Ｈｅｘａｇｏｎａｌ、Ｓｙｍｍｅｔｒｙ６&６２

六方晶ＥＢＳＤデータの解析（ＭＴＥＸ，ＬａｂｏＴｅｘ）

１．概要

Ｈｅｘａｇｏｎａｌは、D-Hexagonal、C-Hexagonal の解析方法があります。

Symmetry		Cubic**		Hexagonal		Tetragonal		Trigonal		Ortho-rhombic	Mono-clinic	Triclinic
		O	T	D_6	C_6	D_4	C_4	D_3	C_3	D_2	C_2	C_1
LaboTex structure code		7	6	11	10	5	4	9	8	3	2	1
ϕ_1	triclinic* (C_1)	360°	360°	360°	360°	360°	360°	360°	360°	360°	360°	360°
	monoclinic* (C_2)	180°	180°	180°	180°	180°	180°	180°	180°	180°	180°	180°
	orthorhombic*(D_2)	90°	90°	90°	90°	90°	90°	90°	90°	90°	90°	90°
	axial*	-***	-	-	-	-	-	-	-	-	-	-
Φ		90°	90°	90°	180°	90°	180°	90°	180°	90°	180°	180°
ϕ_2		90°	180°	60°	60°	90°	90°	120°	120°	180°	180°	360°

* - sample symmetry
** - there are three non-linear basic region inside described region
*** - for any ϕ_1 angle

Ｈｅｘａｇｏｎａｌでは

168	P6	6	10
169	P61	6	10
170	P65	6	10
171	P62	6	10
172	P64	6	10
173	P63	6	10
174	P6	6	10
175	P6/m	6	10
176	P63/m	6	10
177	P622	62	11
178	P6122	62	11
179	P6522	62	11
180	P6222	62	11
181	P6422	62	11
182	P6322	62	11
183	P6mm	62	11
184	P6cc	62	11
185	P63cm	62	11
186	P63mc	62	11
187	P6m2	62	11
188	P6c2	62	11
189	P62m	62	11
190	P62c	62	11
191	P6/mmm	62	11
192	P6/mcc	62	11
193	P63/mcm	62	11
194	P63/mmc	62	11

C21H39O18-Hexa-C6DISP
Hexagonal
23.725 (1.0)
23.725 (1.0)
7.935 (0.3345)
90.0
90.0
120.0

_symmetry_space_group_name_H-M 'P6'
_symmetry_Int_Tables_number 168
_Symmetry 6

Titanium-Ti-D6DISP
Hexagonal
2.95 (1.0)
2.95 (1.0)
4.686 (1.5885)
90.0
90.0
120.0

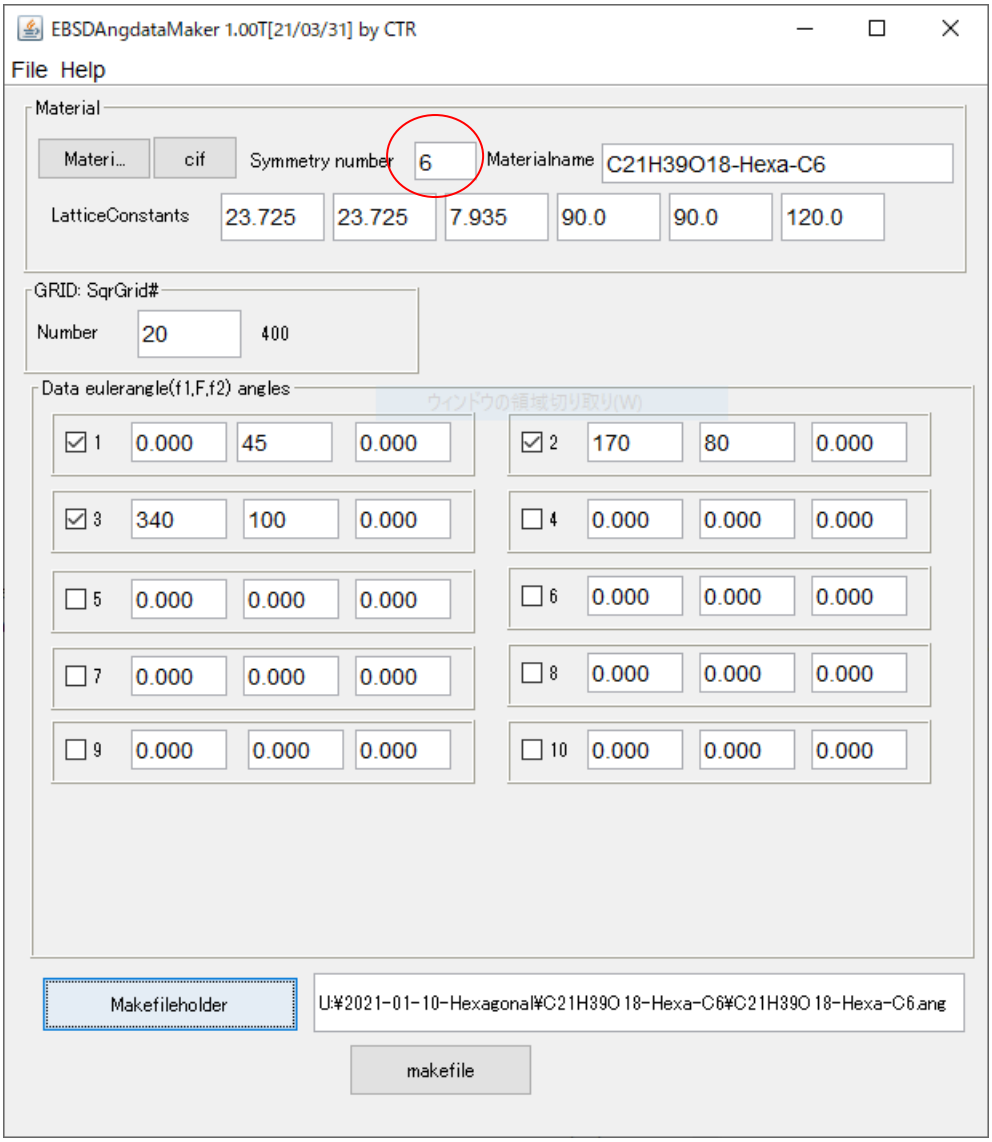
_symmetry_space_group_name_H-M 'P63/mmc'
_symmetry_Int_Tables_number 194
_Symmetry 62

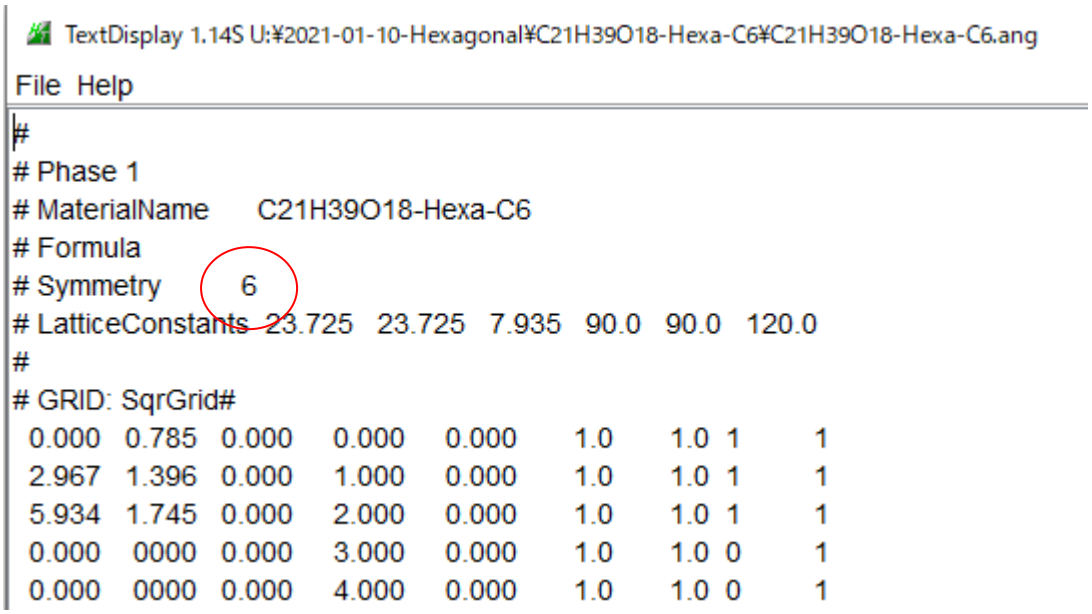
があり、ＴｉやＭｇはＳｙｍｍｅｔｒｙ（６２）である。
本資料では、Ｔａｂｌｅ No168 の C21H39O18　と No194 のＴｉを扱ってみます。

