配向が強い極点図の解析を想定した

ＭＴＥＸソフトウエアにおけるα範囲と結晶方位密度

２０１９年０２月０２日

ＨｅｌｐｅｒＴｅｘ　Ｏｆｆｉｃｅ

概要

同一データでもＯＤＦ解析方法により計算される結晶方位密度は異なる。

資料 http://helpertex.sakura.ne.jp/Soft/DOC3-MTEX/LaboTex-TexTools-MTEX-compare.pdf

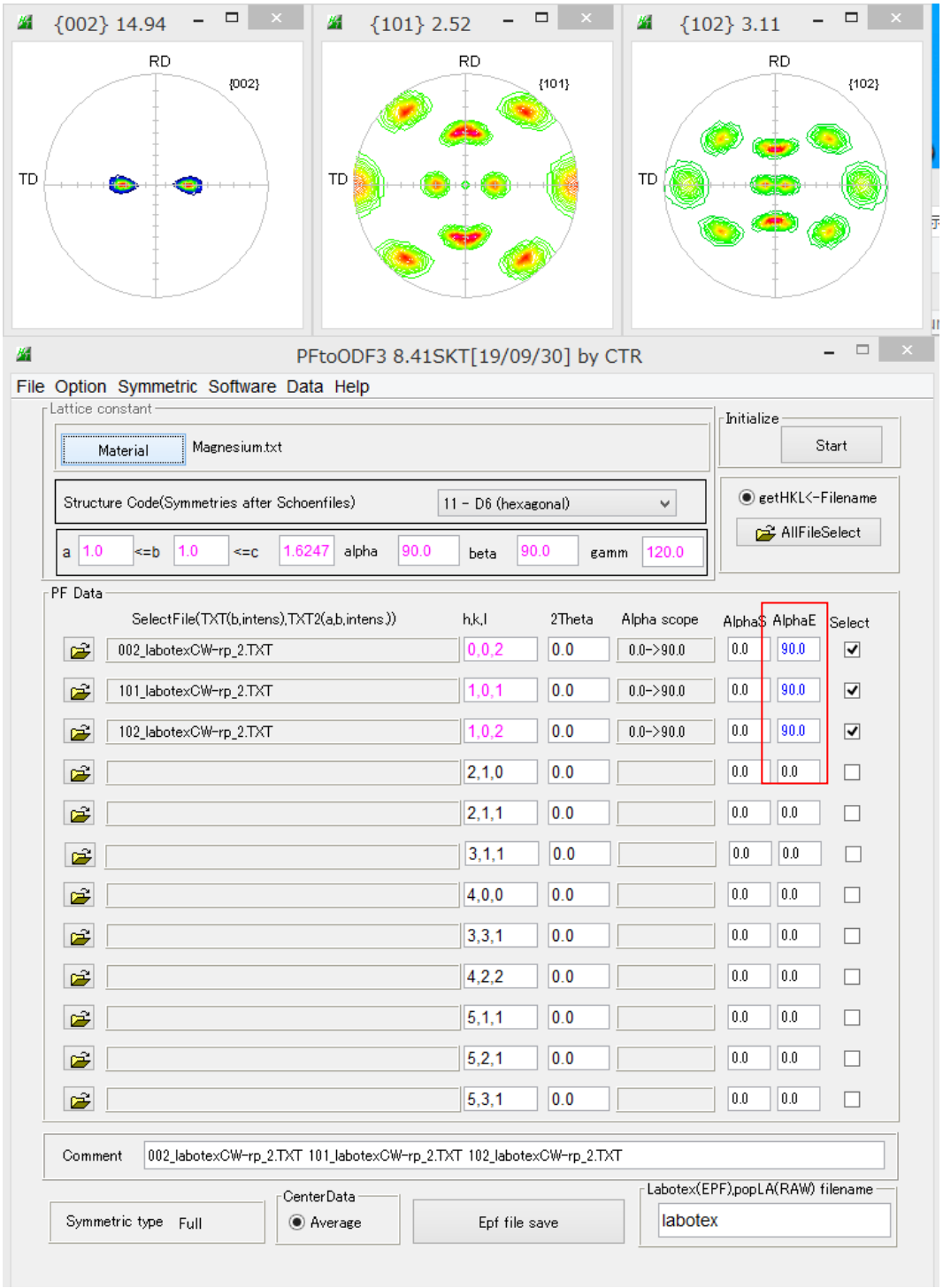
により、MTEX は Hermonic の可能性が高い。もし Hermonic の場合、StandardODF と同様に

