

# Cubic以外の解析 E B S D データから配向関数計算

T e t r a g o n a l   C u F e S 2

MTEX5.1.1/data/EBSD/olivineopticalmap.ang

2023年03月28日

H e l p e r T e x   O f f i c e

# Angデータ変換(複数相からCuFeS2を選択)

The screenshot shows the EBSDtoODF software interface. The 'InputData' section has 'InputFile' set to 'C:\mteX-5.1.1\data\EBSD\olivineopticalmap.ang'. The 'MaterialData' section has 'Material' set to 'cif' and '.TXT .cif file'. The 'Group' is 'P1', 'Symmetry(OIM)' is '42', 'HKLCode' is '5', and 'LaboTex' is 'AllPhase'. The 'Aaxis' is '5.24', 'Baxis' is '5.24', 'Caxis' is '10.3', 'alpha' is '90.0', 'beta' is '90.0', and 'gamma' is '90.0'. A list of phases is shown below, with 'Chalcopyrite' selected. The 'Makefile' section at the bottom has 'DataStartline' set to '180', 'PhasePotision' set to '8', and 'LaboTex-SOR' selected. The 'Holder' is 'C:\mteX-5.1.1\data\EBSD\olivineopticalmapEtoO.SOR'. The 'SOR Variance' is '15 deg.>= Step 5.0'. The 'Filemake' button is visible.

Line	h	k	l	Intensity	Phase	h	k	l	Intensity	Phase	h	k	l	Intensity	Phase
183	1.64198	2.64795	1.39764	12.00000	0.00000	184750.5	0.263	1	0	1.169	0.000000	0.000000	0.000000	0.000000	0.000000
184	1.64511	2.64658	1.40167	16.00000	0.00000	190592.6	0.425	1	0	0.975	0.000000	0.000000	0.000000	0.000000	0.000000
185	1.65003	2.65055	1.40223	20.00000	0.00000	175735.8	0.281	1	0	1.139	0.000000	0.000000	0.000000	0.000000	0.000000
186	1.64906	2.64736	1.40763	24.00000	0.00000	164054.9	0.282	1	0	1.315	0.000000	0.000000	0.000000	0.000000	0.000000
187	1.64619	2.64662	1.40882	28.00000	0.00000	170213.3	0.420	1	0	0.831	0.000000	0.000000	0.000000	0.000000	0.000000
188	1.65036	2.64843	1.41355	32.00000	0.00000	173071.2	0.360	1	0	1.168	0.000000	0.000000	0.000000	0.000000	0.000000
189	1.64426	2.65091	1.40409	36.00000	0.00000	105087.5	0.205	1	0	1.580	0.000000	0.000000	0.000000	0.000000	0.000000
190	6.01848	0.47948	0.86507	40.00000	0.00000	53562.4	0.001	3	0	2.242	0.000000	0.000000	0.000000	0.000000	0.000000
191	1.02674	1.55019	5.37942	44.00000	0.00000	43186.9	0.025	1	0	2.359	0.000000	0.000000	0.000000	0.000000	0.000000
192	1.76871	1.76511	4.64990	48.00000	0.00000	42109.0	0.007	1	0	2.419	0.000000	0.000000	0.000000	0.000000	0.000000
193	6.27863	1.34746	1.31240	52.00000	0.00000	35992.3	0.000	1	0	2.285	0.000000	0.000000	0.000000	0.000000	0.000000
194	4.36202	1.44591	5.43568	56.00000	0.00000	76183.5	0.060	1	0	1.737	0.000000	0.000000	0.000000	0.000000	0.000000
195	4.36117	1.44460	5.43966	60.00000	0.00000	153203.4	0.533	1	0	1.062	0.000000	0.000000	0.000000	0.000000	0.000000
196	4.35841	1.44285	5.44178	64.00000	0.00000	200322.3	0.315	1	0	1.106	0.000000	0.000000	0.000000	0.000000	0.000000
197	4.35997	1.44273	5.44119	68.00000	0.00000	214971.7	0.466	1	0	1.142	0.000000	0.000000	0.000000	0.000000	0.000000
198	4.36095	1.44459	5.43964	72.00000	0.00000	202979.6	0.463	1	0	1.102	0.000000	0.000000	0.000000	0.000000	0.000000
199	4.36150	1.44219	5.43721	76.00000	0.00000	159648.7	0.614	1	0	1.193	0.000000	0.000000	0.000000	0.000000	0.000000
200	4.43858	0.84443	4.99301	80.00000	0.00000	71151.6	0.001	1	0	2.223	0.000000	0.000000	0.000000	0.000000	0.000000

