1 independent parameter) and misorientation axis, **l**, (2 independent parameters);

b) normal to the grain boundary plane, **n**, (2 independent parameters);

c) rigid body translations (2 parameters);

d) other parameters, e.g. describing segregation.

The population of grain boundaries in a polycrystal can be described by means of distribution functions of the respective parameters. The distribution function of the misorientation parameters, f(Θ,**l**), has attracted a great deal of interest since it has been postulated that it controls the energy, diffusivity and other properties of grain boundaries.

The values of Θ and **l** are from continuous space. In common applications the set of values of possible grain boundary parameters is reduced to a discrete set of some characteristic parameters. Such a situation is exemplified by the procedure based on the Coincidence Site Lattice - CSL model (Grimmer et al. 1974). In this case the space of misorientations f(Θ,**l**) is divided into intervals represented by Σ parameters, Σ is an odd number characterized density of coincidence place in mutuall superlattice for adjusent grains, which are computed for each misorientation angle. Those grain boundaries with $\Sigma \leq 29$ usually are assumed to have special properties (Sutton & Balluffi 1987, Svindlerman & Straumal 1985) and these special properties of grain boundaries are retained despite small deviations from the exact CSL Σ relationship. The maximum value of this deviation $\Delta\Theta_{max}$, is commonly calculated from the Brandon criterion (Brandon 1966):

$$\Delta\theta_{max} = 15^{o}\ \Sigma^{-\frac{1}{2}} \tag{2}$$

Grain boundaries in polycrystals form a system of surfaces connected along threefold (grain) edges, TEs, and at four-fold (grain corners) points, FPs. On a cross-section, TEs are revealed as so called triple points, TPs. These three-fold edges and four-fold points play an important role in a number of processes taking place at grain boundaries, especially in micro- and nano- grain sized polycrystals.

The populations of grain boundaries are described in terms of the distribution functions of TE properties in a way similar to that adopted for the individual boundaries. In a simplified approach four specific types of TEs can be distinguished: RRR, RRS, RSS, SSS; where R, S stand for random and special grain boundaries respectively.

Consequently, to a first approximation a system of grain boundaries in a polycrystal can be described additionally by a distribution function, $f_{TE}(q)$, with q equal to 0,1,2 or 3; where q is the number of special grain boundaries at a given TE. (Kurzydłowski et al. 1993).

THE PHYSICAL AND GEOMETRICAL PROPERTIES OF GRAIN BOUNDARIES

Under quasi-equilibrium conditions, for example in annealed polycrystals, the geometry of grains can be expected to be related to their physical properties. Simple considerations show that in a polycrystal with all grain boundaries with the same properties, grains assume a regular geometry which can be approximated by a set of equal-volume tetrakaidekahedra (Underwood 1970; Rhines 1986). The system of such grains is distinguished by the condition CV(V)=0. In this case the grain boundaries are joined along their common edges at an angle close to 120° (termed frequently dihedral angles). The larger are the differences in energy of GBs the larger is the departure of these angles from 120° (Kurzydłowski 1993).

For polycrystals characterized by a variation in the energy of their grain boundaries it should be expected that under near equilibrium conditions grains will differ in their size; the effect reflected in distributions of geometrical and physical properties. It is therefore suggested that the concept of a TE distribution function should be studied from the point-of-view of its applicability to the analysis of processes of grain growth in polycrystals. This is based on the assumption that the common edges of random boundaries, RRR, are more likely to be balanced in terms of their surface tensions than those at RSS, RRS, SSS edges and as such will move under the action of different driving forces. The RRR edges might also have a different mobility since the motion of random boundaries can not, in general, proceed through the motion of dislocations, which are an element of the structure of special grain boundaries.

AN ANALYSIS OF THE DISTRIBUTION OF GRAIN BOUNDARY CHARACTERISTICS AND GRAIN GEOMETRY FOR ALUMINUM POLYCRYSTALS

In the present study the normal distribution N(0, σ) and the Roe formalism were used to approximate the deviation of the components from the ideal texture <hkl> and the standard deviation of this distribution, σ, was a measure of the sharpness of the texture (More details are given in the paper by Garbacz & Grabski 1993).