資料 http://helpertex.sakura.ne.jp/Soft/DOC/StandardODF/StandardODF-PoleErea.pdf の傾向の可能性があるため調査する。

データは、FWHM=10deg、VF%の低いデータを用い直接法 LaboTex と比較する。

入力データ　半価幅 10deg、VF10%の極点図を LaboTex で作成し PFtoODF3 を介して入力する。

調査結果は、方位密度が高いと,Hermonic 的な挙動を示す。

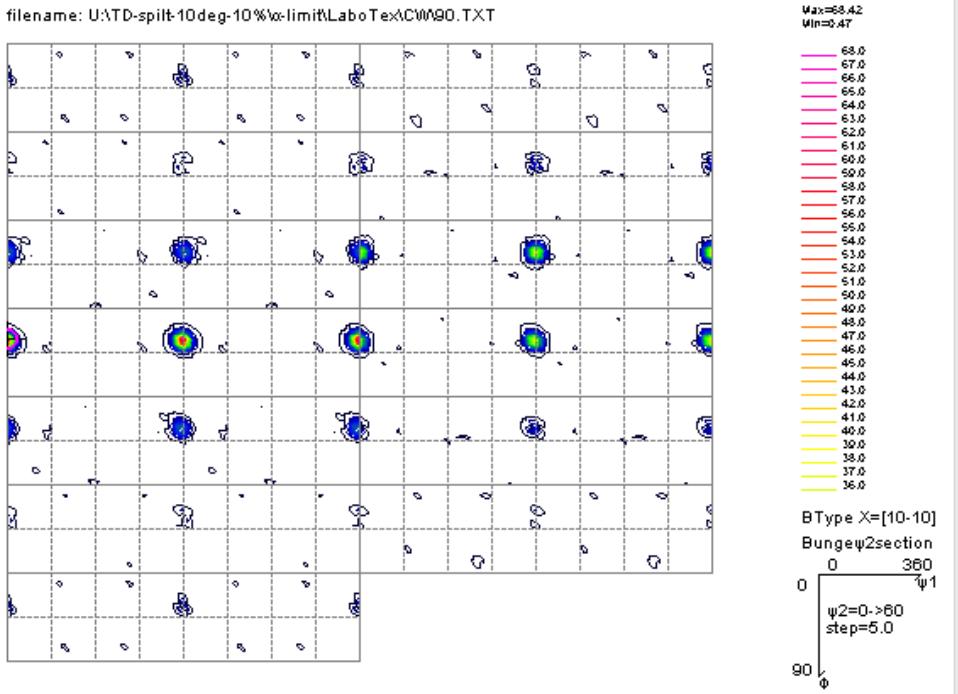


α範囲を６０－＞９０とする。

各データを ODF で解析、データ Export、GPODFDisplay の hkluvwlist で計算する。

α範囲が 0->90 の場合

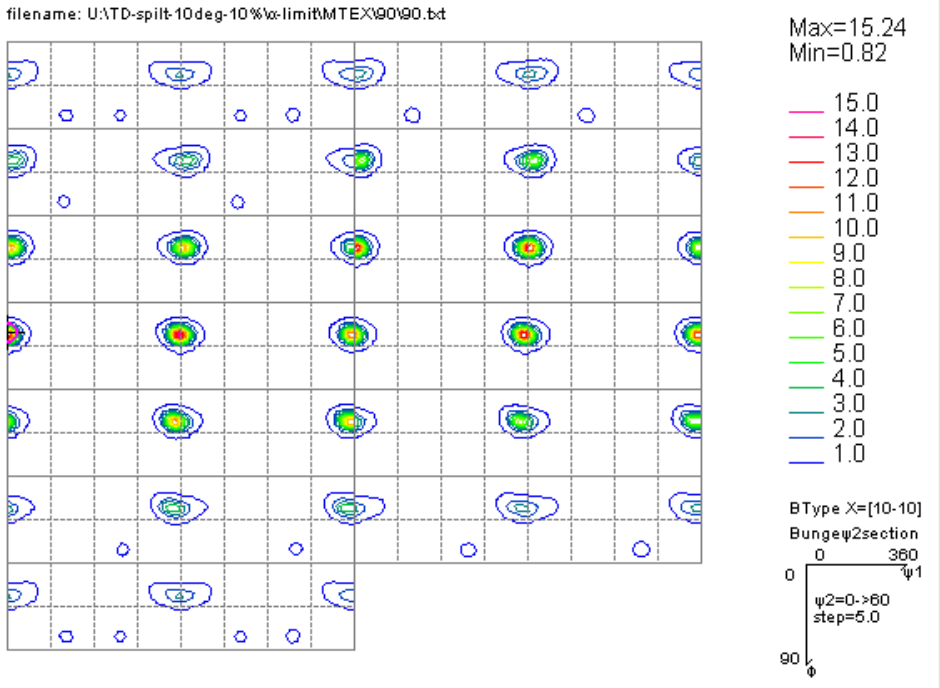
LaboTex



{hkl}<uvtw>,labo90
{0001}<10-10>,0.83
{0001}<2-1-10>,0.86
{-12-10}<10-10>,0.76
{01-10}<2-1-10>,0.96
{-12-10}<0001>,0.92
{01-10}<0001>,0.77
{-12-15}<10-10>,0.84
{01-13}<2-1-10>,68.42
{-12-14}<10-10>,1.89
{02-25}<2-1-10>,58.63
{-12-18}<4-843>,0.81
{01-14}<0-221>,0.93
{-12-16}<1-211>,0.93
{01-13}<0-332>,0.95

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=68.42

