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Report on the PhD thesis of Mr Krzysztof GŁOWIŃSKI

« METHODS FOR QUANTITATIVE CHARACTERIZATION OF THREE-DIMENSIONAL GRAIN BOUNDARY NETWORKS IN POLYCRYSTALLINE MATERIALS»

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The PhD thesis presented by Mr Krzysztof Głowiński is devoted to the problems of characterization and analysis of grain boundaries and their networks in polycrystalline materials. The development of software for handling boundary parameters, essential in tailoring of materials with required properties, is an important part of this thesis. It is well known that in order to characterize a grain boundary or a set of grain boundaries, one has to use five parameters: three of them define misorientation and the remaining two - the orientation of grain boundary plane. The calculation methods developed in the thesis of Mr. Krzysztof Głowiński enable to extract these parameters from 3D electron backscatter diffraction technique (EBSD) and/or from transmission electron microscopy (TEM) measurements.

Structure of the thesis

Generally, the text is written in very good English.
The manuscript consists of 134 pages, it is well structured and correctly presented. It contains 9 chapters, two appendices, the list of abbreviations and the list of bibliography.

Chapter 1 contains a general introduction to the problems of grain boundary characterization.

Next, in Chapter 2, the current state of the field and literature review is presented. In this part, a reader finds basic definitions, a review of parameters and computational methods used in the field of grain boundary characterization as well as remarks concerning their limitations.

In Chapter 3, the objective of the work is defined. The most important are: creation of effective tools to distinguish different types of boundaries (tilt, twist, symmetric and 180^0 tilt boundaries), an alternative approach to computation of the boundary distribution based on the kernel density estimation (KDE), creation of a new scheme of grain boundary distribution and elaboration of new calculation tools for the above purposes.

Chapter 4 is devoted to the problem of the reconstruction of boundary networks. The Author presents here the examples of visualisation of grain boundary networks extracted from three experimental data sets.

Chapter 5 is essential for the presented thesis, because different methods for quantifying the character of a boundary are reviewed. Especially, it deals with the problem of distinguishing different types of boundaries (i.e., twist, tilt, twin, symmetric and 180^0). Also new parameters for estimation of the distance between two orientations are proposed. Moreover, the example sections through the experimental distributions of WC/WC boundaries are shown.

In Chapter 6, the new approach to computation of boundary distributions is presented. This approach is based the use of kernel density estimation. It has an advantage over discretization by binning because it gives more precise results. Example sections through the distribution of grain boundaries, obtained with kernel density estimation, are presented. A new result is also the calculation of boundary planes distribution in the laboratory reference frame.

In Chapter 7 the Author presents the package of computer programs used in the thesis.

An interesting result is contained in Chapter 8 entitled 'Final Remarks'. Besides comments on particular problems encountered in grain boundary analysis, there is a comparison of boundary distributions to computed boundary energies. The main conclusion is that in many cases the grain boundaries with the lowest energy are most numerous. This result could be expected, because it confirms a general principle of minimization of energy in physical systems.

Finally, Chapter 8 contains concluding remarks, and Chapter 9 is devoted to the summary of the thesis.

One should also note Appendix B, where the Charts for interpreting functions of macroscopic parameters, created by the Author, are shown.

Main achievements of Thesis

The thesis makes a contribution to the material science in the field of grain boundary geometry and, more specifically, in the methods of determination of their distributions.
I would underline the following achievements of the thesis of Mr. Krzysztof Głowiński:
* Elaboration of precise criteria for the distinction between tilt, twist and mixed boundaries. Three different sets of parameters have been analyzed as possible measure of this closeness:
- the smallest angles of boundary components obtained from Fortes decomposition,
- strictly defined distances to pure twist or tilt boundaries: δ_L and δ_N, and
- new parameters α_L and α_N defined as the maximal values between the misorientation axis and the normal to the boundary plane. It was found that the latter parameters are very strongly correlated to strictly defined distances to pure twist or tilt boundaries: δ_L and δ_N, but their calculation is much simpler and it needs much less computer time. These parameters were mostly used in the thesis.
* The methods for identification of symmetric and 180^0-tilt boundaries have been studied and applied.
* Distributions of the newly defined closeness parameters were calculated for three experimental data sets concerning grain boundaries. The studied material were WC-Co composite, ferrite and two nickel based superalloy.
* The new method of the computation of boundary distributions, based on kernel density estimation was proposed and used.
* The kernel density estimation technique has also been used for computing the distributions of boundary planes. These distributions were analyzed not only in the crystal reference frame, but also in the laboratory coordinates system. The latter result is original and enables new types of analyses.
* The calculation of grain boundaries energy was performed. It revealed that generally one observes a high density of grain boundaries when their energy is low.
* A complete set of calculation methods and corresponding computer programs for grain boundary analysis was elaborated. In the case of application of new parameters of distance closeness between grain boundaries (α_L and α_N) - the calculation time was drastically reduced.

Critical Remarks

I have found two places which are not clear for me;

- what is the sense of Eq. 2.4 (p. 23) if the condition $\mathbf{l}\cdot\mathbf{u}=0$ has to be fulfilled ?

- Figs. 5.11 and 5.12 have exactly the same captions. So, what is the difference between them?

Conclusions

The PhD Thesis presented by Mr. Krzysztof Głowiński is dedicated to the study and analysis of grain boundaries and their distributions using a full five-parameter description. Such kind of grain boundary characterization will enable examination and tailoring of polycrystalline materials with required properties.

It can be concluded that the PhD Thesis presented by Mr. Krzysztof GŁOWIŃSKI is original and has many theoretical and practical implications.

Mr. GŁOWIŃSKI showed that he can solve theoretical, computational and practical problems using different tools and showing scientific criticism. This work brings a real progress in the studied field and proves the scientific maturity of Mr. Krzysztof GŁOWIŃSKI.

I wish to underline that the presented work fulfils all the criteria concerning the doctoral theses in respect to the law concerning scientific degrees and titles.

In conclusion, I express my very favourable evaluation of the PhD thesis presented by Mr. Krzysztof GŁOWIŃSKI and I recommend that the permission for a public defence of his thesis is granted.

Moreover, I propose to distinguish this thesis.

Kraków, 10-th April 2015

Professor K. Wierzbanowski

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