ＩＣＤＤからＣＴＲのＤａｔａＢａｓｅへの登録は Yb2O3 の ODF 解析を参照してください。

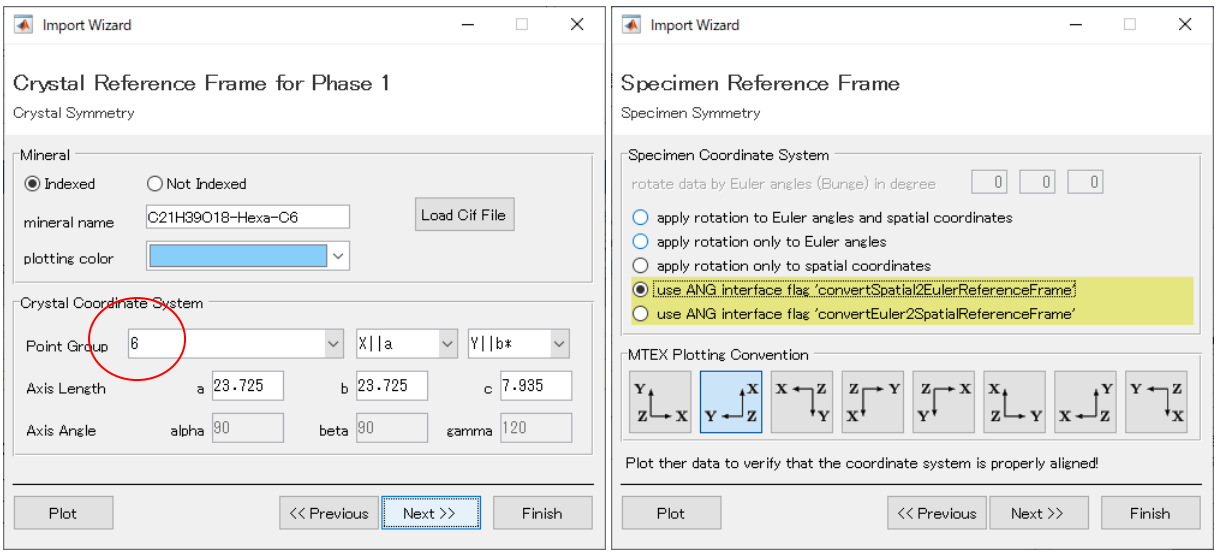
２．Ｃ２１Ｈ３９Ｏ１８、Ｓｙｍｍｅｔｒｙ（６）の解析

２．１　ＥＢＳＤデータ作成

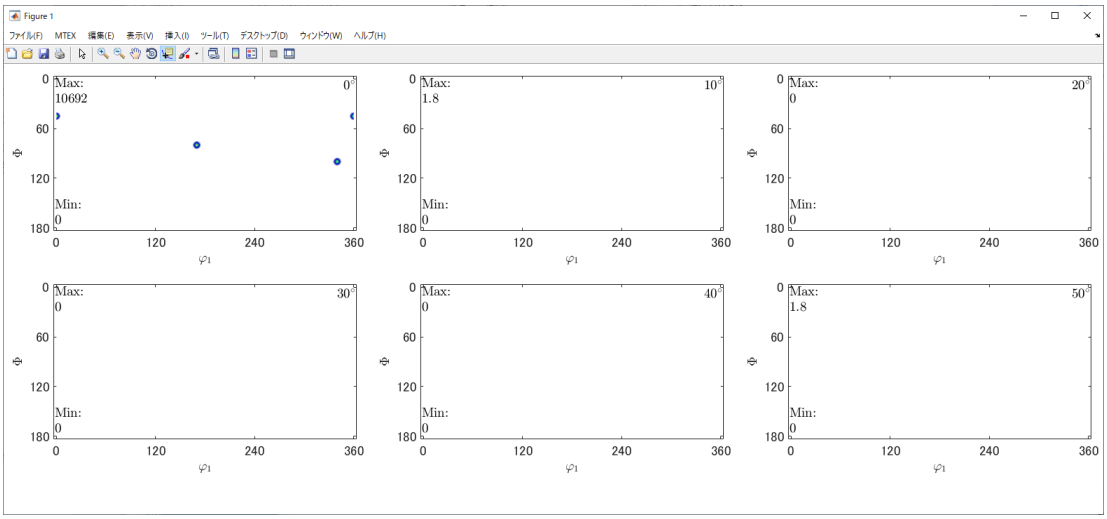




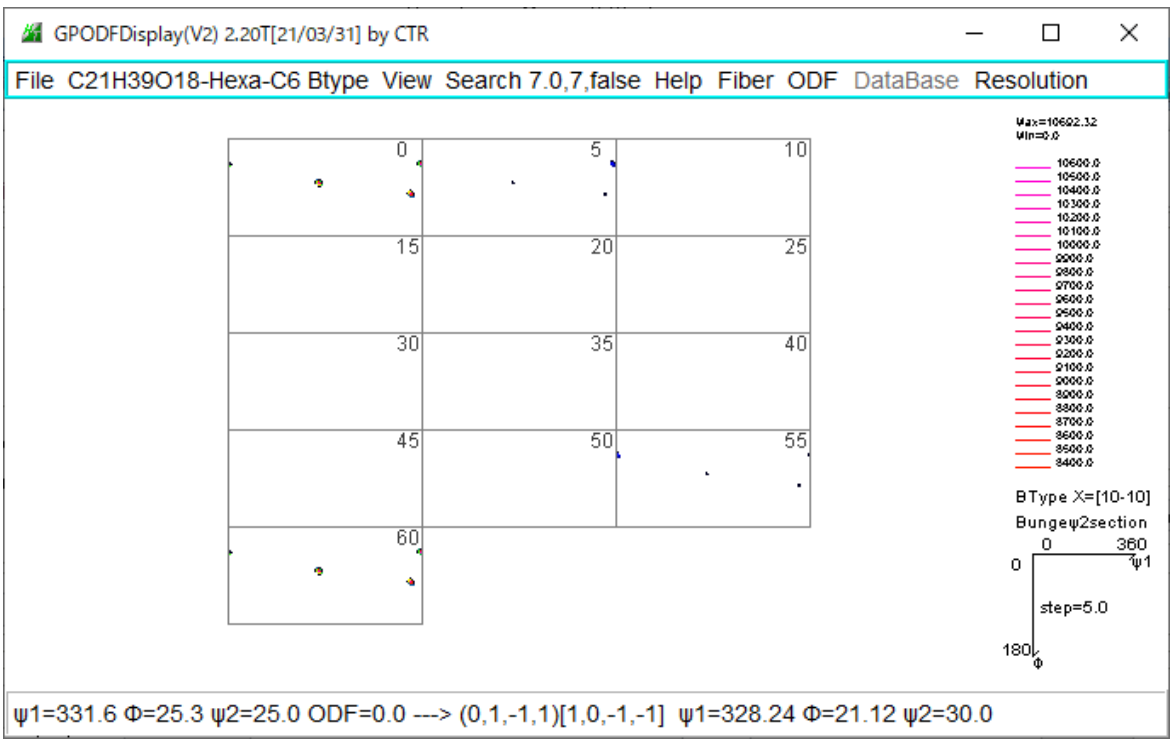
２．２　ＭＴＥＸの解析



odf = calcDensity(ebsd('C21H39O18-Hexa-C6').orientations,'halfwidth',2*degree)