MTEX

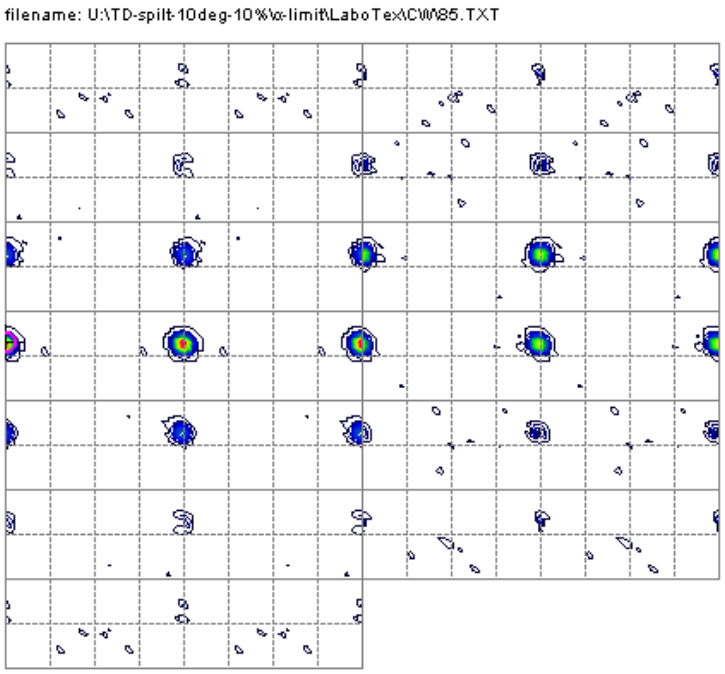


{hkl}<uvtw>,mtex90
{0001}<10-10>,0.82
{0001}<2-1-10>,0.82
{-12-10}<10-10>,0.83
{01-10}<2-1-10>,0.92
{-12-10}<0001>,0.83
{01-10}<0001>,0.87
{-12-15}<10-10>,3.19
{01-13}<2-1-10>,14.98
{-12-14}<10-10>,1.95
{02-25}<2-1-10>,14.75
{-12-18}<4-843>,1.02
{01-14}<0-221>,0.87
{-12-16}<1-211>,0.86
{01-13}<0-332>,0.88

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=14.98

α範囲が 0->85 の場合

LaboTex



{hkl}<uvtw>,labo85
{0001}<10-10>,0.84
{0001}<2-1-10>,0.86
{-12-10}<10-10>,0.85
{01-10}<2-1-10>,0.8
{-12-10}<0001>,0.84
{01-10}<0001>,0.87
{-12-15}<10-10>,0.91
{01-13}<2-1-10>,70.57
{-12-14}<10-10>,1.88
{02-25}<2-1-10>,61.24
{-12-18}<4-843>,0.81
{01-14}<0-221>,0.87
{-12-16}<1-211>,0.96
{01-13}<0-332>,0.93

