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ON THE COMPUTER AIDED DESCRIPTION OF GRAIN SIZE DISTRIBUTION IN POLYCRYSTALLINE MATERIALS

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ABSTRACT

Population of grains in polycrystals is characterized by the distribution functions of their size and shape. The volume of grain is a desired parameter to describe its size, because grain is a 3-D object. Commonly available experimental techniques can be used to measure only 2-D and 1-D parameters of grain size. Stereological computer aided method to describe grain volume distribution parameters on the basis of grain section area measurement is presented in this work. This method is designed especially for computerized image analysis system. The developed method is based on interactive, computer aided modelling of polycrystalline aggregate. The method uses non-standard approach to reconstruction of 3-D parameters of polycrystal microstructure. Algorithm consisting of modelling 3-D grain structure, and modelling preparation process of 2-D section is used in presented method. The modelled section is then compared with section of real sample by means of comparison of 2-D size and shape distributions. The method takes into account resolution limit that result in small sections of grains not to be revealed on 2-D images. This factor, if not considered, can lead to significant errors in 3-D size parameters estimation. Using proposed method one can obtain such parameters describing grain size inhomogeneity as coefficient of variation, skewness or kurtosis of grain volume distribution function.

Key words: polycrystal, grain size distribution, image analysis, computer modelling.

INTRODUCTION

Among the parameters used to describe size of grains in polycrystal only the grain volume V reflects the size of the individual grain. The other two commonly used parameters: grain section area A and intercept length l depend on the grain volume and shape, and on the position of intersecting plane or line with respect to the grain center. These two parameters are mainly used to characterize the mean size of grains. On the other hand grain area and intercept length which are measured on 2-dimensional sections of polycrystals can be much more easily experimentally determined, especially with the help of automatic image analysis systems, while measurements of grain volume are complicated and time consuming. In this

situation it is desirable to define the relationship between the parameters defining the grain volume distribution and the parameters defining grain area (or intercept length) distribution. It should be pointed out, that it is not theoretically possible to uniquely relate any distribution measurements in 2-D section to the true size-shape distribution in 3-D. However, approximate estimation of 3-D distribution is possible under certain conditions. In the proposed method there is assumption, that the structure is isotropic and grains are of close to equiaxial shape.

The problem of the relationship between parameters describing the grain volume distribution function f(V) and the parameters describing the grain area distribution function f(A) can be viewed as a special case of the relationship for an aggregate of particles. Such a relationship has been investigated in earlier works, for instance in classical works by DeHoff and Rhines (1961), DeHoff (1964) and Hilliard (1968). It should be noted however that the previous approach was oriented mostly towards simple counting type procedures. Such procedures are characterized by relative simplicity of measurements. On the other hand they are based on rather sophisticated considerations and in consequence do not offer much flexibility in model case studies of various types of polycrystals. They also impose considerable limitations on modelling experimental conditions of the measurements, characterized for example by resolution limit.

The importance of a proper description of the experimental conditions can be concluded from the fact that the estimations based on the assumption of unlimited resolution capacity (see for example (Hull and Houk, 1953) or (Szala et al., 1988)) predict the value of grain area variance for homogeneous constant grain volume polycrystals that is higher than the variance frequently measured for the polycrystals characterized by a distribution of grain size.

METHOD

There are two general types of the approach to the relationship between f(V) and f(A): "forward" and "backward" procedures. They are shown in Fig.1.

In the traditional, backward procedure, the results of grain area measurements $f(A)_{meas}$ are adopted as a starting point, and on their basis, for a given shape of grains, the distribution $f(V)_{calc}$ is calculated.

In the forward procedure, one assumes certain type of distribution function $f(V)_{theor}$ which has some adjustable parameters. Then, taking into account the physical limitations of sectioning and imaging process, the distribution function $f(A)_{calc}$ is calculated. The values of the f(V) parameters are then determined in a procedure based on examination of the fit between $f(A)_{calc}$ and $f(A)_{meas}$.

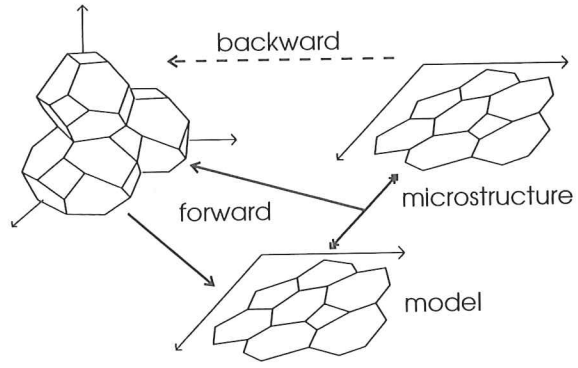

Fig. 1. Schematical difference between backward and forward approach to f(V) reconstruction

Apart from numerical details these two methods differ in fact that the first approach emphasizes the role of the data collected as a $f(A)_{meas}$ while in the second, the attention is focused on the $f(V)_{theor}$ function. In view of this the second approach is more convenient in modelling of a polycrystal behavior.
Computer programs have been implemented in the present work for this approach. The main part of the flow chart is shown in Fig.2.