The close-up shows the 'Makefile' section. The 'DataStartline' is '180', 'PhasePotision' is '8', and 'LaboTex-SOR' is selected in the dropdown menu. The 'Holder' is 'C:\mteX-5.1.1\data\EBSD\olivineopticalmapEtoO.SOR'. The 'Step' is '5.0'. The 'Filemake' button is visible.

SOR: LaboTex向け  
Ctf: MTEX向け

# LaboTex SORファイル作成, LaboTex読み込み

EBSDtoODF 1.02GaussT[23/12/31] by CTR

File Help

InputData  
InputFile: C:\mtex-5.1.1\data\EBSD\olivineopticalmap.ang  
Chalcopyrite

MaterialData  
Material: cif  
.TXT .cif file

Group: P1  
Symmetry(OIM): 42  
HKLCode: 5  
LaboTexCode: 5 - D4 (teragonal)

Aaxis: 5.24  
Baxis: 5.24  
Caxis: 10.3  
alpha: 90.0  
beta: 90.0  
gamma: 90.0

183:	4.5591	2.1189	4.1201	1
184:	1.1542	0.4078	5.6447	1
185:	6.0507	0.8127	1.6050	1
186:	6.0505	0.8145	1.6068	1
187:	6.0524	0.8138	1.6043	1
188:	6.0511	0.8141	1.6053	1
189:	6.0526	0.8132	1.6052	1
190:	6.0482	0.8153	1.6066	1
191:	6.0495	0.8117	1.6067	1
192:	2.9058	2.3300	4.6748	1
193:	2.9042	2.3312	1.5345	1
194:	6.0464	0.8047	1.6087	1
195:	6.0476	0.8091	1.6077	1
196:	2.6517	0.0892	0.3833	1
197:	5.7824	3.0525	2.7461	1
198:	5.7877	3.0512	2.7546	1
199:	5.7692	3.0566	2.7331	1
200:	5.7297	3.0582	2.6995	1

outfiledisp

Makefile  
DataStartline: 180  
PhasePotision: 8  
Selectphase: 1  
f1: 1  
F: 2  
f2: 3  
X: 4  
Y: 5

LaboTex-SOR  
Holder: C:\mtex-5.1.1\data\EBSD\olivineopticalmapEtoO.SOR

SOR Variance  
 15 deg.>= Step: 5.0

Filemake: C:\mtex-5.1.1\data\EBSD\olivineopticalmapEtoO.SOR make complete !!

New Sample

Choose Experimental Data (LaboTex Single Orientations Files)  
 EPF  PFF  SOR  NJC  NJA  RW1  epf Selected: 1

ACOMEtO.SOR  
dataEtoO.SOR  
DC06\_2uniaxEtoO.SOR  
ForsteriteEtoO.SOR  
olivineopticalmapEtoO.SOR  
single\_grain\_aluminumEtoO.SOR

Path: C:\mtex-5.1.1\data\EBSD\  
Info: C:\mtex-5.1.1\data\EBSD\olivineopticalmap.ang

Choose Defocussing Correction  
 Correction (On/Off)  
 Correction Data from File  Correction Data from Formula  
(COR\_POW\_DFB\_ASC\_PFG\_NJA\_DAT\_POL\_NJC\_COA\_RWA\_UXD\_EXP)  
Cor(1x1).cor  
Cor(5x5).cor