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=70.57

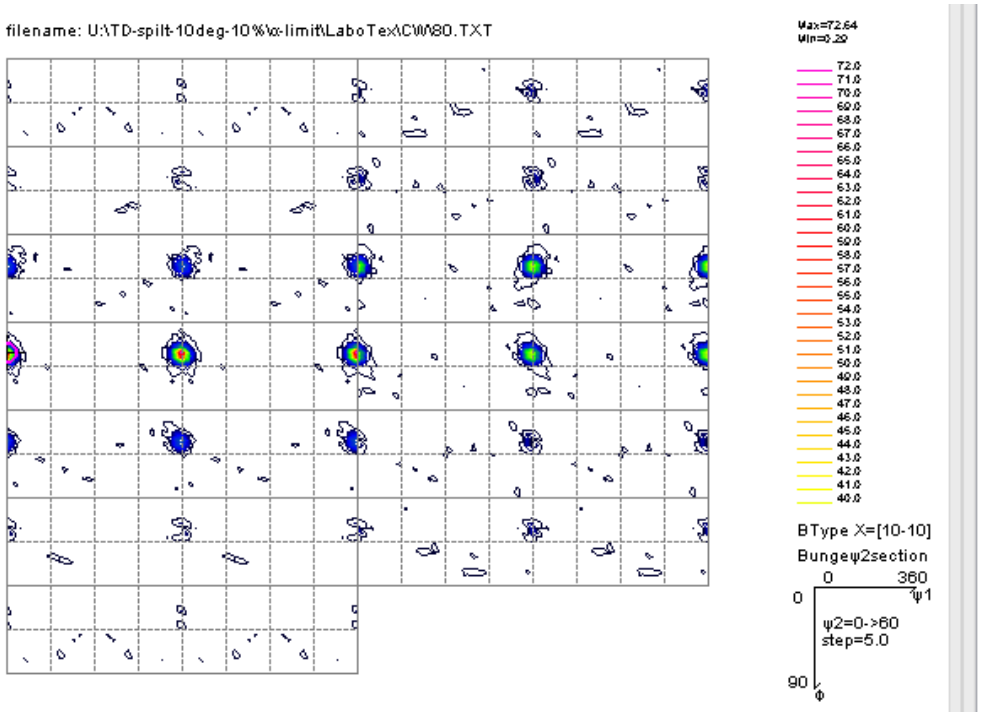
MTEX

{hkl}<uvtw>,mtex85
{0001}<10-10>,0.81
{0001}<2-1-10>,0.81
{-12-10}<10-10>,0.84
{01-10}<2-1-10>,1.01
{-12-10}<0001>,0.82
{01-10}<0001>,0.89
{-12-15}<10-10>,4.0
{01-13}<2-1-10>,14.66
{-12-14}<10-10>,2.24
{02-25}<2-1-10>,14.91
{-12-18}<4-843>,1.09
{01-14}<0-221>,0.87
{-12-16}<1-211>,0.84
{01-13}<0-332>,0.89