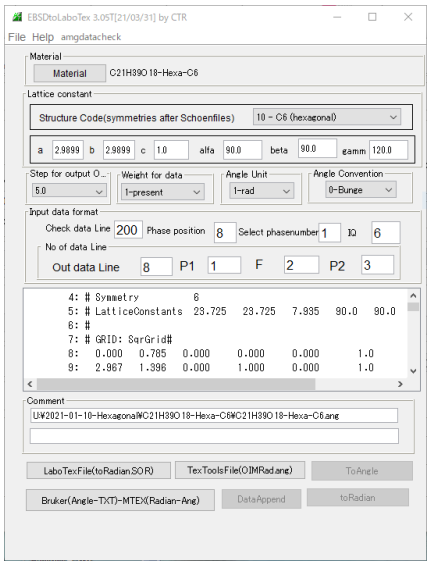


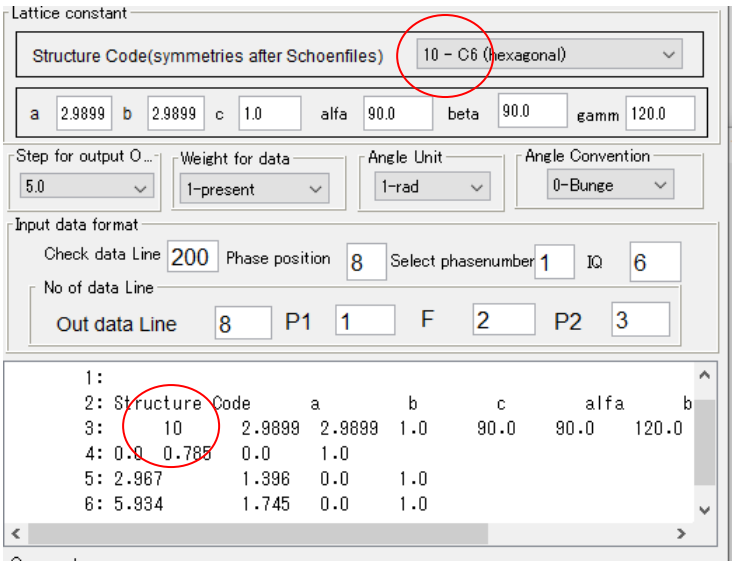
ODFデータをＥＸｐｏｒｔし、ＧＰＯＤＦＤｉｓｐｌａｙで表示



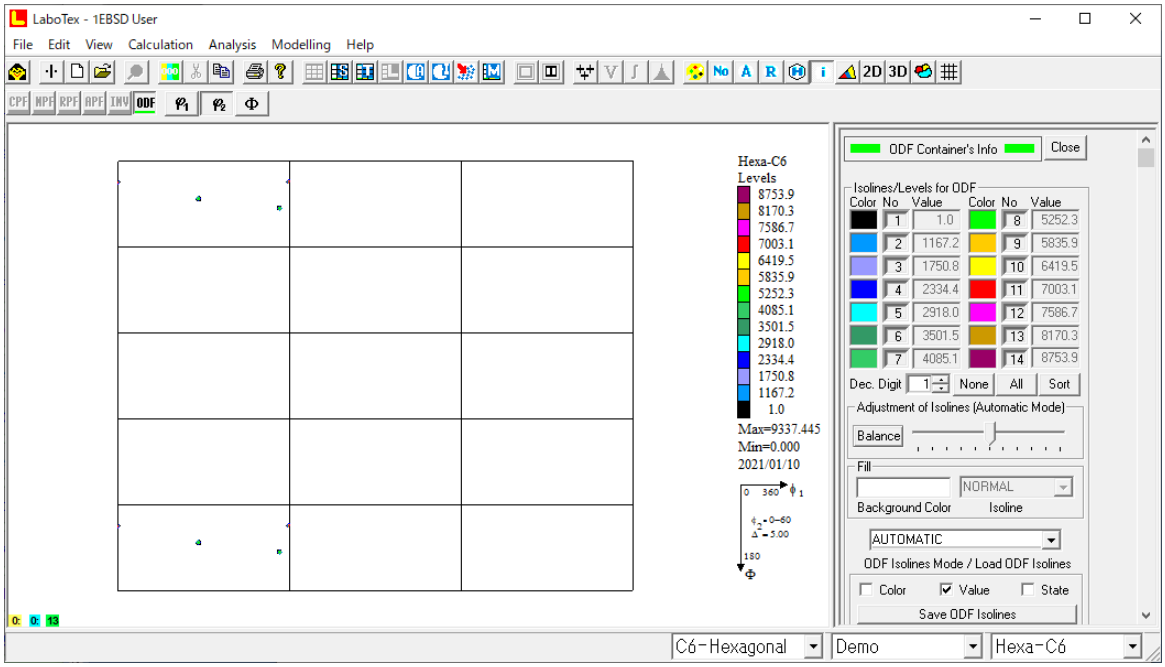
２．３　ＬａｂｏＴｅｘの解析

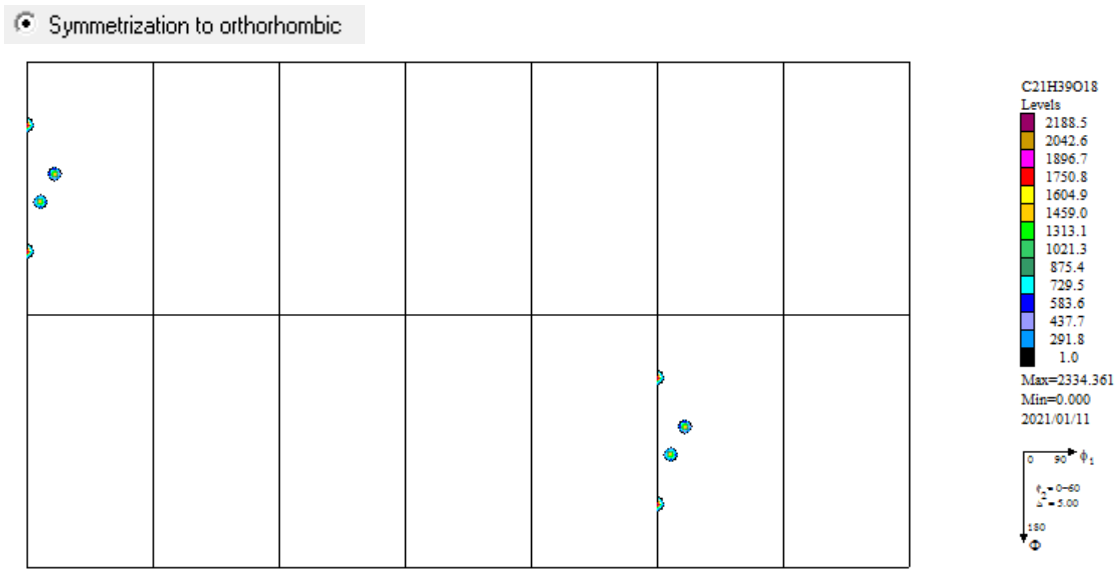
Angデータから ＳＯＲデータ変換





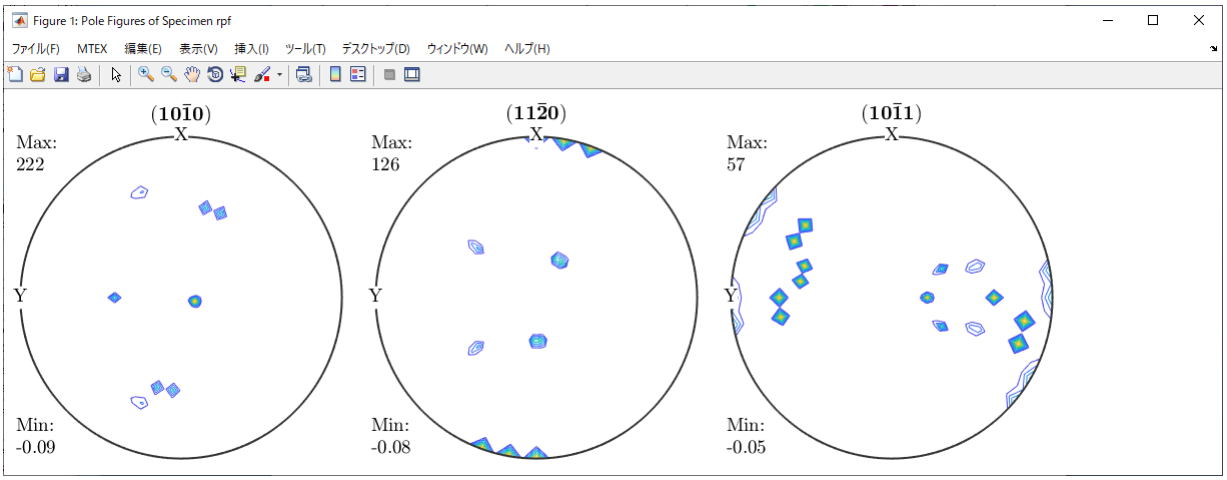
ＬａｂｏＴｅｘのＯＤＦ解析結果



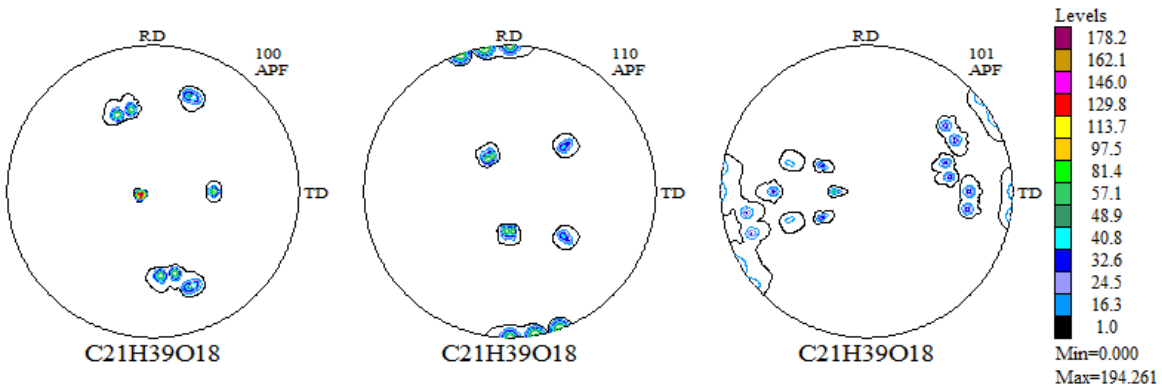


２．４　ＭＴＥＸ，ＬａｂｏＴｅｘ再極点図比較

```
cs=ebsd('C21H39O18-Hexa-C6').CS
h={Miller(1,0,0,cs),Miller(1,1,0,cs),Miller(1,0,1,cs)}
rpf=calcPoleFigure(odf,h)
plot(rpf,'contour','projection','eangle')
```



