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AN APPLICATION OF CLUSTER ANALYSIS TO THE STUDIES OF GRAIN GROWTH PATTERN IN POLYCRYSTALS

Tomasz CZUJKO, Jerzy BYSTRZYCKI
and Krzysztof J. KURZYDŁOWSKI*

Department of Metallurgy and Metal Technology
Military University of Technology, 01-489 Warsaw,
Kaliskiego 2, POLAND
*Department of Materials Science and Engineering,
Warsaw University of Technology, 02-524 Warsaw,
Narbutta 85, POLAND

ABSTRACT

Analysis of the evolution of grain geometry during grain growth have been performed by cluster analysis method. Size and shape of grains have been described by points in 3-dimensional space of geometrical features. Population of grains have been divided into clusters (sub-population) which vary depending on the condition for the process of grain growth.

Key words: Size and shape of grains, cluster analysis, grain growth.

INTRODUCTION

Grain growth is an important phenomenon taking place in polycrystalline materials exposed to temperatures exceeding approximately 0.4 of the material melting point T_m. Generally, the process results in a systematic increase of the mean equivalent diameter of grains, $E_t(d)$, as function of annealing time t. However, depending on the experimental conditions it can proceed along different paths which are distinguished by specific changes in the shape of grains and the equivalent diameter distribution functions $f_t(d)$.
Normal grain growth is a special case of grain growth path characterized by a constancy of the normalized distribution functions $f(d/E_t(d))$ and self-similarity of the subsequent grain structures. Łazęcki et al (1993) have shown that normal grain growth is rarely observed in commercial alloys. As a result, in experimental studies of grain growth it is usually necessary to record and categorize changes in the distribution functions of the size of grains and the distribution functions observed assume complicated, multi-modal character.
In the general case the process of grain growth brings about changes in both size and shape of grains (Kurzydłowski 1992). As a result additional geometrical parameters, and their distribution functions, are included in the studies of grain growth. In the modern approach to the phenomenon of grain growth

this process is analyzed in multi-dimensional space of random variables and special tools are required to handle and analyze the collected data.
It has been assumed in the present paper that analysis of the evolution of grain geometry during different variants of grain growth and identification of the grain growth paths can be much facilitated by cluster analysis methods.

MATERIAL AND THE METHODS

The chemical composition of the material used in the present studies is given in Table 1. One set of the specimens have been annealed at 0.7 T_m for the annealing times varying from 5 to 160 minutes.

Table I. Chemical Composition of the Material.

Element	Mn	C	S	N	O_2
Concentration	2.1	0.068	0.002	0.0015	0.0045

H_2	Fe	Si	Mg	Co	Cr	Ni
0.0008	0.01	0.00X	0.00X	0.00X	brak	reszta

Specimens of the second set were strained, in uniaxial straining to 4% elongation and subsequently annealed in the same annealing condition as for the first set. Specimens for metallographic observations were prepared according to standard procedures. Individual grains revealed on cross-section of the specimens were characterized in terms of:
a) d - equivalent diameter;
b) d_{max} - maximum chord length;
c) p - perimeter.
These parameter were used to calculate:
the normalized size $d_n=d/E(d)$ (1)
and two shape factors α and β, previously used by Kurzydłowski et al (1989), defined in the following way:

$$\alpha=d_{max}/d \quad (2)$$

$$\beta=p/d. \quad (3)$$

In this way geometry of individual grains revealed on a section of the polycrystals is described by 3 parameters:

$$(d_n,\ \alpha,\ \beta)$$

and can be represented by a point q_i in a 3-dimensional space. Accordingly, population of grains characteristic of a given specimen form a set of points, Q, in such a space.
The Q sets, i.e. the points representing geometry of grains in a given polycrystal, are arranged in the space of geometrical features in specific configurations of varying density. These configurations evolve in the course of grain growth according to specific patterns, characteristic of a given grain growth path. The Q set configurations and their evolutions can be studied and systemized using the method of cluster analysis.
Cluster analyses have been successfully used in a wide range of applications; including biology and medicine. The method helps to divide the populations studied, for example grains in a polycrystalline material, into distinctive sub-populations

(groups, clusters) in an optimal way or according to some specified criteria. Elements, for example grains in a polycrystal, showing similar values of their features can be found and be characterized by some average values common to a given sub-population. At the same time the grains that are categorized to be in different groups radically differ among themselves.

Without an "a priori" knowledge of the potential cluster positions it is convenient to base the grouping of elements using as a criterion the distance from the nearest neighbor.