Path: C:\LaboTex2\USER\CuFeS2.LAB\COR\  
Info:

Crystal Symmetry: D4 (Tetragonal)

Project Name: Demo

Sample Name: D4\_Tetragonal

Sample Name: CuFeS2

Cancel Create of ODF from Single Orientations Data

# LaboTex

100.0 % ODF Creations from Single Orientations

Project: Demo

Sample: CuFeS2

Crystal Symmetry: D4-Tetragonal

Cell Parameters (Relative): a: 1.0, b: 1.0, c: 1.9

Angle Convention for Data: Bunge

Grid Cells for Output ODF: 5.0\*5.0

Angle Unit: Radians

Weight: Yes

Phase: 0

Descriptions: C:\mtex-5.1.1\data\EBSD\oliveopticalmap.ang

Single Orientations Files: [List of files]

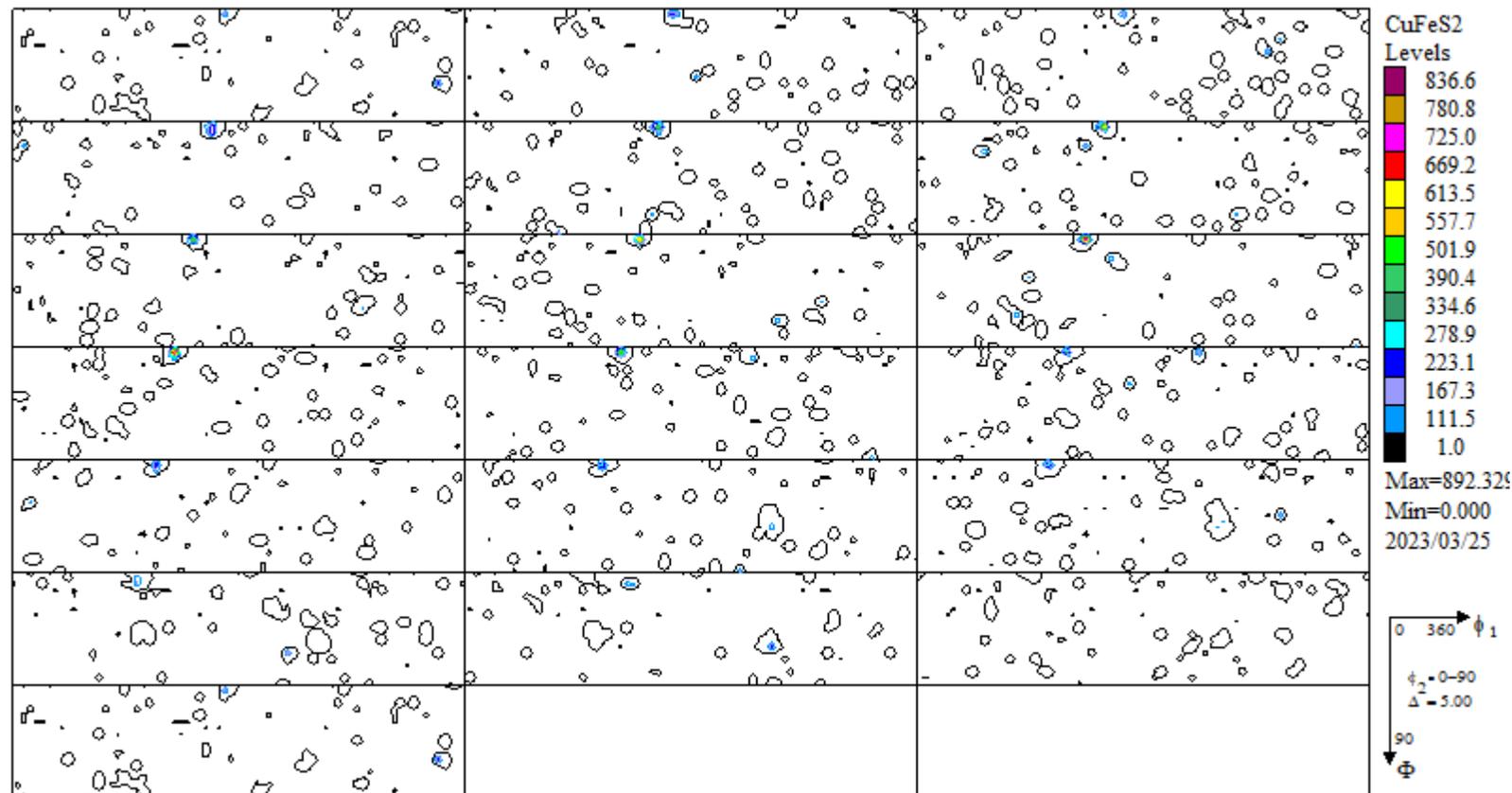
Calculations Progress: Merge (files): 1/1, No of single orien.: 44953, Calculation Finished: 100.0%