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=14.66

α 範囲が 0->80 の場合

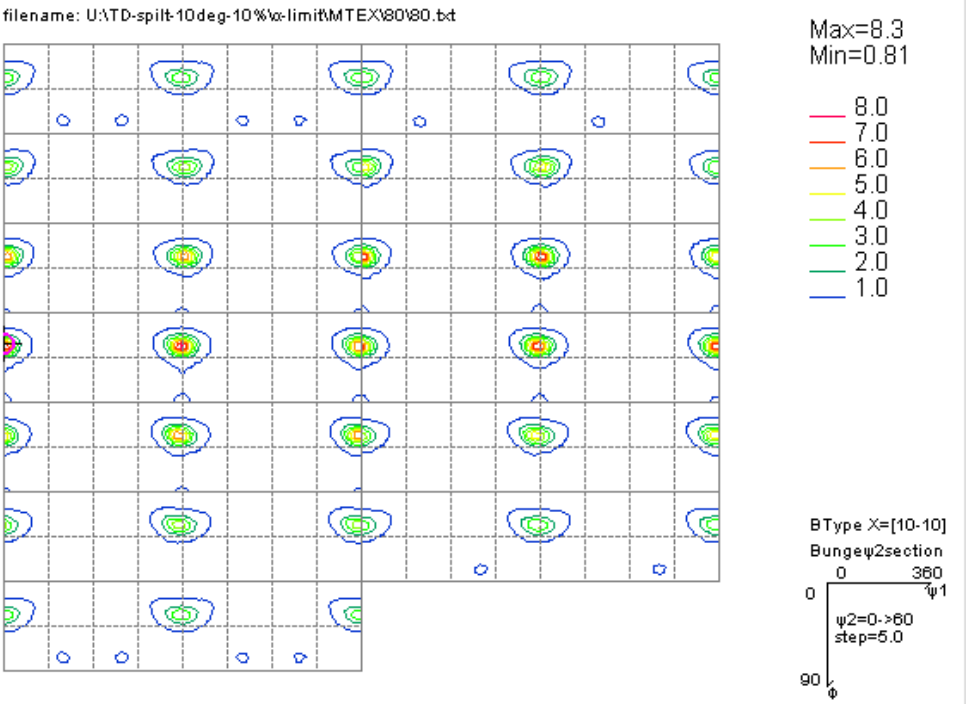
LaboTex



{hkl}<uvtw>,labo80
{0001}<10-10>,0.83
{0001}<2-1-10>,0.86
{-12-10}<10-10>,0.79
{01-10}<2-1-10>,0.73
{-12-10}<0001>,0.82
{01-10}<0001>,0.88
{-12-15}<10-10>,0.84
{01-13}<2-1-10>,72.64
{-12-14}<10-10>,1.67
{02-25}<2-1-10>,60.74
{-12-18}<4-843>,0.84
{01-14}<0-221>,0.88
{-12-16}<1-211>,0.83
{01-13}<0-332>,0.91

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=72.64

MTEX

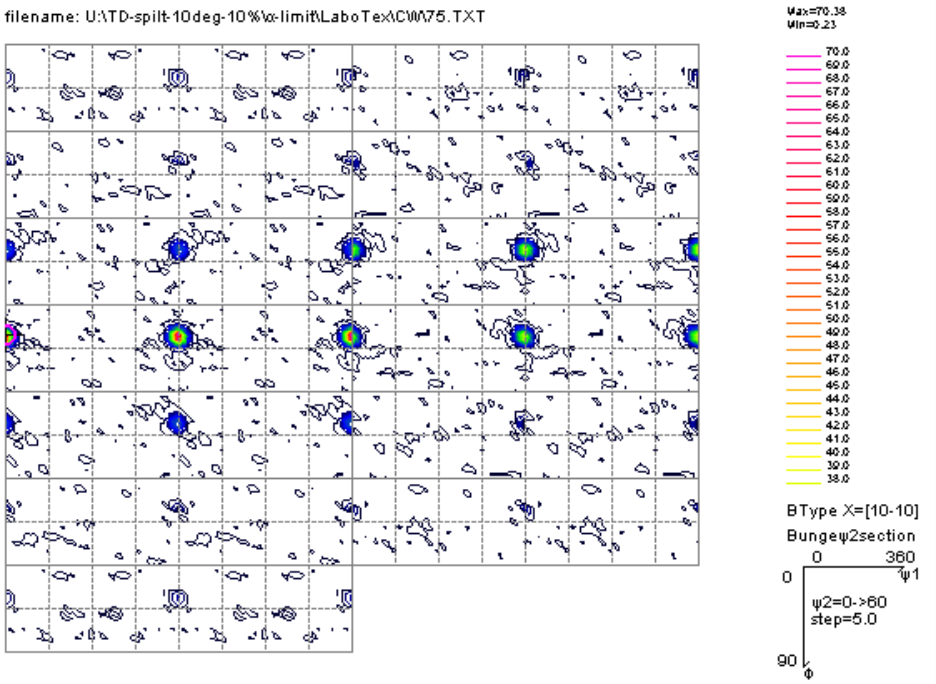


{hkl}<uvtw>,mtex80
{0001}<10-10>,0.81
{0001}<2-1-10>,0.81
{-12-10}<10-10>,0.89
{01-10}<2-1-10>,1.11
{-12-10}<0001>,0.87
{01-10}<0001>,0.95
{-12-15}<10-10>,3.92
{01-13}<2-1-10>,8.1
{-12-14}<10-10>,2.42
{02-25}<2-1-10>,8.3
{-12-18}<4-843>,1.2
{01-14}<0-221>,0.91
{-12-16}<1-211>,0.86
{01-13}<0-332>,0.93

