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Analysis of grain misorientation distribution in polygonal ferrite of low-carbon steel

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ABSTRACT

A method to deduce the origin and crystallographic features of the polycrystalline state basing on the analysis of misorientation distribution function is considered. According to this approach, the misorientation distribution is represented in the form of linear superposition of partial distributions, each distribution corresponding to the boundaries of a specific physical nature. Then the fractions of the boundaries of different types in the overall structure are determined from the best fit of the computed distribution to the experimental data. In the present work the method is applied to a low-carbon ferrite-pearlite steel. The emphasis is made on the boundaries, whose misorientations are predetermined by orientation relationship between parent austenite and ferrite, i.e. on the so-called crystallography-specified or inter-variant boundaries. It was shown that they constitute about one third of the total amount of boundaries in the polygonal ferrite microstructure.

1. Introduction

The polycrystalline structure of metallic materials is often formed in the course of complex multistep process. In addition to crystallization from the melt, this process may include phase transformations in the solid state, plastic deformation as well as recrystallization and grain growth. Analysis of the distribution of misorientations between crystallites can be utterly useful in order to study the nature and crystallographic features of the polycrystalline state and to provide information on the processes involved in the microstructure formation during plastic deformation, recrystallization and phase transformations [1–13]. Recently the quantitative analysis of that kind has been used for investigation of the microstructure developed during explosive bonding of copper plates [10,11]. A misorientation distribution was represented by the sum of partial distributions, each of which corresponds to the boundaries of a specific nature, whereupon the fractions of the boundaries of different kinds in the overall microstructure are determined from the best fit of the computed distribution to the experimental data. Using this approach, it has been shown, in particular, that the microstructure of bonding interface zone forms substantially by deformation twinning.

A polycrystalline structure formed during phase transformation may contain peculiar boundaries, which misorientations are predetermined by an orientation relationship (OR) between the final and the parent phase. These boundaries arise between distinct orientation variants appeared due to a symmetry of the crystal lattices of the phases. In an early study [14], where their possible misorientations have been calculated for steels and titanium alloys, they were called crystallography-predetermined boundaries. At present the term "inter-variant boundaries" is used in the literature [15–16].

In steels, in the cases of martensite or bainite transformations, the crystals of the final α phase grow only into that grain of the parent γ phase, with which they have strict OR [16–18]. As a result, all boundaries formed between α crystals inside the parent γ (austenite) grain are the inter-variant ones. Correspondingly, their fraction within steel microstructure is always rather high, usually about 90% [19].

Quite otherwise the microstructure of polygonal ferrite is formed in the course of diffusional transformation. In this case an α (ferrite) crystal nucleated at an austenite grain boundary has slow-moving coherent boundary with the austenite grain, with which it has the OR [20]. Then this crystal will grow more rapidly into other austenite grain, with which it has highly mobile random boundary [20–21], Fig. 1. Under these circumstances, as one can see in Fig. 1, the ferrite crystal α_1 will form inter-variant (I-V) boundary with the crystal α_2, which has OR with the same austenite grain (γ_1), while it will form random (R) boundary with the crystal α_3, which has OR with other austenite grain (γ_3). It is difficult to predict the fraction of inter-variant boundaries within the ferrite microstructure, though anyway it is expected to be much lower than in the case of displacive transformation. Nevertheless, as far as we know, the quantitative

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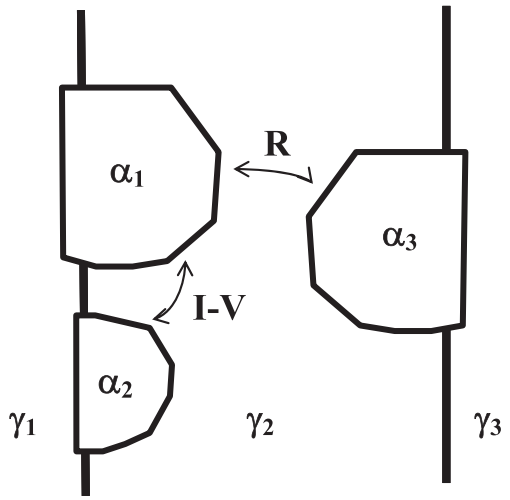

Fig. 1. Schematic image of the growth of the ferrite grains (α_1, α_2, α_3) nucleated at the boundaries of austenite grains (γ_1, γ_2, γ_3). Growing nuclei form inter-variant (I-V) or random (R) boundaries depending of their nucleation conditions [21].

characterization of inter-variant boundaries in polygonal ferrite hasn't been carried out up to date.

In the next part of the present article the method of misorientation distribution analysis is considered on the simple example of polycrystalline copper. Then the method is developed as applied to the polygonal ferrite microstructure formed as a result of phase transformation in low-carbon steel. The main purpose of this study is to characterize quantitatively a fraction of the boundaries, whose misorientations are predetermined by orientation relationship between γ and α phases.