ＬａｂｏＴｅｘ



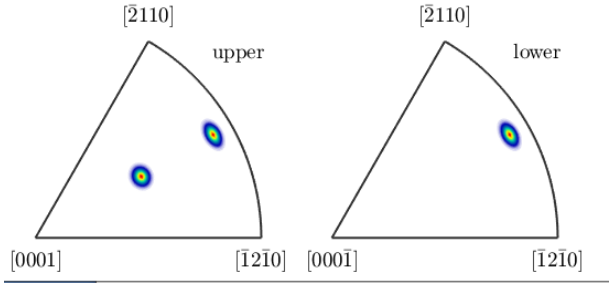
極点図の TD 方向

ＭＴＥＸは左、データはＣＣＷ方向に並ぶ

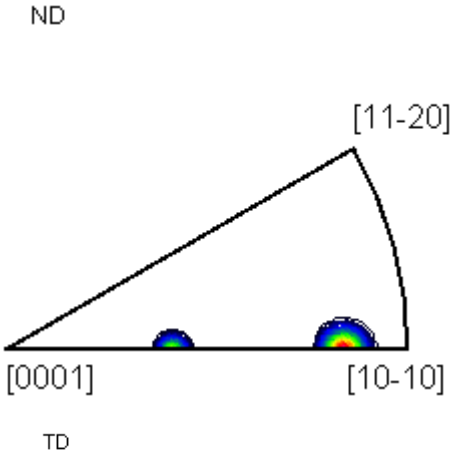
ＬａｂｏＴｅｘは右、データはＣＷ方向に並ぶ

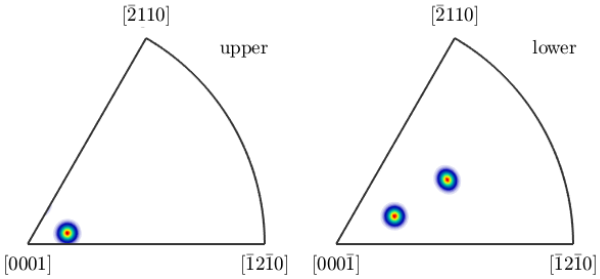
２．５　逆極点図比較

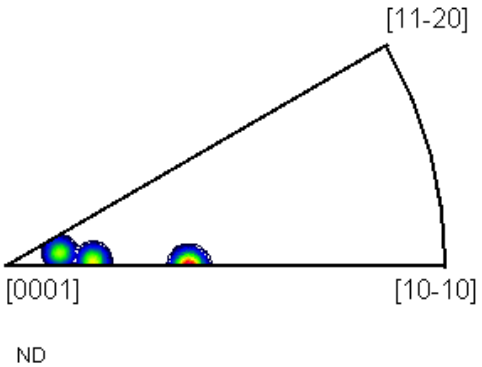
ＭＴＥＸ（１度間隔データ）

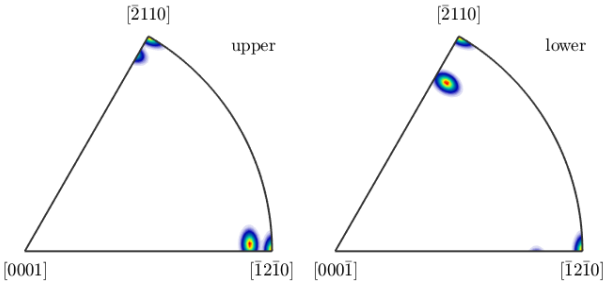