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=8.1

α範囲が 0->75 の場合

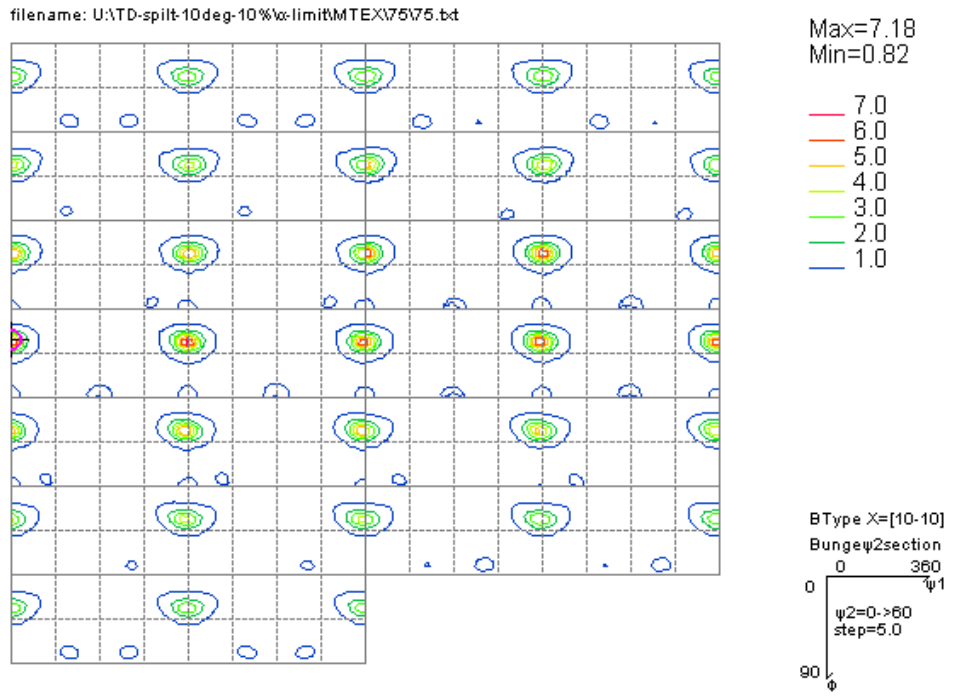
LaboTex



{hkl}<uvtw>,labo75
{0001}<10-10>,0.78
{0001}<2-1-10>,0.9
{-12-10}<10-10>,0.81
{01-10}<2-1-10>,0.74
{-12-10}<0001>,0.71
{01-10}<0001>,0.82
{-12-15}<10-10>,3.17
{01-13}<2-1-10>,70.38
{-12-14}<10-10>,2.04
{02-25}<2-1-10>,64.3
{-12-18}<4-843>,0.77
{01-14}<0-221>,0.86
{-12-16}<1-211>,0.77
{01-13}<0-332>,1.03

