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Computer-aided analysis of grain growth in metals

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ABSTRACT

Isothermal grain growth in aluminium, copper and α -iron was investigated experimentally at elevated temperatures and quantitatively interpreted by computer simulation on the base of a statistical model described in [4,5,6]. As it is demonstrated for the grain growth kinetics, the experimental data can be fitted satisfactorily.

INTRODUCTION

Analysis of grain growth in metals and alloys is a basic problem of materials science and technology and the subject of extensive work. But because an adequate characterization of the phenomenon requires the knowledge of a lot of parameters (e.g. the initial grain-size distribution, driving and dragging forces, grain boundary energies and mobilities) the interpretation of experimental data is often a complicated task. In order to improve the situation computer simulation may be helpful, which took a fast development during the last years (e.g. [1,2,3]). In this connection the following problems are of interest:

- * development and control of theoretical ideas concerning grain growth
- * prediction of microstructure characteristics (mean grain size, grain - size distribution) in annealing processes
- * estimation of grain growth parameters (grain-boundary mobilities and energies) by fitting of experimental results.

The present paper informs about a computer-aided analysis of isothermal grain growth experiments which was performed with several pure metals (aluminium, copper, and α -iron) at elevated temperatures. In all cases the mean grain sizes and the grain-size distributions were measured and compared with numerical simulations based on the statistical grain-growth model developed by ABBRUZZESE et al. [4,5,6]. A statistical model was chosen because it works threedimensionally, uses real scales of time, grain size and temperature, and permits the incorporation of textures and drag forces.

METHODOLOGICAL BACKGROUND

Computer simulation

Grain growth in metals and alloys is usually described statistically in terms of the size distribution $f(R)_{t=\text{const}}$ of spherical crystallites and the well - known growth kinetics

$$R^m - R_0^m = k t \quad \text{or} \quad R = k t^{1/n} \quad \text{for} \quad R \gg R_0, \quad (1)$$

with R - mean grain radius at the time t , R_0 - initial grain radius at $t = 0$, and m, n - growth exponents.

In order to get the temporal changes of the distribution $f(R)$ the continuity equation

$$\partial f / \partial t = - \partial / \partial R (f(R) v) \quad (2)$$

has to be integrated numerically in the (R, t) -space on the base of the equation

$$v = dR/dt = M \Gamma (1/R_c - 1/R) \pm M \Gamma D \quad (3)$$

for the growth rate of the crystallites. R_c is a critical grain radius separating the growing ($R > R_c$) and the shrinking particles ($R < R_c$) of the distribution $f(R)$, M and Γ are the grain boundary mobility and the grain boundary energy, and D is a drag force due to solutes or precipitations.

The simulation of grain growth was realized by means of the programme system SIMU [7] written in Fortran 77 for IBM-compatible PC's. The procedure requires the following input data: the initial grain size distributions $f_k(R_i)$ of the texture components being present, the class width ΔR_i of the grain-size distributions, the time step Δt , the fractions N_k and the total number N of grains at $t = 0$, matrices M_{kj} and Γ_{kj} of grain boundary mobilities and grain boundary energies related to the texture of the sample material, and (if necessary) the drag term D .

In the calculations presented here it was assumed that texture changes can be neglected. This is, of course, an oversimplification, but X-ray investigations showed that in all sample materials the texture variations were small during the annealing treatments used.

Experimental grain size determination

The grain - sizes of the isothermally annealed materials were derived from chord length distributions $f(l)$, which were constructed, in general, from about 2000 chord lengths measured via light microscopy.

The comparison of the experimental results with those of the computer simulation requires a stereological transformation of either $f_{exp}(l)$ into $f(R)$ or $f_{sim}(R)$ into $f(l)$. In the present work the BARTHEL-BÄLTHNER procedure [8,9] was used for this purpose, which also assumes spherical grains and is characterized by the transitions

$$f_{exp}(l) \rightarrow f(r) \rightarrow f(R) \quad \text{or} \quad f_{calc}(R) \rightarrow f(r) \rightarrow f(l)$$

with $f(l)$ - chord-length distribution, $f(r)$ - planar grain-radius distribution, and $f(R)$ - spatial grain-radius distribution.

RESULTS AND DISCUSSION

The sample materials and the annealing treatments used in the present work are given in Table 1.

Table 1 : Sample materials and treatments

Material	Sample treatment	Annealing temperature	Time intervall
Al 99.99	cold-rolling, $\epsilon=90\%$	400°C	60 - 3600 s
Cu 99.99	cold-rolling, $\epsilon=90\%$	400°C	300 - 11100 s
α -Fe 99.95	cold-rolling, $\epsilon=88\%$	750°C	60 - 10800 s

The mean grain sizes $R = R(t)$ derived directly from the annealing experiments and the grain-growth kinetics obtained by computer simulation are illustrated in Fig. 1, 2 and 3.

Fig. 1:
Isothermal grain growth in
Aluminium ($T = 400^{\circ}\text{C}$)

Fig. 2:
Isothermal grain growth in
Copper ($T = 400^{\circ}\text{C}$)

Fig. 3:
Isothermal grain growth in
 α -Iron ($T = 750^{\circ}\text{C}$)

The grain-growth exponents m, n as measured directly and obtained in the best fit of the growth kinetics are summarized and compared in Table 2.

Table 2: Grain growth exponents m, n

Material		m_{exp}	m_{sim}	n_{exp}	n_{sim}
Al	a)	1.34 ± 1.96		0.22 ± 0.03	
	b)	-	1.08 ± 0.59	0.20 ± 0.06	0.24 ± 0.02
Cu	a)	2.66 ± 0.36		0.33 ± 0.02	
	b)	2.68 ± 0.20	2.86 ± 0.04	0.39 ± 0.02	0.37 ± 0.00
α -Fe	a1)	5.45 ± 0.01	3.48 ± 0.21	0.15 ± 0.01	0.20 ± 0.03
	a2)	6.87 ± 0.81	6.16 ± 1.49	0.02 ± 0.07	0.005 ± 0.002
a) mean chord length l				b) mean grain radius R	
a1) $t < 1800$ s a2) $t > 1800$ s					

Both the table 2 and the graphs can briefly be commented as follows :

* Computer simulation by means of the statistical model of ABBRUZZESE et al. [4,5,6] allows a satisfactory formal interpretation of experimentally observed isothermal grain growth. The grain boundary parameters (mobility M , energy Γ , drag D) estimated in this manner are in good correspondence with experimental data [7]. For instance, for Cu the quantities $M = 3.1 \cdot 10^{-5} \text{ cm}^4/\text{Js}$ and $\Gamma = 6.5 \cdot 10^{-2} \text{ mJ/cm}^2$ were found which well agree with the values $M = (1.6 - 3.3) \cdot 10^{-5} \text{ cm}^4/\text{Js}$ and $\Gamma = (5.0 - 6.5) \cdot 10^{-2} \text{ mJ/cm}^2$ given in the literature.

* As it can be understood easily, the remaining differences between experiment and computer simulation increase with decreasing purity of the sample material (e.g. Cu, Al $\rightarrow$ α -Fe) and (or) with decreasing statistical reliability of the experimental data (e.g. Cu $\rightarrow$ Al due to the stereological transformation $f_{exp} \rightarrow f(R)$).

In α -Fe two stages of isothermal grain growth were observed at 750°C and formally explained by a drag term. However, as it shall be mentioned yet, the apparent stagnation of the grain growth can also be caused by various growth rates of the crystallites of different texture components (A more detailed investigation of the effect is just performed) which must not be accompanied by a drastic change of the character of the orientation distribution.

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