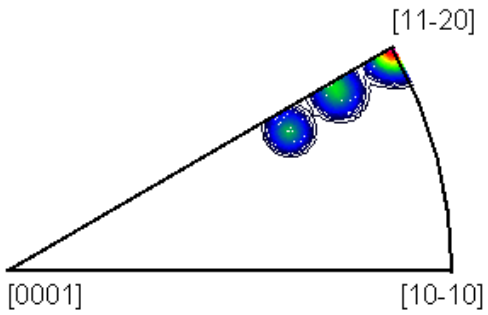
MTEXExport　GPInverseDisplay で表示



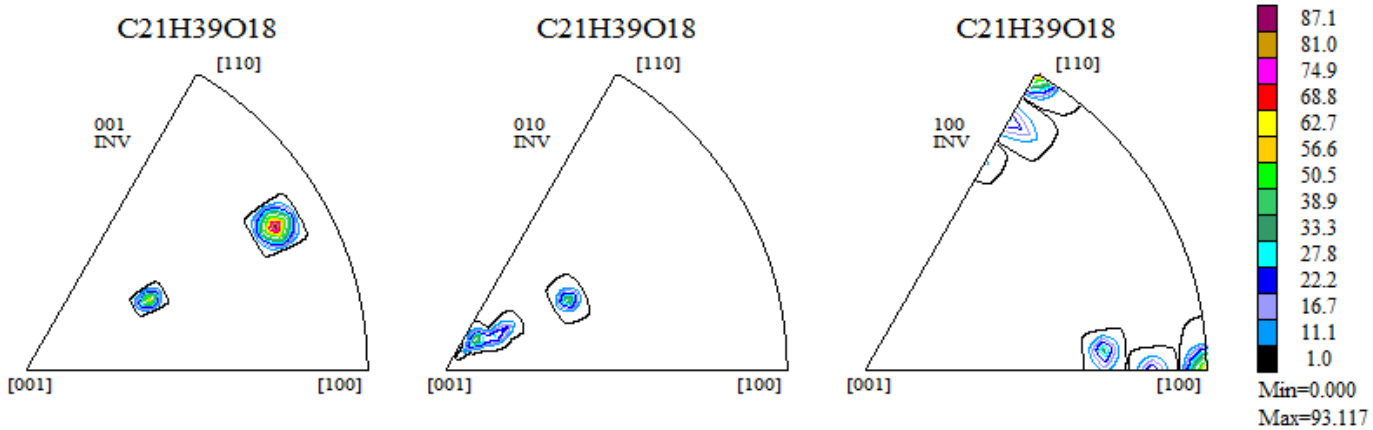






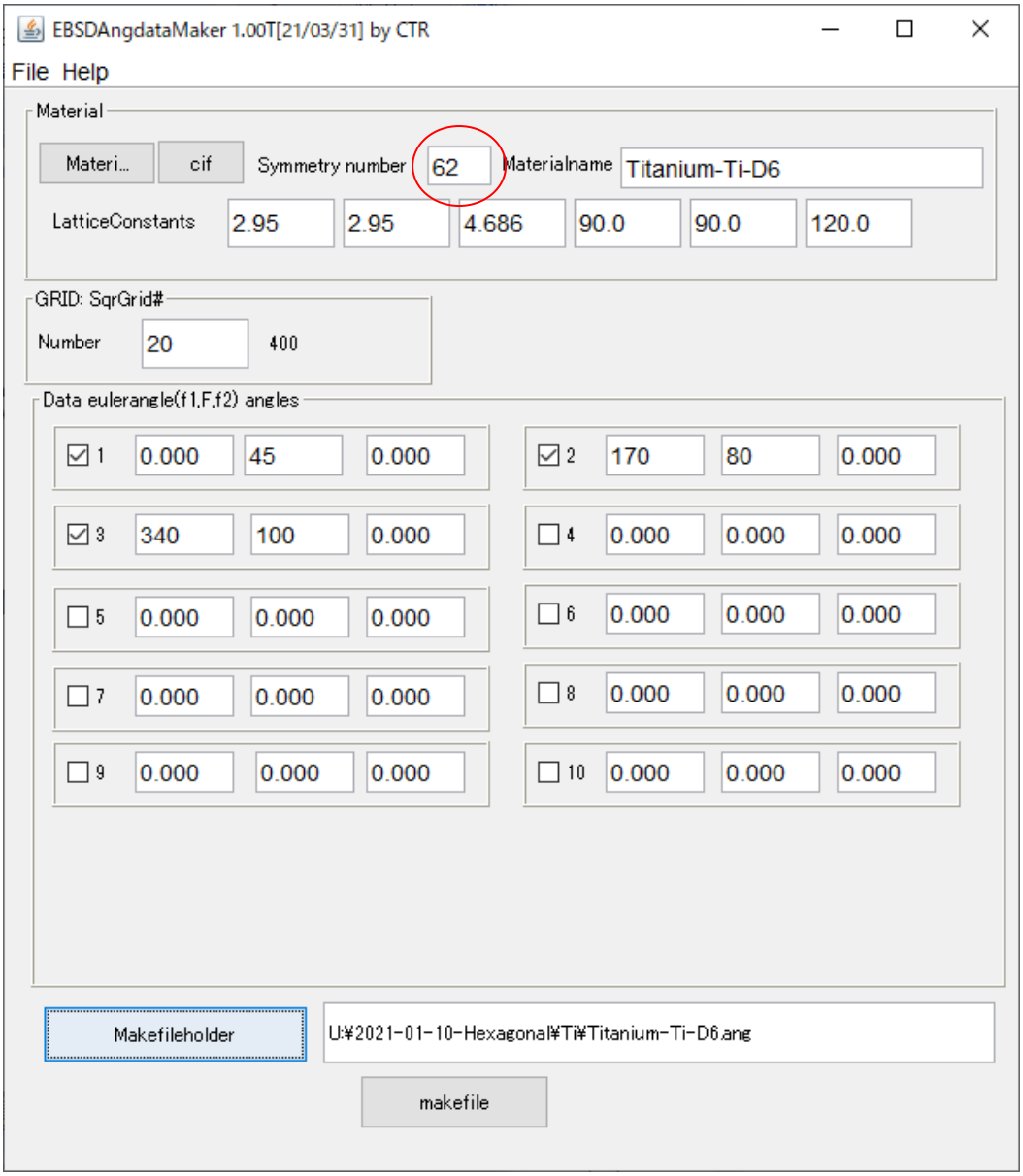


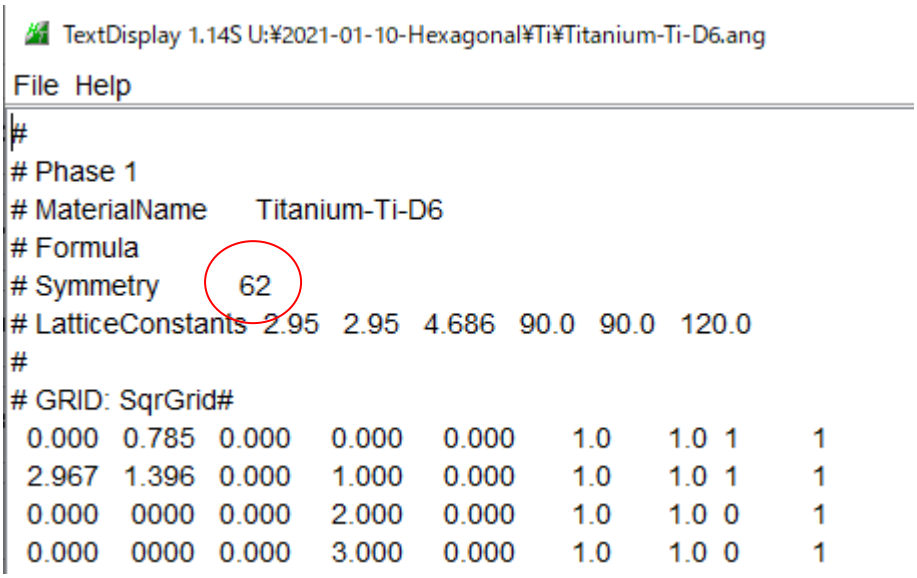
ＬａｂｏＴｅｘ（５度間隔データ）



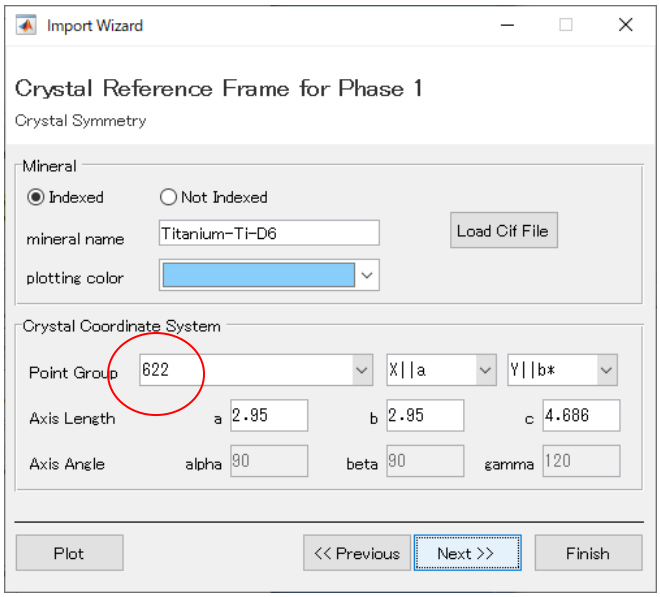
３．Ｔｉｔａｎｉｕｍ、Ｓｙｍｍｅｔｒｙ（６２）の解析