It is assumed in this case that a cluster C is formed by the points/elements such that:

a) for any point X_i in the cluster there is another point X_j in the cluster that is placed at a distance smaller than a certain critical value R,

b) each point outside the cluster is at a distance larger than R from any point in the cluster.

The distance d_{ij} between the points $q_i(x_{i1},x_{i2}..x_{im})$ and $q_j(x_{j1},x_{j2}..x_{jm})$ which represent geometry the i-th and j-th grain, has been defined using the formula:

$$d_{ij}=\sqrt{\frac{\sum_{k=1}^{n}(x_{ik}-x_{jk})^2}{\sqrt{\sum_{k=1}^{n}x_{ik}^2\sum_{k=1}^{n}x_{jk}^2}}} \qquad (4)$$

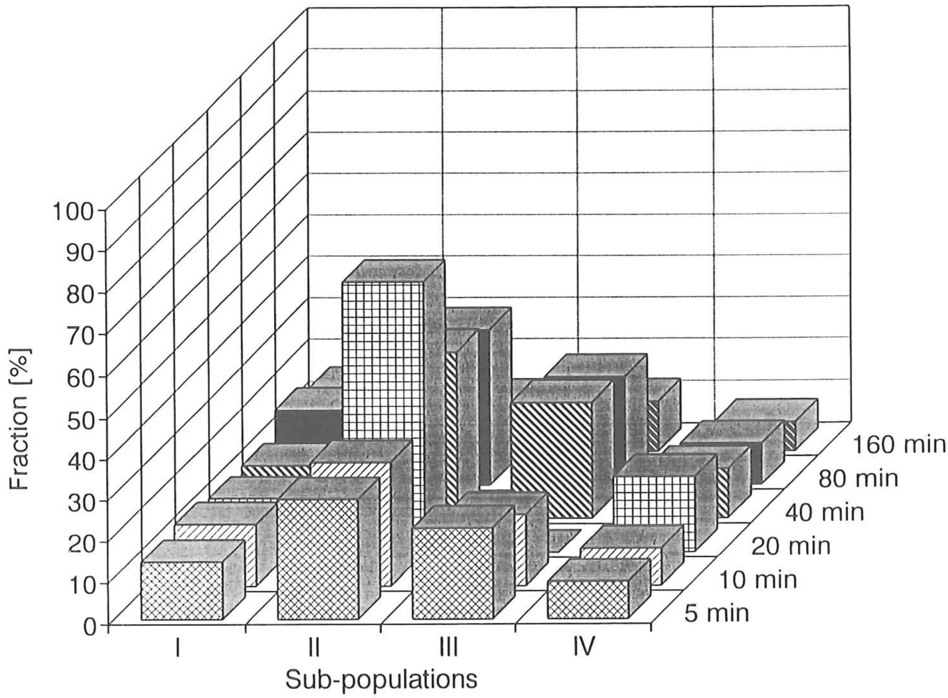
where n is the number of studied grains. In the present example, three parameters (d_n, α, β) have been measured for each grain. It means that m=3 and $x_{i1}=(d_n)_i$, $x_{i2}=\alpha_i$, $x_{i3}=\beta_i$.

RESULTS AND DISCUSSION

The results of grouping are shown in Figures 1 and 2. It has been found generally that the grains in polycrystals of the first set of specimens, annealed at a constant temperature, show much more uniform geometry than the grains in the specimens strained before the annealing. However, in most cases the cluster analysis lead to identification of cluster of grains. The results suggest that population of grains in these specimens can be viewed as build up of two or more sub-populations. One of these sub-populations consist of large grains (d_n>1) and the other consists of small grains (d_n<1). It can be further found that the larger grains show significantly smaller elongation in terms of the mean value of α shape factor.

In one case, annealing time t=40 min., the population of grains has been found to be totally uniform (see Table 2). This is an indication that the degree of homogeneity of the geometrical features of grains varies during the process of grain growth in a non-monotonic way.