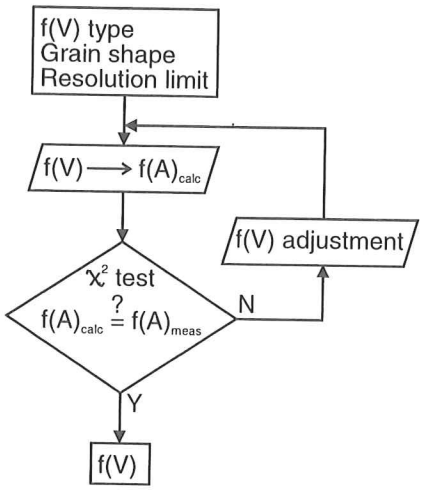

Fig. 2. Simplified main part of implemented program flow chart

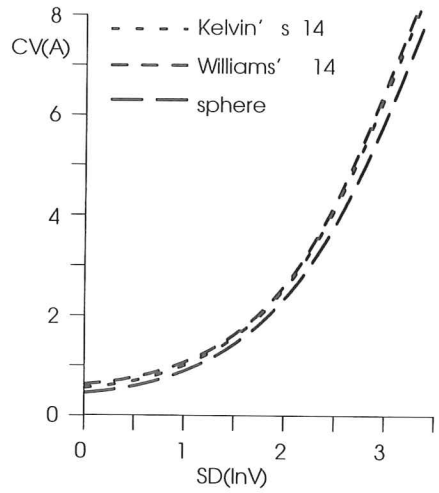

Fig. 3. Influence of SD(lnV) on CV(A) for CShG polycrystals

RESULTS

The results of the computations for Constant-Shape Grains (CShG) polycrystals characterized by a log-normal distribution function LN(V) are depicted in Fig.3. The plot shows the relationship between standard deviation of grain volume logarithm SD(lnV) and coefficient of variation of grain area CV(A) for different grain shapes. It has been shown in previous work of authors (Bucki and Kurzydłowski, 1992) that this relationship is much less grain shape sensitive than the relationship between standard deviation of grain volume logarithm SD(lnV) and standard deviation of grain section area logarithm SD(lnA). The relationship shown in Fig. 3 is recommended therefore for practical applications and further examination.
The values of CV(A) and SD(lnA) calculated for CShG polycrystals for the case of $SD(lnV) = 0$ (the polycrystal with constant size grains) set the unlimited-resolution lower bounds for the values of polycrystals characterized by the distribution of grain volume. In the work (Bucki and Kurzydłowski, 1992) these bounds have been determined as: $CV(A) \approx 0.55$ and $SD(lnA) \approx 1.0$. The values of CV(A) and SD(lnA) higher that given above should be treated as an indication of non-homogeneity of the size of grains.
The results obtained for the case of limited resolution are presented in Fig.4. It shows the CV(A) - resolution limit δ relationship for different grain shapes in the case of $SD(lnV) = 1.0$. Resolution limit δ is here defined as a ratio of the smallest measured area to the mean area E(A) measured in a given experimental conditions. The plot shows that for a given value of SD(lnV) the value of CV(A), decreases

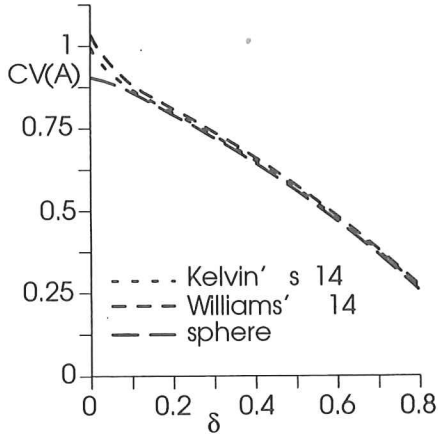

Fig. 4. The influence of resolution limit δ on CV(A) for polycrystals characterized by SD(lnV) = 1

with an increasing value of the resolution limit δ. The other observation is, that for values of δ greater than ca. 0.1 the grain shape influence on the SD(lnV)-CV(A) relationship can be neglected.

The method can be also used to describe bimodal grain volume distribution, quite common in metal structures (for example obtained during abnormal grain growth). For such a structures another $f(V)_{theor}$ function should be used. As a first approach the bi-log-normal function could be used. The adjustable parameters of this function are the mean and variation of both log-normal functions, and the ratio of their amplitudes, so description of both subpopulations of grains can be obtained.

FINAL REMARKS

The proposed method is designed especially for computer image analysis system, and can be easily used in model studies on polycrystal behavior. Because of non-standard approach to reconstruction of 3-D grain size distribution parameters used in the method the resolution limit of experimental procedure can be considered.

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