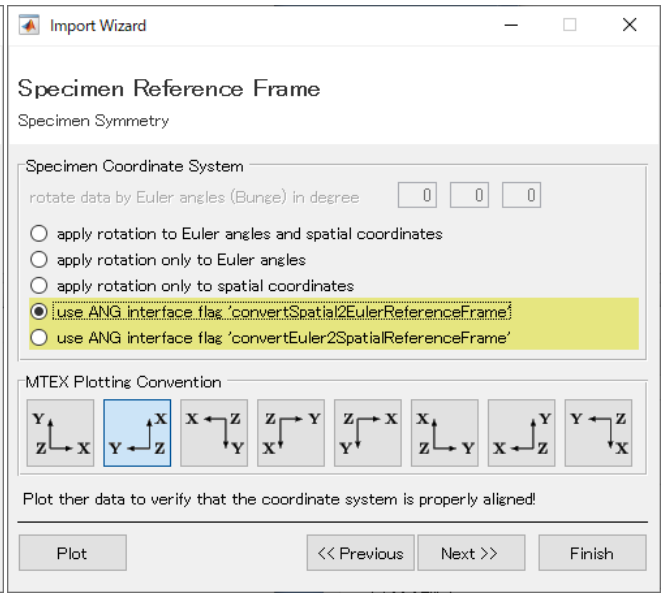
３．１　ＥＢＳＤデータ作成



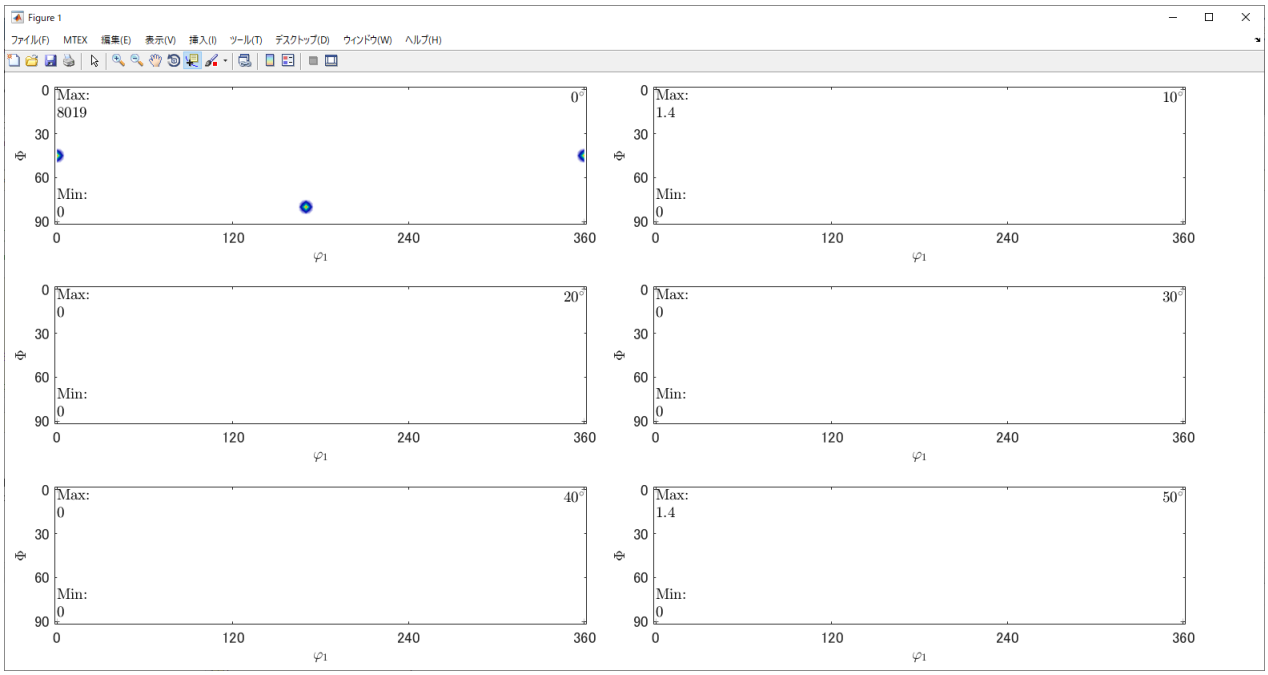


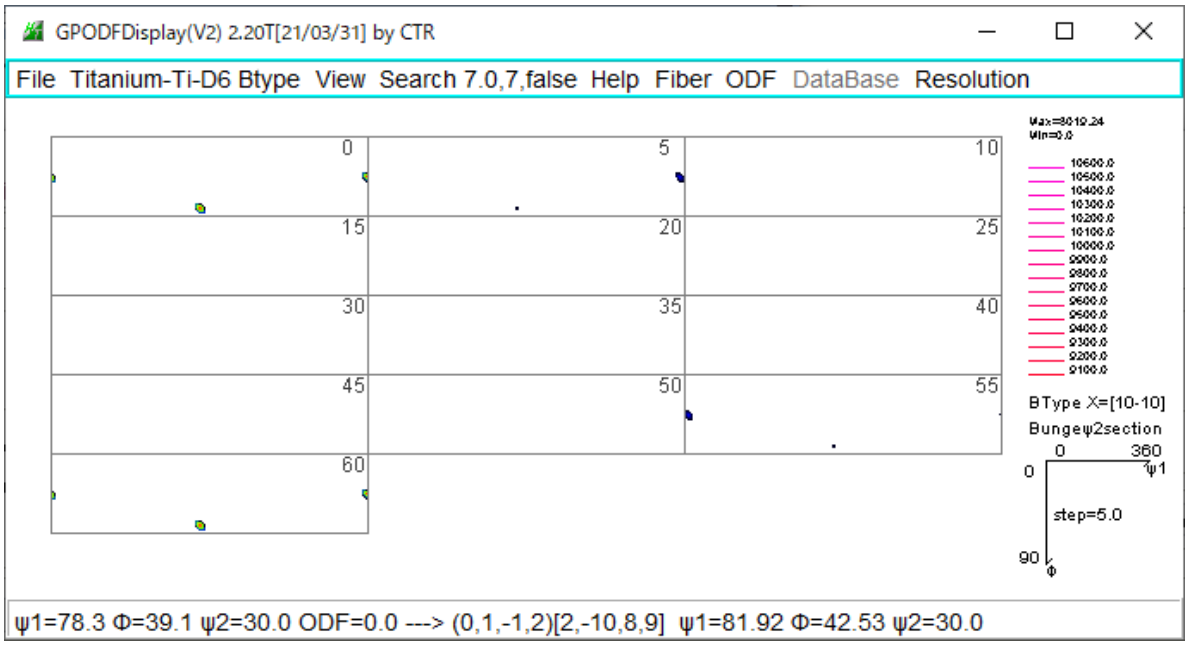
３．２　ＭＴＥＸの解析



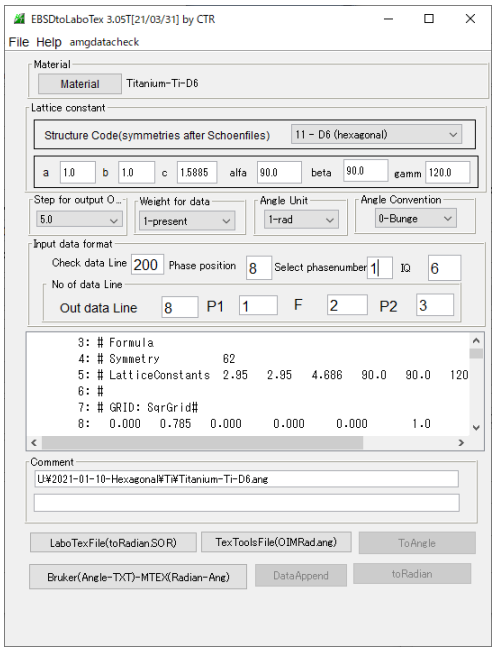


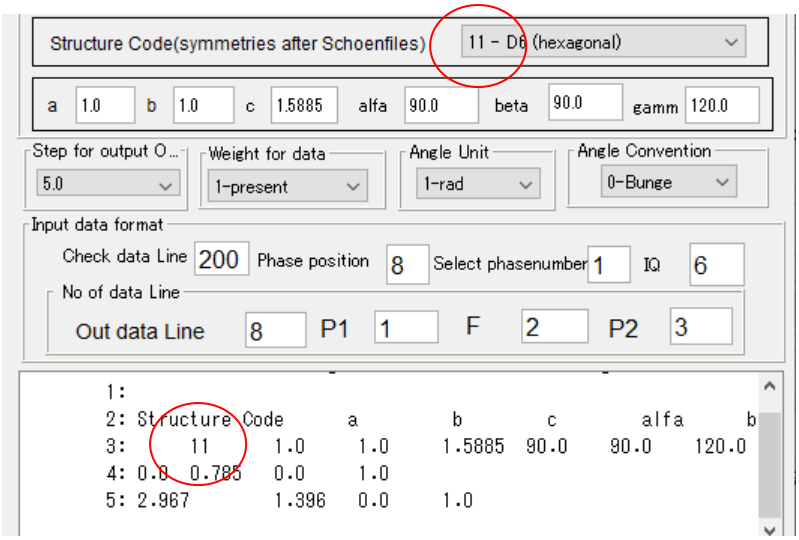
odf = calcDensity(ebsd('Titanium-Ti-D6').orientations,'halfwidth',2*degree)