'SOR' Output File Options: Add {HKL}<UVW>  Max. Value of Miller Indice = 15

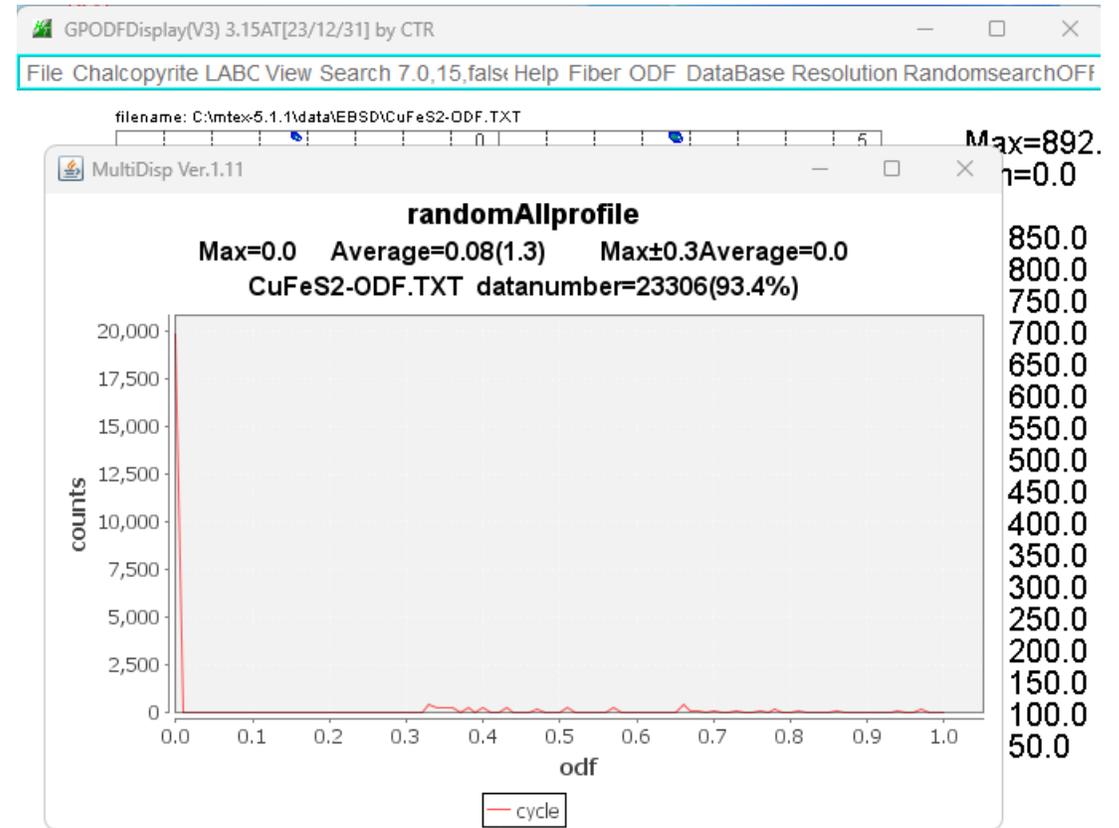
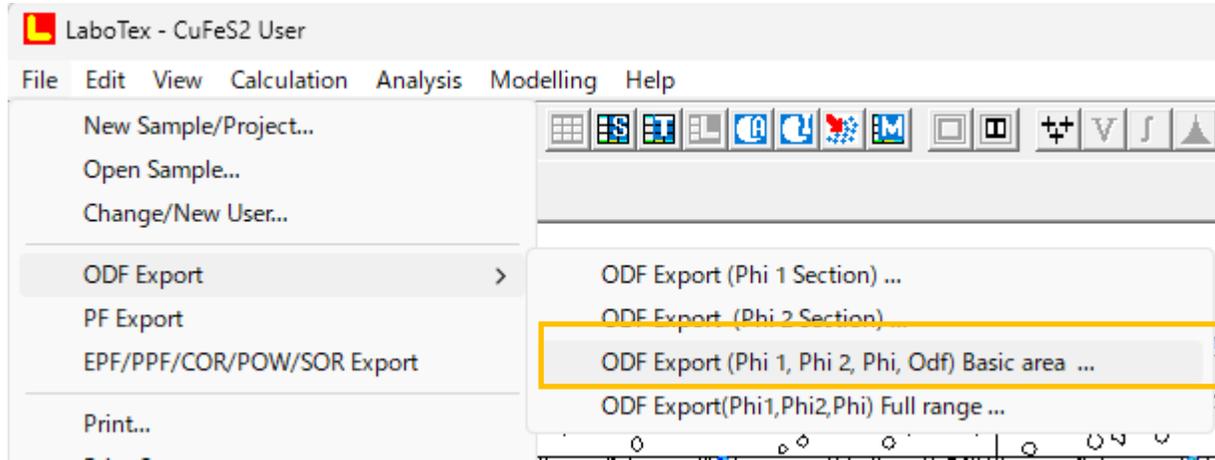
Hexagonal Axis Convention of Data (important only in Hexagonal C.S.):

