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Grain Boundaries of Primary Crystallization

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The interest of researchers to the problems of the physics of grain boundaries is caused by the great role these defects play in the formation of the properties of real materials.

The appearance of large-angle boundaries close to the special Kronberg-Wilson boundaries in polycrystalline materials is of special importance due to their unique physical properties [1, 2].

A large number of investigations carried out recently in this field was aimed at the study of integrain disorientation in artificially created model polycrystalline structures and also in deformed and recrystallized structures of real metals and alloys [1–6].

However, a very important type of real polycrystalline structures that is initial crystallization structures has remained unexplored from the point of view of its quantitative assessment of intergrain disorientation ensemble despite the wide usage of such materials in technics and the importance of initial crystallization grains in the succeeding processes of deformation and recrystallization.

The aim of the present investigation is to give quantitative assessment of grain boundaries ensemble of two industrially produced alloy with f.c.c. solid solution structure in casting by means of precision analysis of individual disorientations of grains.

The subject of investigation

The investigated materials were Al-Zn-Mg alloy (about 91 % of Al) and German silver Cu-Ni-Zn (about 65 % Cu). Both specimens were cut of the centre of an initial crystallization slab with the average size of grains about 1 mm and without distinct texture, which was proved by direct pole figures method.

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Experiment

Precision data on individual disorientations of grains were obtained by means of local X-ray diffractometry method with the use of an original goniometric set to the standard X-ray diffractometer, a micro X-ray collimator and optical appliance supplied with optical aiming at individual grains of the polycrystal.

Angular parameters of basis lattice vectors measured in the laboratory system by means of putting each grain into "reflecting" position served as initial experimental data for the calculation of grain boundaries parametres. Computerized evaluation of grain boundaries parametres was done with the use of matrix algebra and Gibbs vectors technique [7, 8].

The method which has been recently successfully used in investigation of large grain structures of recrystallized materials enables us to calculate grain parameters with the accuracy of 6 angular minutes [2, 7–10].

Experiment resulted in full crystalgeometrical description of grains and their boundaries including the following characteristics;

1. Gibbs vector for each grain describing its orientation in a coordinate system of the specimen;
2. Direct point pole figure <100> of each grain (projection of axes <100> in stereographic circle);
3. Inverse pole figure of each grain for any macroscopic axis of a specimen (coordinates of the given axis in the standard stereographic triangle);
4. Disorientation angle Θ for each pair of grains and their directional cosines p, q, r of the axis $[pqr]$ with respect to mutual positions of the said grains in the crystalline basis (these values are given in terms of minimal angles Θ as to exclude discrepancies in the symmetry of lattice orientation);
5. Orientation of the $[pqr]$ axis for each pair of grains in the coordinate matrix of the specimen (the $[pqr]$ axis projections in the stereographic circle);
6. Orientation of the $[pqr]$ axis for each pair of grains in the crystalline matrix (coordinates of $[pqr]$ axis in the standard stereographic triangle).

Additional data was obtained: by means of computer analysis of the parameters of each experimental boundary as to their proximity to Kronberg-Wilson values using Brandon criterion.

7. The number of a boundary (numbers of grains of their respectiv pair- related to the class of the boundaries close to these of special Brandon boundaries and their parameters Θ, p, q, r;
8. Canonic parameters of the special Kronberg-Wilson boundary, the closest to the estimated CS boundary: special disorientation angle Θ_{0i}, indices of rotation axis p_{0i}, q_{0i}, r_{0i} and the value of recirpocal density of coinciding centres Σ_i;
9. Angle of total "additional rotation" $\Delta\Omega_i$ of the given CS disorientation to reach the nearest special disorientation;
10. The angle of "specific additional rotation" $\Delta\Omega_i$, $\sqrt{\Sigma_i}$, that is the quantitative

evaluation of proximity of the given experimental boundary to the closest special boundary (in the case when $\Delta\Omega_i \sqrt{\Sigma_i} < 15°$ the given boundary is of the CS type according to Brandon).

The set of above named parameters obtained for a considerable enough number of individual disorientations allows to describe the grain boundaries ensemble as a whole and to plot the distribution of grain boundaries against most important values and also evaluate the percentage of CS boundaries in the experimental set.