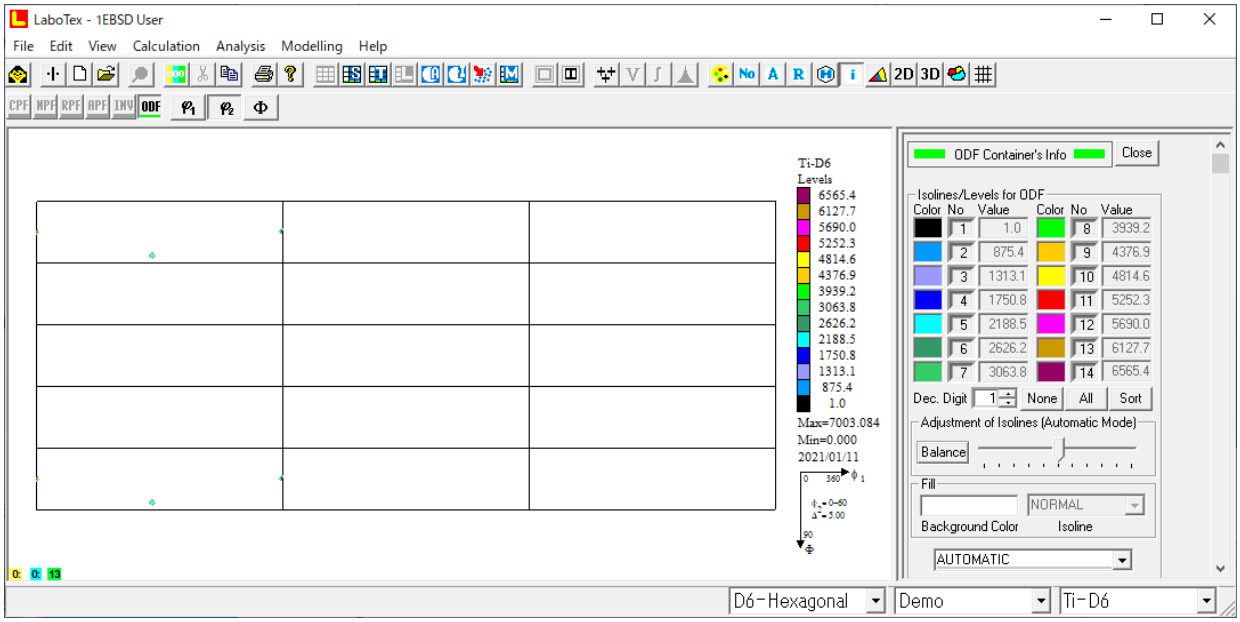




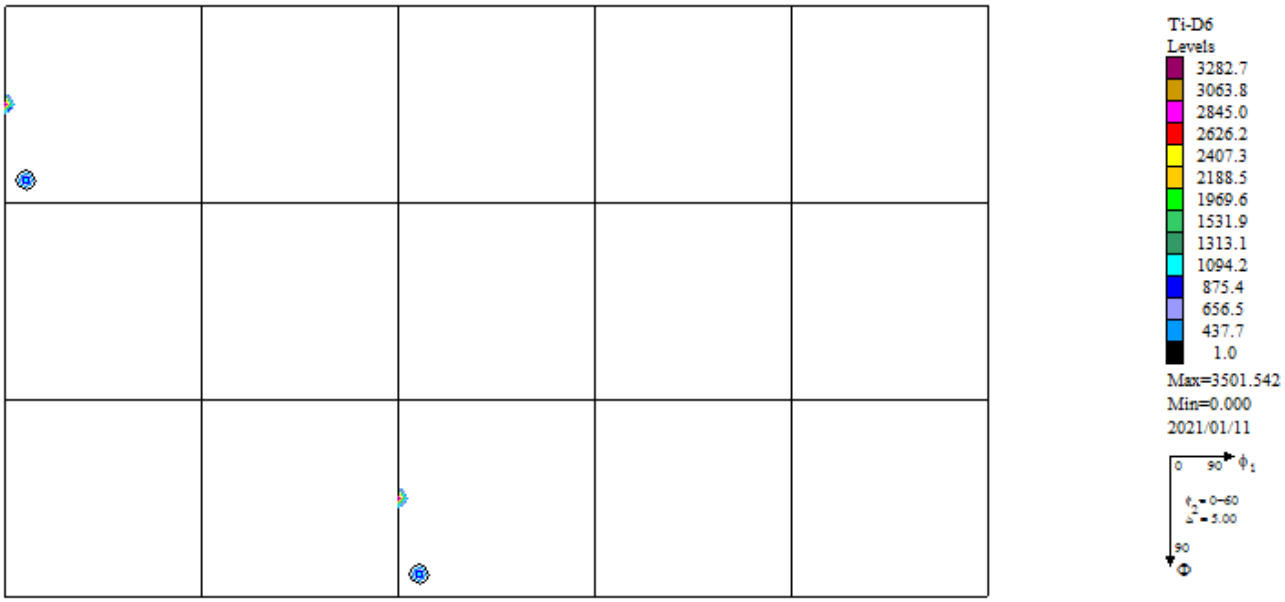
３．３　ＬａｂｏＴｅｘの解析





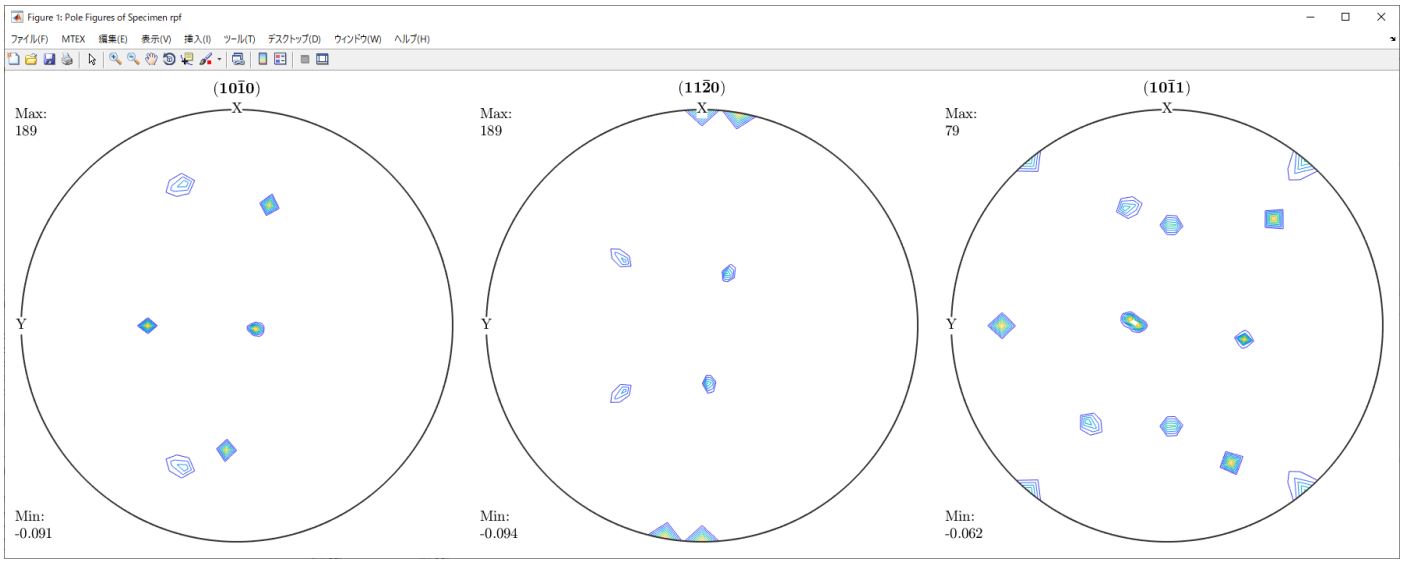


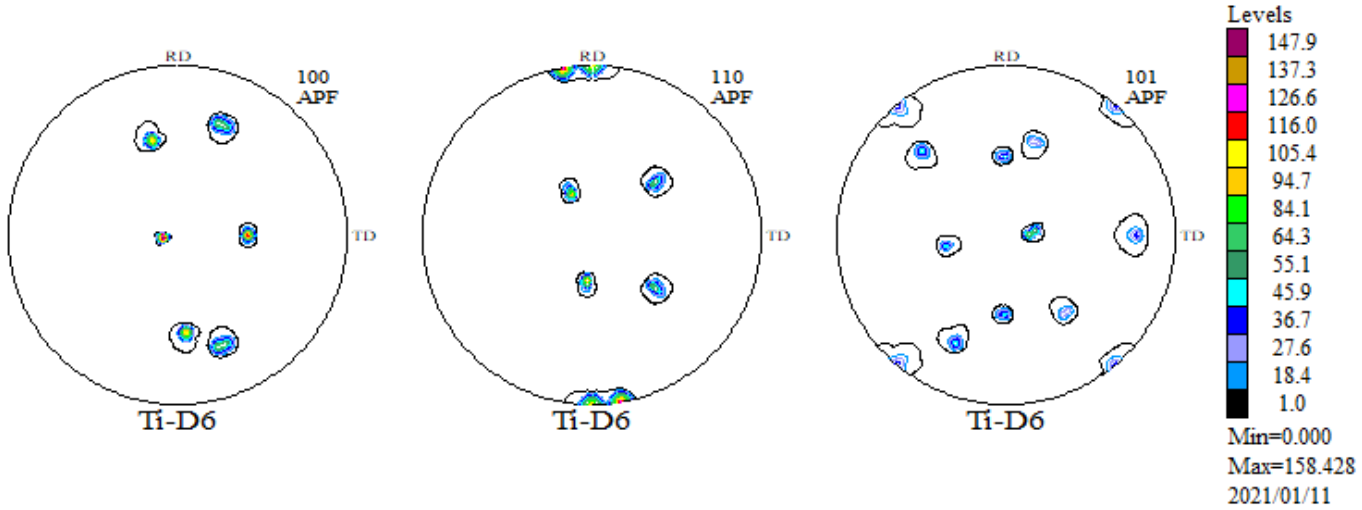
Symmetrization to orthorhombic



３．４　ＭＴＥＸ，ＬａｂｏＴｅｘ再極点図比較

plot(rpf,'contour','projection','eangle')