2. Experimental

Low-carbon plain steel Fe-0.18C-0.21Si-0.33Mn (wt%) was studied in the as-delivered state, after austenitization at 920° and subsequent air cooling (normalization). As a result, the fine-grained ferrite-pearlite microstructure containing 16% pearlite was obtained (Fig. 2). EBSD with SEM Quanta 3D FEG was carried out at the accelerating voltage of 20 kV; EDAX Pegasus system was used to process the obtained data. The specimen area 180 * 250 μm^2 was scanned with the step of 0.15 μm. Since quality of diffraction patterns from thin cementite lamellae of pearlite is rather poor, EBSD maps only ferrite orientations. Meanwhile, as shown earlier with different techniques [22–24], proeutectoid ferrite continues to grow during lamellar pearlite formation as part of a pearlite colony without a change in crystallographic orientation. Hence, EBSD orientation mapping can hardly discriminate a pearlitic region from an adjacent ferrite grain. A modest fraction of such regions, however, is expected not to have any notable effect on the statistics of misorientations of ferrite-ferrite boundaries. The analysis of EBSD data was carried out with MTEX software [25].

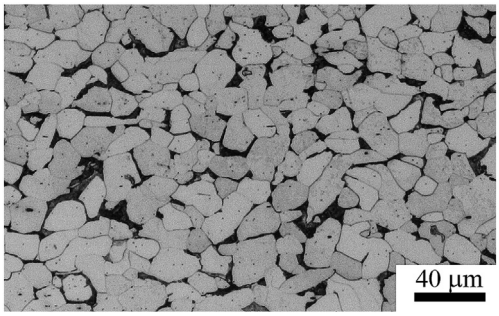

Fig. 2. Optical microscopy micrograph of the steel sample.

3. Method of Misorientation Distribution Analysis

A misorientations distribution function $F_\alpha(\theta)$ is represented by the expansion in terms of partial misorientation functions $F_\alpha(\theta)$, each function describing boundaries of a certain type:

$$F(\theta) = \sum_\alpha \eta_\alpha F_\alpha(\theta), \quad (1)$$

where η_α is a fraction of boundaries of the type α. The Eq. (1) is supplemented by the normalization requirement $\sum_\alpha \eta_\alpha = 1$. At first, the functions $F_\alpha(\theta)$ describing adequately the partial misorientation distribution are to be defined. After that the values of the coefficients η_α are fitted, which provide agreement of the numerical model to the experimental data.

Let us consider the application of this approach on the simple example of recrystallized copper [10]. The misorientation distribution obtained by electron backscatter diffraction (EBSD) is presented in Fig. 3 by a histogram. As long as many twins are formed during annealing of copper, its microstructure includes boundaries of the following types: random boundaries ($\alpha = 1$), Σ3 boundaries of 1st order twins ($\alpha = 2$) and Σ9 boundaries of 2nd order twins ($\alpha = 3$). Contribution of twins of higher orders was not considered since their amount is negligible. Each of these three boundary types has individual misorientation distribution, that has to be generated by numerical modeling.

An array of misorientation for random boundaries can be produced assuming grain orientations to be fully random if the material under consideration has no crystallographic texture. Corresponding misorientation distribution distinguished by the maximum at 45° is well known [1,12]. It can be generated by numerical modeling as follows. A random orientation is specified by three Euler angles (φ_1 Φ φ_2) using a random-number generator, and then the Euler angles are transformed to the orientation matrix $\mathbf{A}_1$ [1]. Similarly a matrix of another random orientation $\mathbf{A}_2$ is obtained. Their misorientation is determined by matrix equation

$$\mathbf{R}_r = \mathbf{S}_m \cdot \mathbf{A}_1 \cdot \mathbf{A}_2^{-1}, \quad (2)$$

Here $\mathbf{S}_m$ is a matrix of one of 24 symmetry operations, where index m corresponds to the operation providing minimum angle of

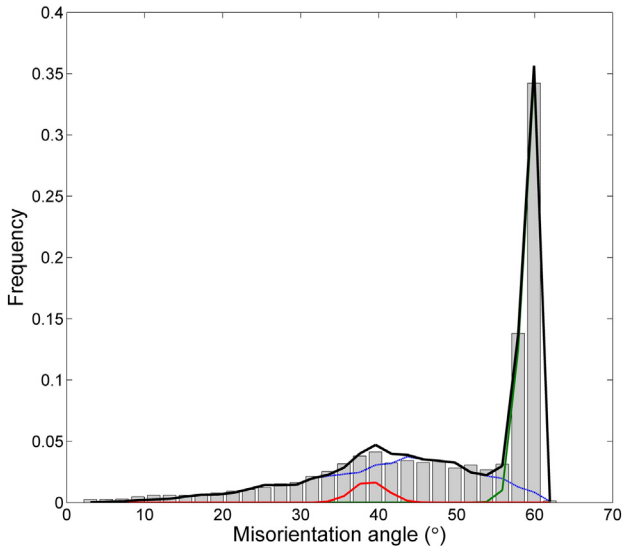

Fig. 3. Experimental (histogram) and computed (thick line) misorientation distributions in copper. Partial distributions for 1st order twin ($\theta_{\Sigma 3} = 60°$, thin brown line), 2nd order twin ($\theta_{\Sigma 9} = 38.9°$, thin green line) and random boundaries (dotted blue line) are also represented. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)