Warning: If your file contains non-indexed data, then you should use "EBSD Format - Defined by User" (Menu "Edit", "LaboTex Options", "Data Formats")  
In this format you can exclude non-indexed data from ODF calculation.  
Non-indexed data can create false maximum on the ODF!  
In case of problems, please contact the office@labosoft.com.pl

BREAK END

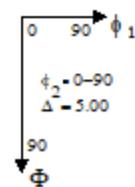
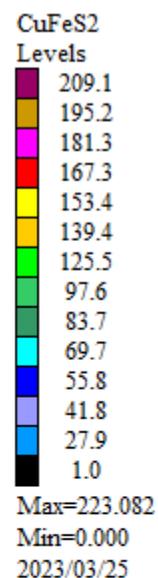
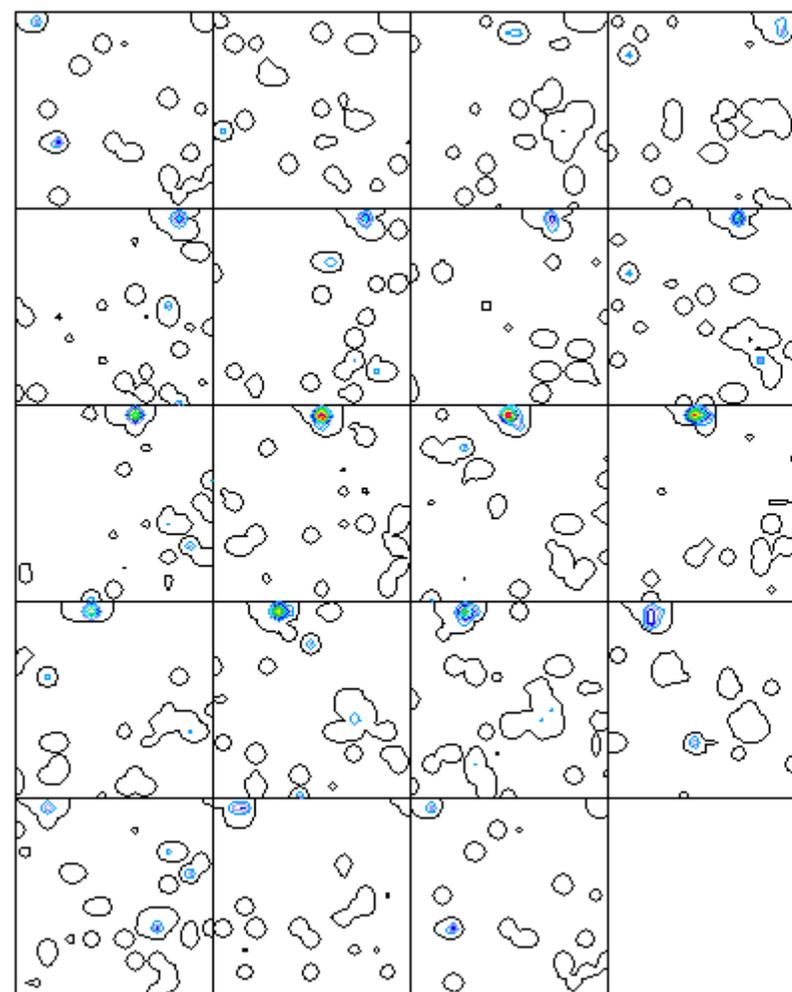
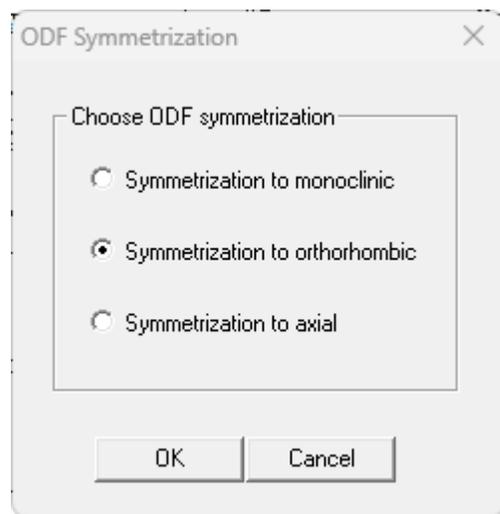
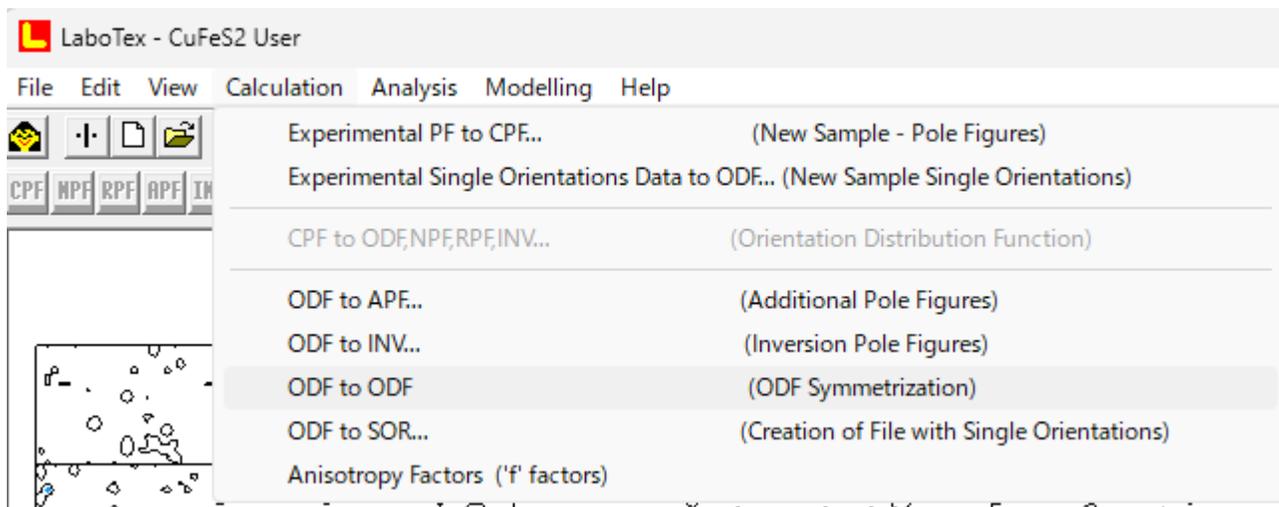