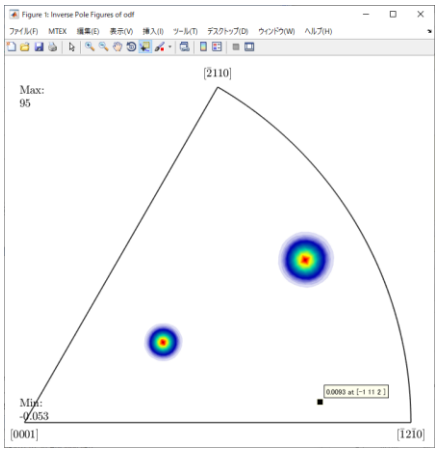
３．５　逆極点図比較

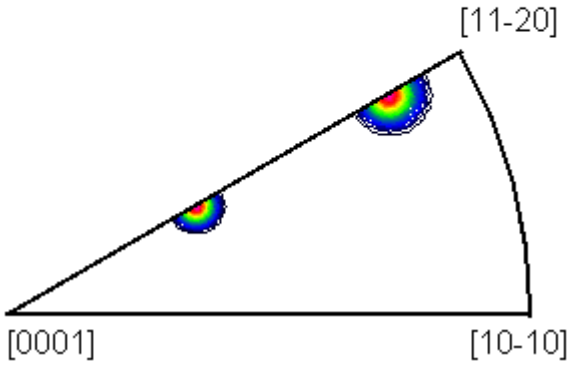
ＭＴＥＸ

plotIPDF(odf,zvector,'projection','eangle')

U:\2021-01-10-Hexagonal\Ti\ND.TXT

ND

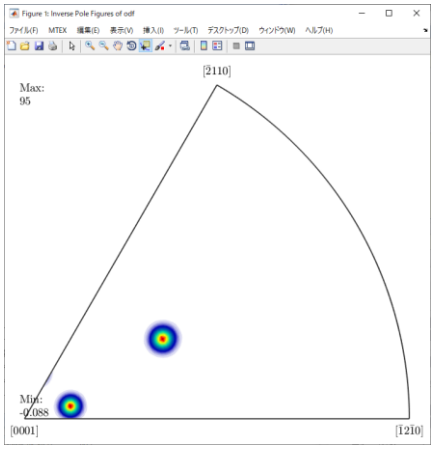


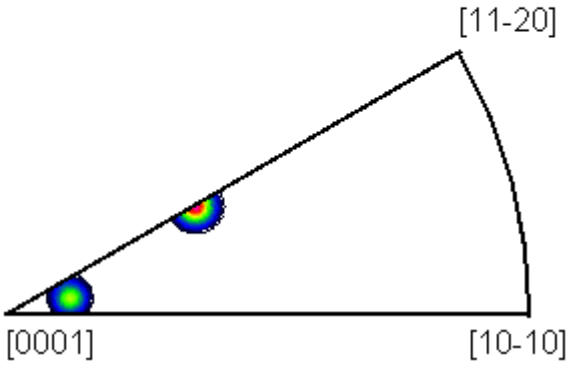


plotIPDF(odf,yvector,'projection','eangle')

U:\2021-01-10-Hexagonal\Ti\TD.TXT

TD

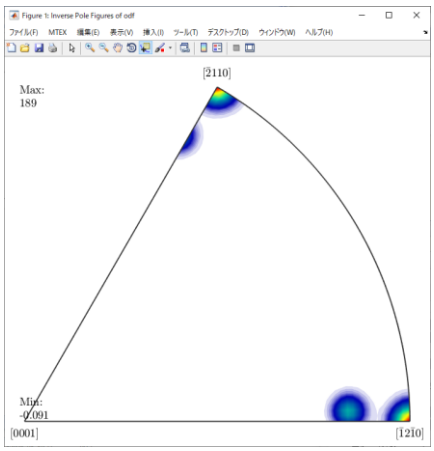


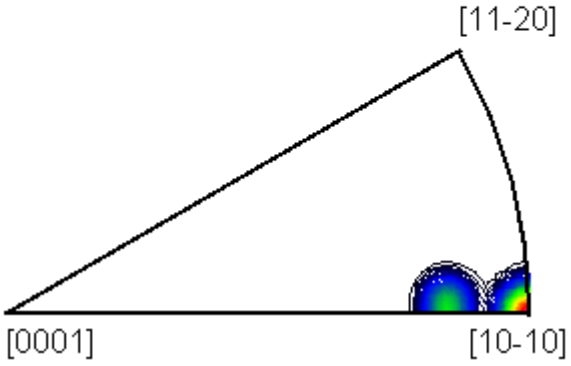


plotIPDF(odf,xvector,'projection','eangle')

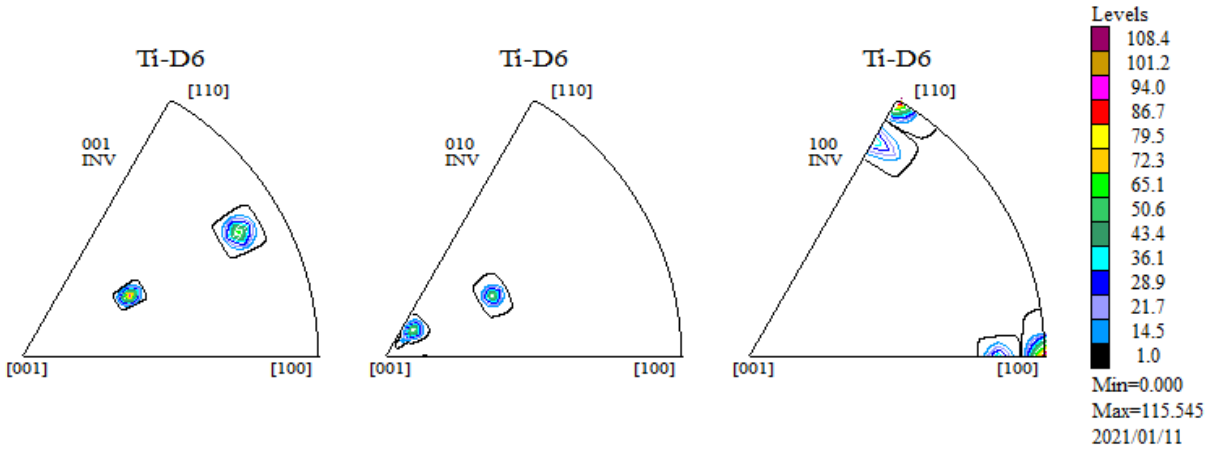
U:\2021-01-10-Hexagonal\Ti\RD.TXT

RD

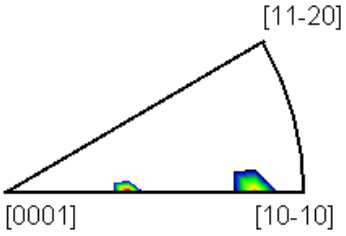




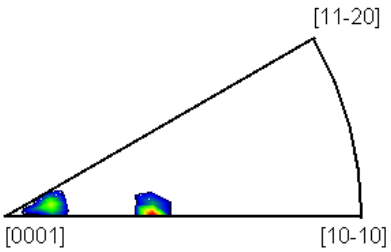
L a b o T e x



U:\2021-01-10-Hexagonal\Ti\Ti-D6-Inverse.TPF
ND



U:\2021-01-10-Hexagonal\Ti\Ti-D6-Inverse.TPF
TD



U:\2021-01-10-Hexagonal\Ti\Ti-D6-Inverse.TPF
RD