The results of earlier studies have shown that the type, sharpness and character of the texture exert a strong influence on the distribution of CSL boundaries (Garbacz & Grabski 1993) and characteristic triple edges (Kurzydłowski et al. 1993). For diffuse textures, the distributions of TEs and FPs approach that of a random texture-free polycrystal, with the following fractions of particular types of TPs: RRR - 67.9%, RRS - 27.7%, RSS - 4.3%, SSS - 0.2%. On the basis of the results obtained it has been established that the relationship between the fraction, F_0, of RRR TEs and the fraction, F_C, of CSL boundaries can be described by the formula:

$$F_0 = 0.82 \log(F_C^{-1}) - 0.07 \qquad (3)$$

The relation between the texture and CV(V) has been studied for high purity aluminum (99.99%). Polycrystalline specimens of this material were extruded and then recrystallized, for one hour at various temperatures. The microstructures obtained differed in their grain size distributions (Wyrzykowski & Grabski 1986), annealing textures and the distribution of the diffusivity properties of their grain boundaries (Kwieciński & Wyrzykowski 1989). The modelled distributions of grain orientations for aluminum polycrystals were used (Garbacz & Wyrzykowski 1993) to simulate distributions of grain boundary misorientations and distributions of CSL boundaries. The main conclusions of the Garbacz and Wyrzykowski (1993) paper were that there exists a relationship between grain boundary diffusivity and grain boundary coincidence distribution functions. This indirectly confirms the adequacy of the model used to compute the distribution function of the grain boundary misorientation parameter.

In the present study, the approach proposed by Garbacz and Grabski (1993) has been extended to obtain the characteristics of the triple edges, TEs, of the grain boundary system for each texture. For each type of texture, associated with a given annealing temperature, three independent simulations of TEs were performed for a model of the polycrystal consisting of 10 layers of 20x20 grains, which permitted examination of a total of 24000 TEs. Each CSL boundary with coincidence, Σ, ranging from 1 to 29 was counted into an "S" category. The common edges in the system of grain boundaries have been examined in terms of the number of special/random grain boundaries which they connect.

The geometry of the grains in the series of aluminum polycrystals have been determined with an automatic image analyzer (Kurzydłowski et al. 1991). The grain geometry was described, as a function of the annealing temperature of the polycrystal, using the mean equivalent diameter, d, and shape factors, α.

CONCLUDING REMARKS

The results of these measurements (Fig.1) indicate that the polycrystals annealed at various temperatures differ in size. This is reflected by a systematic increase in the mean equivalent diameter, E(d). The systematic increase in the mean size of grains is accompanied by changes in the normalized grain size distribution function, f(V/E(V)) and in changes in the coefficients of variation CV(d) which are monotonic functions of CV(V).