Results and discussion

Fig. 1 and 2 represent distribution of 38 grain boundaries in the cast Al-Zn-Mg alloy and that of 26 boundaries in the cast German silver according to their disorientation angles Θ. It can be seen that in initial crystallization structures of both

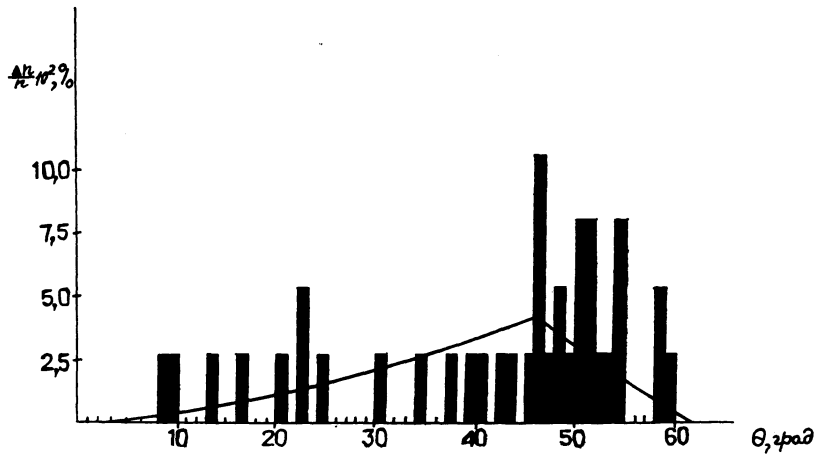

Fig. 1. The angular disorientation distribution histogram for the grains of cast Al-Zn-Mg alloy. The solid line shows the distribution for the chaotically disoriented grains (CDG).

alloys the intergrain disorientation angles were formed at all possible angles. It should be noted that the number of small-angle disorientations ($\Theta < 15°$) is relatively small but that for the range 45–50° is essentially greater for both distributions. Comparison of these spectra and the results of computer modelling for the chaotically disoriented grains (CDG) [9, 10] (solid lines in fig. 1 and 2) shows certain resemblance of the real spectra and the model one. This results is not unexpected because of the absence of distinct crystalline texture of grains and the specimens having been cut from the central part of slabs.

Some differences between the investigated sets of disorientations and the CDG ensemble can be noted as to the distribution of grain axes in the standard stereographic triangle. For the cast Al-Zn-Mg alloy the area around ⟨100⟩ pole is the least

preferable, the same is right for the area ⟨111⟩ in the case of German silver, but for the CDG ensemble the stereographic triangle is approximately evenly filled with [*pqr*] axis projections [11].

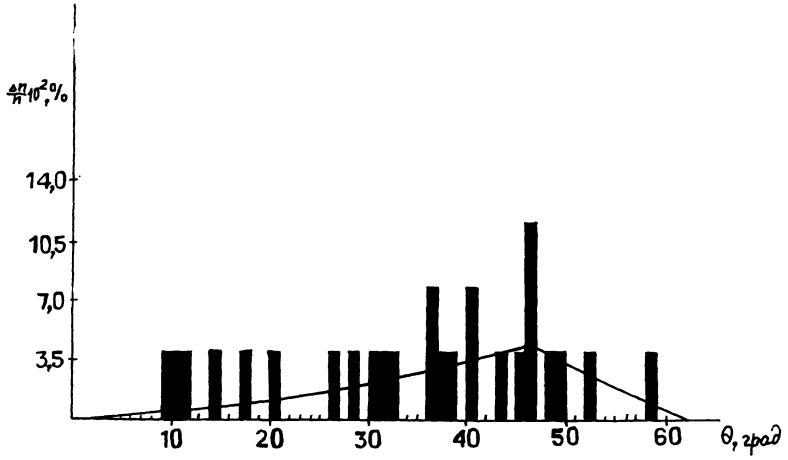

Fig. 2. Angle disorientation distribution histogram for the grains in cast German silver; the solid line corresponds to distribution for the CDG.

The potentialities of the described method can be proved in the process of analysis of proximity of the given boundary to the special disorientations. The results of this analysis are given in table 1, containing additional data on boundaries, referred to the CS type. In computerized analysis of boundaries ensemble in Al-Zn-Mg alloy (table 1) a standard set of special boundaries for $\Sigma_i \leqq 49$, was used; while analysis for German silver a vater range of boundaries was used, namely $\Sigma_i \leqq 99$ (table 1).

The total number of CS boundaries in each of the investigated materials can be compared with the similar quantity for the model CDG ensemble where only randon distribution of CS boundaries exist.

The percentage η of CS boundaries in the model spectrum of CDG comprises 14,7 % for special disorientations at $\Sigma_i \leqq 49$ and 21,0 % at $\Sigma_i \leqq 99$ [9, 10]. Corresponding values of η for grain boundaries ensemble of cast German silver are 23,1 % and 30,8 % and for cast Al-Zn-Mg alloy is 26,3 % at $\Sigma_i \leqq 49$ (the data at $\Sigma_i \leqq 99$ have not been obtained).

