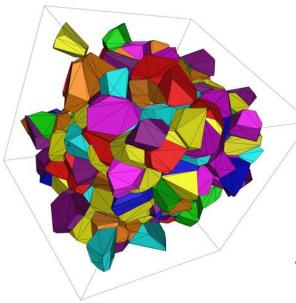




EUROPEAN UNION





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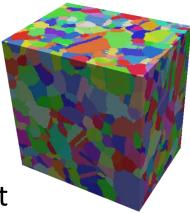
Introduction

Recently, progress in 3D microstructure imaging techniques has been made

Resulting data sets are large enough for carrying out statistical studies

Our goal is to get quantitative information about grain boundary networks based on all five macroscopic parameters

□ For this purpose, dedicated software tools are needed









Software toolbox for geometric grain boundary characterization

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Distribution of boundary plane normals: Count boundaries which are simultaneously (assuming criteria specified in brackets): tilt $(\delta < 3 \circ)$ symmetric $(\delta < 3 \circ)$ tilt (decomposition) $(v < 5 \circ)$ tilt (decomposition) $(v < 5 \circ)$ CSL $(\Delta\omega \le \omega_0 / Z^P,$ • all Σ-values where $\omega_0 = 15 \circ \wedge p = 0.5 \land \Sigma \le 50$	arameters p	present in all files	will be used for analyzes. Total number of boundaries: 1113546		
tilt $(\delta < 3^\circ)$ \checkmark twist $(\delta < 3^\circ)$ \checkmark symmetric $(\delta < 3^\circ)$ \checkmark improperly quasi-symmetric $(\delta < 3^\circ)$ \checkmark tilt (decomposition) $(v < 5^\circ)$ \checkmark twist (decomposition) $(\lambda < 5^\circ)$ \checkmark CSL $(\Delta \omega \le \omega_0 / Z^p)$, \checkmark \checkmark \checkmark \bullet all Σ -valueswhere $\omega_0 = 15^\circ \land p = 0.5$ $\Lambda \Sigma \le 50$ \checkmark		of boundary plan			
tilt (decomposition) $(v < 5^\circ)$ it twist (decomposition) $(\lambda < 5^\circ)$ CSL $(\Delta \omega \le \omega_0 / \Sigma^p)$, it \odot all Σ -values where $\omega_0 = 15^\circ \land p = 0.5^\circ \land \Sigma \le 50^\circ$					
$ \begin{array}{c c} \textbf{CSL} & (\Delta \omega \leq \omega_0 / \Sigma^p, & & \\ \hline \bullet & \text{all Σ-values} & \text{where } \omega_0 = 15 \circ \land p = 0.5 \land \Sigma \leq 50) \end{array} $		laries which are s		(δ < 3 °)	
ⓒ all Σ-values where $ω_0 = 15$ ° ∧ p = 0.5 ∧ Σ ≤ 50)	🗌 tilt		(δ < 3 °) 🔲 🗸 twist		
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■ We have developed pieces of computer software essential for quantitative analysis of grain boundaries

The results and figures on the following slides have been obtained mainly using our program

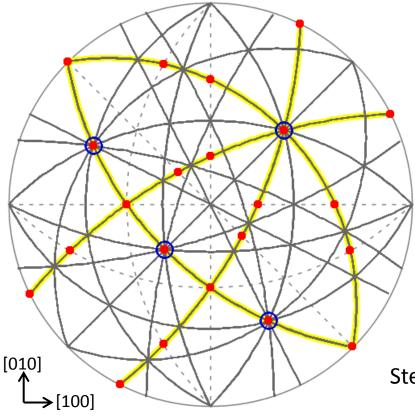
Screenshot of one of the modules included in the package



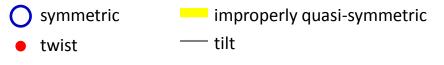




All characteristic GBs for a given fixed misorientation



- Exact locations of characteristic GBs are calculated analytically
- Crystal symmetry is taken into account
- The catalogs can be directly linked to experimentally measured boundary distributions



Stereographic projections of boundary plane normals of various characteristic boundaries for the Σ3 misorientation (cubic symmetry)

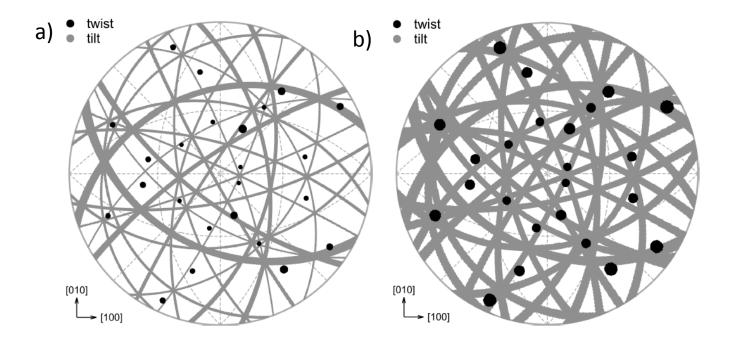






Experimental errors. Classification as tilt, twist, etc.

What do the catalogs look like if we introduce experimental errors?