# ODF図をExportし、random定量

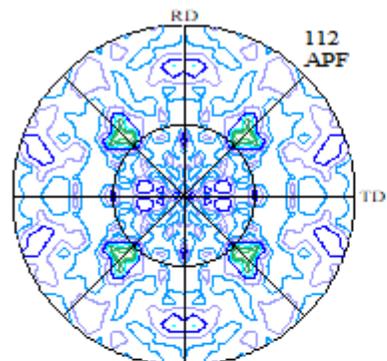


格子点の93.4%が1.0以下でrandom値は0%である。

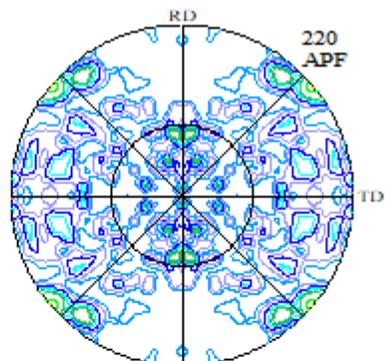
# LaboTex Triclinic->Orthorhombic



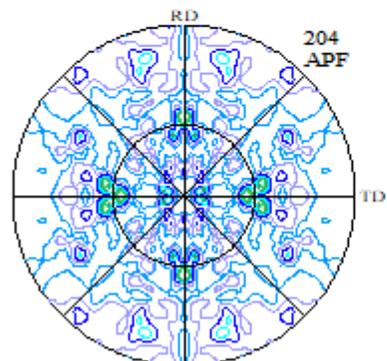
# 配向関数



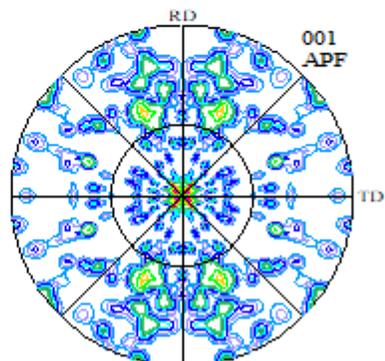
CuFeS2



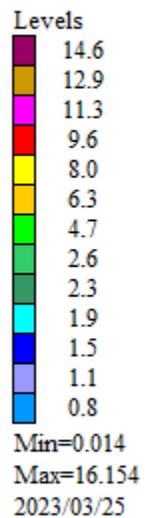
CuFeS2



CuFeS2



CuFeS2



Calculation of Anisotropy Factors

Calculation for Hexagonal, Tetragonal and Orthorhombic Crystal Systems

Fraction of Basal Planes {001} in Sample Directions

LD	TD	ND
0.3702	0.2846	0.3452
f1	f2	f3

Angles between Basal Planes {001} and Sample Directions

LD	TD	ND
50.9	60.0	53.6
a	b	c

Kearns Factors (Fraction in Physical Property)

LD	TD	ND
0.3970	0.2504	0.3525
fL	fT	fN

Texture Index (F2) (normalized) 0.95325  
("0" - Random, "1" - Monocrystal)

Calculate

End

# {001}極点図をExport