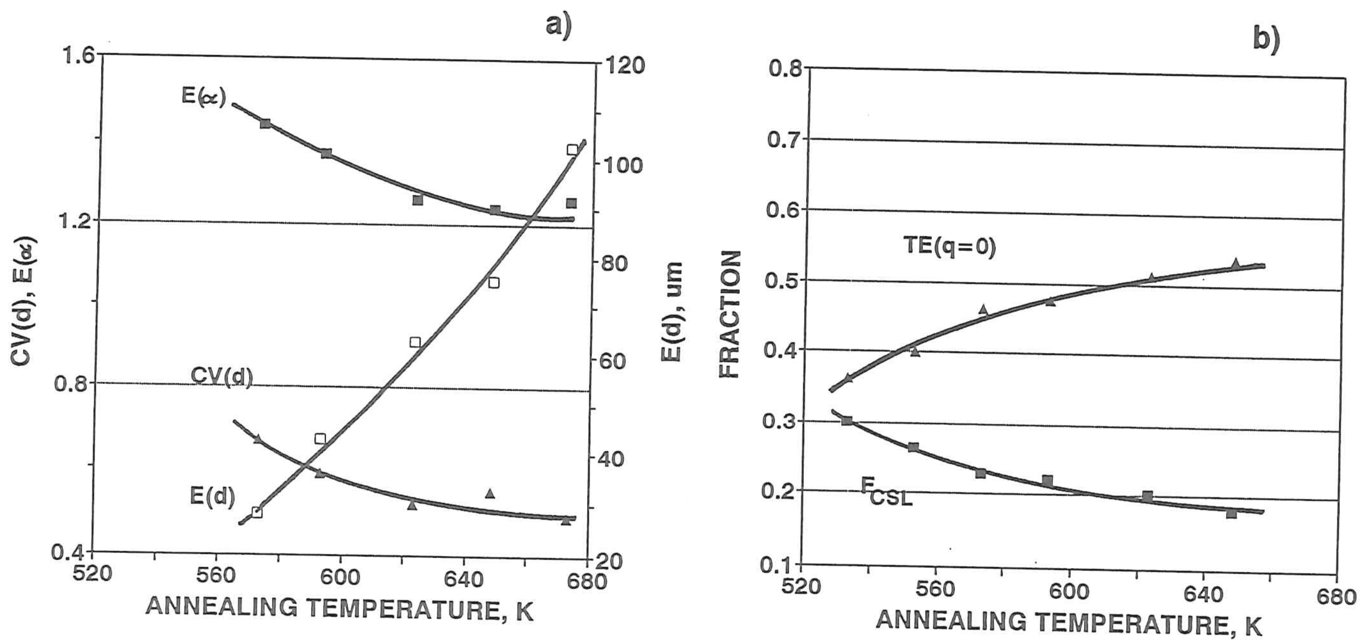

Fig. 1. Temperature of annealing effect on the parameters describing the geometry of grains and the characteristics of the grain boundaries: (a) alterations in the mean size E(d), in the coefficients of variation of the equivalent diameter CV(d) and in shape factor α; (b) variation of the fraction of CSL boundaries and alterations in the fractions of TEs.

The results of the measurements of grain geometry also show that the increase in the size of grains is associated with an equilibration of their shape. There is a clear tendency for the mean values of E(α) to reduce as the mean equivalent diameter, E(d), rises.

It may be noted that extensive changes in the shape of grains, the degree of grain size uniformity and the characteristics of the threefold edges take place as a function of the annealing temperature in the range 533-625K. These changes are accompanied by a systematic decrease in the sharpness of the material texture. Higher temperatures of annealing seem to lead to some steady state in the development of the texture, shape of grains and the degree of the grain size uniformity. This steady state is characterized by approximately 50% of the TEs being of RRR character and corresponds to about 18% of CSL boundaries.

The results obtained from modelling the TE distribution function for different annealing textures/temperatures have shown that there is a clear dependence of the TE character distribution function with the texture of the polycrystals. Generally, the fraction of TEs without special grain boundaries, (q=0), increases with increasing mean grain size while the fractions of all other TEs, (q=1,2,3), decrease.

The results of these computations show that, within the framework of the model adopted, the observed evolution in the texture of the material is accompanied by systematic changes in the distribution function of the TE character. It may be noted that the evolution in the texture of the material causes a systematic increase in the number of TEs joining 3 random boundaries TE(q=0) (RRR). The computed variation in the relative numbers of different types of TE agrees well with the observed variation in the character of the grain size distribution function. The increasing fraction of RRR common edges is accompanied by an increasing degree of grain size uniformity; as reflected by decreasing values of the coefficient of variation of grain volume CV(V). The decreasing fraction of the common edges with at least one special grain boundary correlates also with variations in the grain shape. There is a clear tendency for the grains to assume a more equiax shape with a decreasing fraction of (SSS)+(SSR)+(SRR) common edges.

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