Considering rather poor statistics of experimental disorientations we found the prevalence of energetically profitable CS boundaries at the rate 1,5−2,0 for both cast alloys if compared with CDG ensemble. It should be noted, that every line of the table 1 is not just of a statistical value, but proved the existence of the above named CS boundary and this fact is due to precision of the method.

The results lead to the idea that the centres of craystllization of the studied alloys though having no specific crystalline orientation in the central part of a slab yet

Table 1. Close to special (CS) boundaries in the cast Al-Zn-Mg alloy and German silver alloy.

alloy	number of grains pair	CS boundaries parameters				corresponding special boundaries					total additional rotation $\Delta\Omega_i$, deg.	specific rotation $\Delta\Omega_i\sqrt{\Sigma_i}$ degress
		Θ, degrees	p	q	r	Θ_{0i} deg.	p_{0i}	q_{0i}	r_{0i}	Σ_i		
Al-Zn-Mg	10—11	50.10	0.7729	0.5720	0.2771	50.13	3	2	1	39	2.22	14.50
	12—65	47.27	0.6820	0.6455	0.3436	46.39	2	2	1	29	1.40	8.56
	131—132	51.51	0.7126	0.7013	0.0195	50.47	1	1	0	11	1.44	5.44
	10—11	30.49	0.7363	0.6742	0.0575	31.58	1	1	0	27	2.22	12.15
	11—131	51.12	0.7833	0.5477	0.2939	50.13	3	2	1	39	2.01	12.38
	10—5	59.02	0.6456	0.6248	0.4392	60.76	3	3	2	43	2.05	13.42
	111—5	59.16	0.5891	0.5815	0.5611	59.99	1	1	1	3	1.22	2.22
	77—132	54,15	0.6167	0.5650	0.5481	59.99	1	1	1	3	6.22	11.02
	62—63	42.03	0.9533	0.3016	0.0151	43.13	3	1	0	37	1.24	8.11
	64—63	46.35	0.8845	0.4651	0.0354	48.18	2	1	0	15	2.28	9.34
Cu-Ni-Zn German silver	3—5	36.04	0.9948	0.0754	0.0691	36.86	1	0	0	5	3.45	8.24
	5—7	38.46	0.9848	0.1230	0.1049	36.86	1	0	0	5	6.19	14.08
	6—8	40.51	0.9898	0.1091	0.0913	36.86	1	0	0	5	6.31	14.35
	1—11	40.06	0.9921	0.1254	0.0093	36.86	1	0	0	5	5.44	12.49
	13—17	28.48	0.7154	0.6979	0.0336	26.52	1	1	0	19	2.29	10.50
	13—16	36.37	0.9723	0.2339	0.0033	35.19	4	1	0	93	1.28	14.10
	12—13	14.34	0.9919	0.0904	0.0887	16.26	1	0	0	25	2.35	12.54
	1—3	46.21	0.9432	0.2937	0.1551	48.62	1	3	1	87	1.07	10.20

caused the appearance of the ensemble of large angle disorientations, which is similar to CDG spectrum but special disorientation could be formed at the stage of formation of atomic structure of grains due to energetical profitability of special disorientations which showed itself in the enhanced percentage of relative part of low-energy CS boundaries in the composition of initial crystallization grains.

Very significant is the fact of appearance in the structure of cast Cu-Ni-Zn German silver of considerable amount of CS boundaries with $\Sigma_i = 5$ which can not be practically found in pure Cu polycrystalls and this fact shows the essential influence of alloys on the electronic descrement into intergrain interaction energy which is the most responsible for the realization in the material of definite CS boundaries out of the set of theoretically possible for the given syngony.

Conclusion

1. The grain boundaries ensemble in the central parts of cast aluminium and copper based alloys is similar to model CDG ensemble as to disorientation angles spectrum but distinctly differs from CDG ensemble as to orientation of grain axes distribution.

2. Experimental data indicate the possibility of existance of the conditions for special boundaries realization in the central part of the slab.

3. An essential pereentage of CS boundaries existing in the polycrystalline Cu-based solid solution is not energetically profitable in pure Cu.

4. High precision estimation of crystal geometry of grain boundaries ensemble in metal slab improves our knowledge of the crystallization process and can be used for prediction of cast metals and alloys properties and prediction of structural changes in materials due to deformation and recrystallization.

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