Grains revealed in the specimens pre-strained, by 4% elongation, before the anneal have been found significantly less uniform in terms of their geometrical features. There were at least 3 clusters in each population studied. These clusters., for each annealing time, are characterized in Fig.2. It can be noted that again sub-populations of large and small grains can be



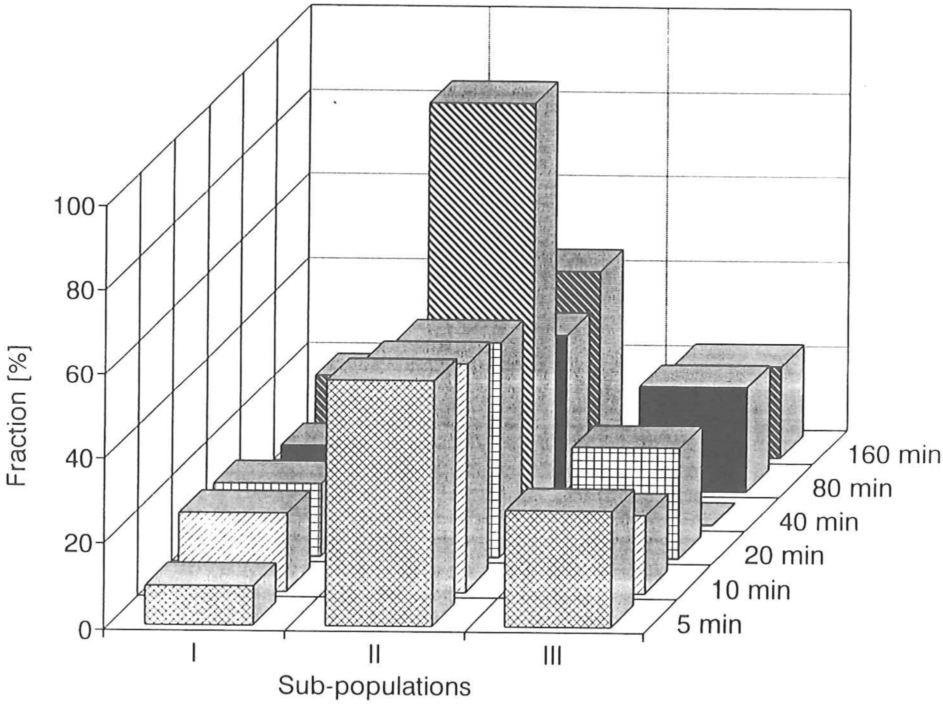
No	F_g	NiMn2, t=5 min, N=636, k=22		
		d_n	α	β
I	14	0.55	1.22	1.16
II	29	0.82	1.26	1.16
III	22	1.23	1.26	1.17
IV	9	1.65	1.27	1.18

No	F_g	NiMn2, t=20 min, N=540, k=7		
		d_n	α	β
I	13	0.46	1.22	1.17
II	65	0.91	1.27	1.17
IV	18	1.56	1.29	1.20

No	F_g	NiMn2, t=40 min, N=425, k=10		
		d_n	α	β
I	13	0.38	1.21	1.16
II	40	0.73	1.28	1.17
III	28	1.26	1.31	1.20
IV	12	1.91	1.33	1.23

No	F_g	NiMn2, t=160 min, N=339, k=29		
		d_n	α	β
I	15	0.43	1.24	1.15
II	12	0.83	1.27	1.15
III	12	1.15	1.29	1.18
IV	7	1.53	1.29	1.18

Fig.1. Number of grains in the clusters (sub-populations) and their characterisaction as a function of annealing time for first set of specimens (see text); No-number of population, F_g-fraction of grains.



No	F_g	NiMn2, t=5 min, N=425, k=8		
		d_n	α	ß
I	9	0.44	1.19	1.16
II	58	0.84	1.26	1.17
III	27	1.37	1.26	1.17

No	F_g	NiMn2, t=20 min, N=241, k=8		
		d_n	α	ß
I	17	0.48	1.24	1.17
II	51	0.88	1.29	1.17
III	26	1.42	1.30	1.17

No	F_g	NiMn2, t=40 min, N=431, k=2		
		d_n	α	ß
I	99.8	1.00	1.29	1.18

No	F_g	NiMn2, t=160 min, N=262, k=11		
		d_n	α	ß
I	19	0.54	1.26	1.16
II	44	0.93	1.28	1.16
III	22	1.38	1.30	1.19

Fig.2. Number of grains in the clusters (sub-populations) and their characterisaction as a function of annealing time for second set of specimens (see text); No-number of population, F_g-fraction of grains.

identified. However, a reversed trend is observed for larger grains to be more elongated that the smaller ones.
In the present the geometrical features of grains have been measured on their 2-dimensional sections. Since the grains are in reality 3-dimensional objects, this simplification significantly reduces possibility for any generalization of the conclusions. Nevertheless, detected changes in the internal structure of the Q-sets describing geometry of grain sections indicate transformations in geometry of 3-dimensional grains and justify further research in this directions.

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