- □ The decomposition (a) and minimization (b) methods have been compared
- The decomposition technique appears to be more dependent on particular geometric configuration
- Moreover, the distance minimization method can be easily extended to search for symmetric, quasi-symmetric boundaries







Frequencies of occurrence of geometrically characteristic boundaries among random grain boundaries

The frequencies have been calculated for various types of boundaries and different crystal symmetries

Cubic symmetry

Tol.	Tilt*	Twist*	Symmetric	Improp. quasi-sym.
1 °	39.2	0.4	0.002	0.3
2 °	66.4	1.7	0.02	1.3
3 °	84.0	3.9	0.07	2.9
5°	98.5	10.7	0.33	8.0

Hexagonal symmetry

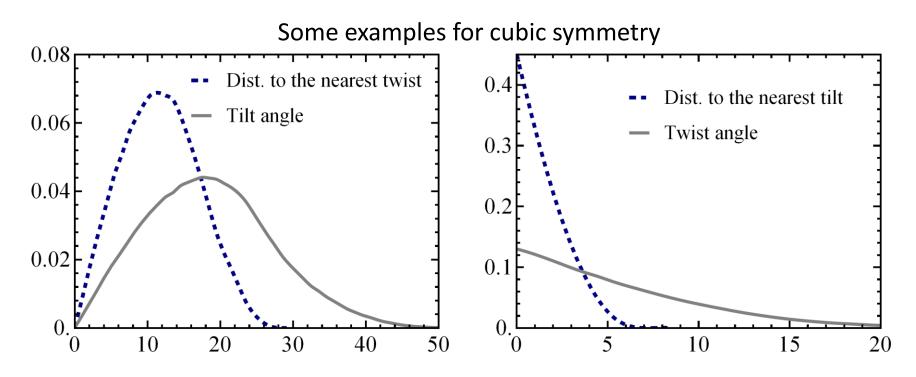
Tol.	Tilt*	Twist*	Symmetric	Improp. quasi-sym.
1 °	21.2	0.2	0.002	0.28
2 °	39.2	0.9	0.01	0.7
3 °	54.3	2.0	0.03	1.5
5°	76.8	5.4	0,16	4.0







Probability density functions for the distances to the nearest characteristic boundaries and for the angles of components



Analogous plots have been obtained also for hexagonal, tetragonal and orthorombic symmetries, and for distances to other types of characteristic boundaries. Moreover, corresponding cumulative distribution functions have been calculated.



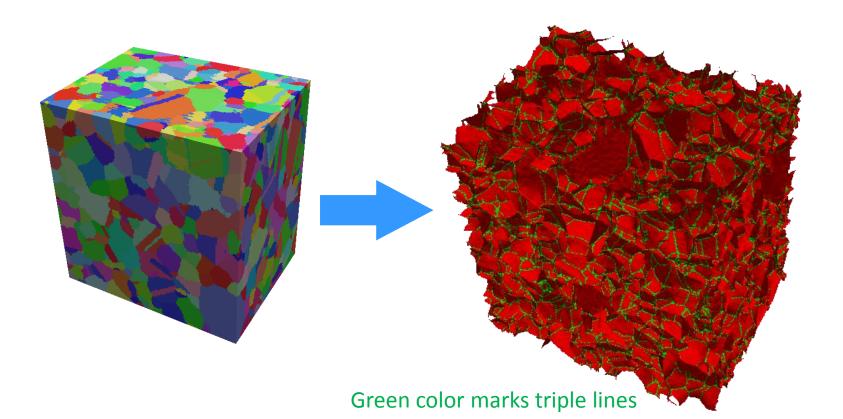




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Reconstruction of grain boundary surfaces from experimental data

Our software tools have been tested on randomly generated boundaries. The next step is to apply our algorithms to experimental data.

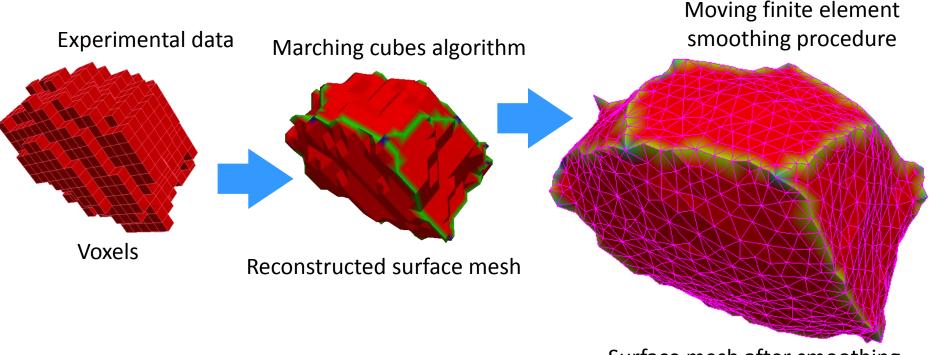








Boundary segments reconstruction



Surface mesh after smoothing

Reconstruction is done using DREAM.3D computer program
 The output from DREAM.3D can be easily read
 These data are then processed by our software (in progress)







Summary

□ The first version of our program is ready

□ Using the package, one can generate catalogs of characteristic boundaries for a fixed misorientation, it is also possible to calculate the frequencies of occurrence of characteristic GBs

□ Tools for analysis of experimental data are being developed