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=70.38

MTEX

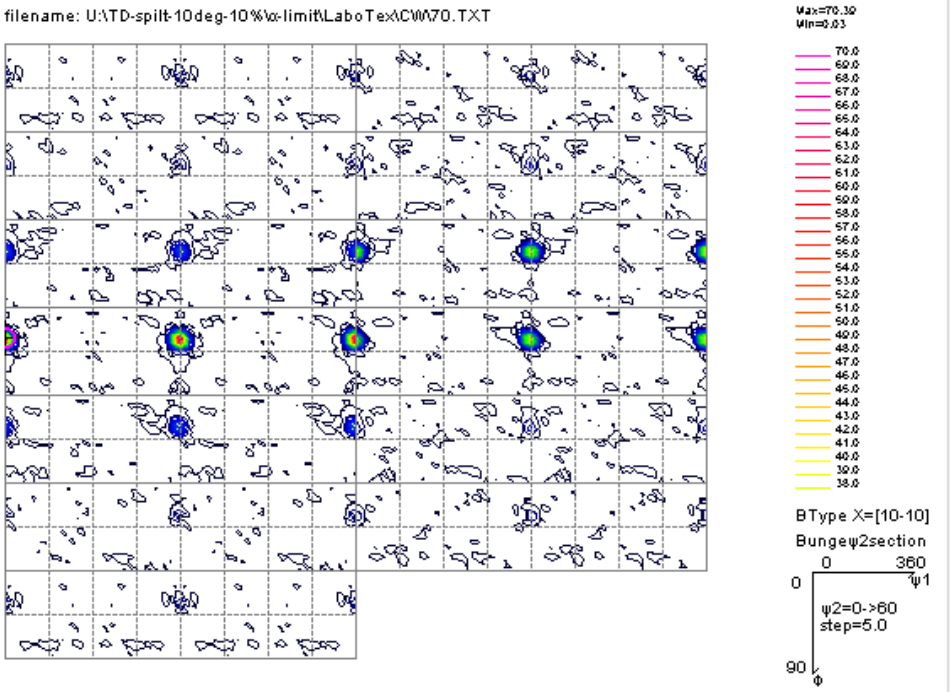


{hkl}<uvtw>,mtex75
{0001}<10-10>,0.82
{0001}<2-1-10>,0.82
{-12-10}<10-10>,0.9
{01-10}<2-1-10>,1.16
{-12-10}<0001>,0.9
{01-10}<0001>,0.99
{-12-15}<10-10>,3.93
{01-13}<2-1-10>,7.03
{-12-14}<10-10>,2.47
{02-25}<2-1-10>,7.18
{-12-18}<4-843>,1.21
{01-14}<0-221>,0.91
{-12-16}<1-211>,0.86
{01-13}<0-332>,0.92

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=7.03

α範囲が 0->70 の場合

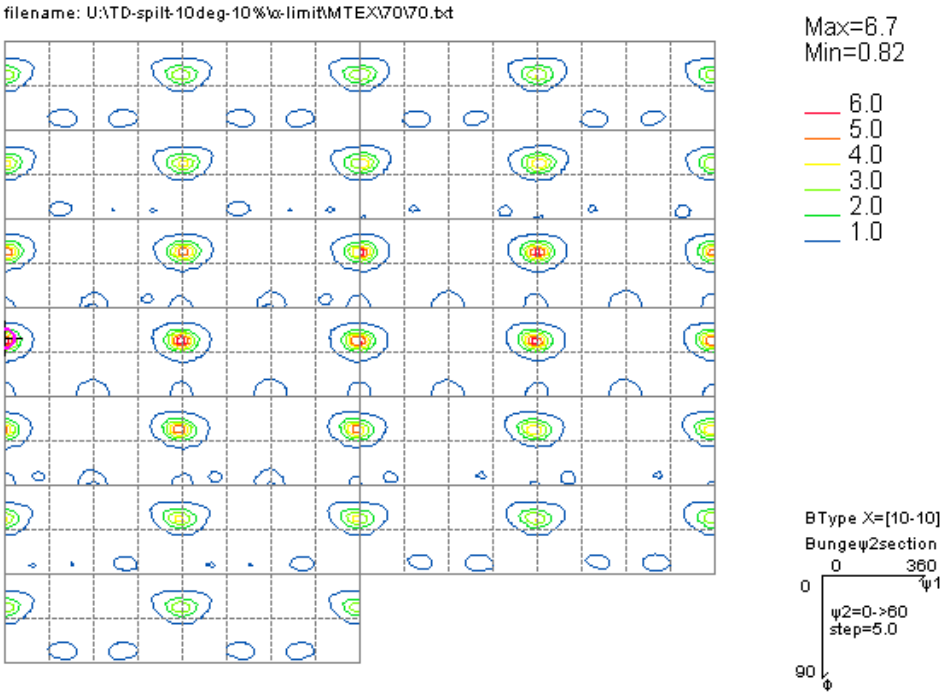
LaboTex



{hkl}<uvtw>,labo70
{0001}<10-10>,0.79
{0001}<2-1-10>,0.87
{-12-10}<10-10>,0.82
{01-10}<2-1-10>,0.86
{-12-10}<0001>,0.43
{01-10}<0001>,0.82
{-12-15}<10-10>,3.41
{01-13}<2-1-10>,70.39
{-12-14}<10-10>,1.56
{02-25}<2-1-10>,60.89
{-12-18}<4-843>,0.89
{01-14}<0-221>,0.83
{-12-16}<1-211>,0.83
{01-13}<0-332>,0.84

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=70.39

MTEX

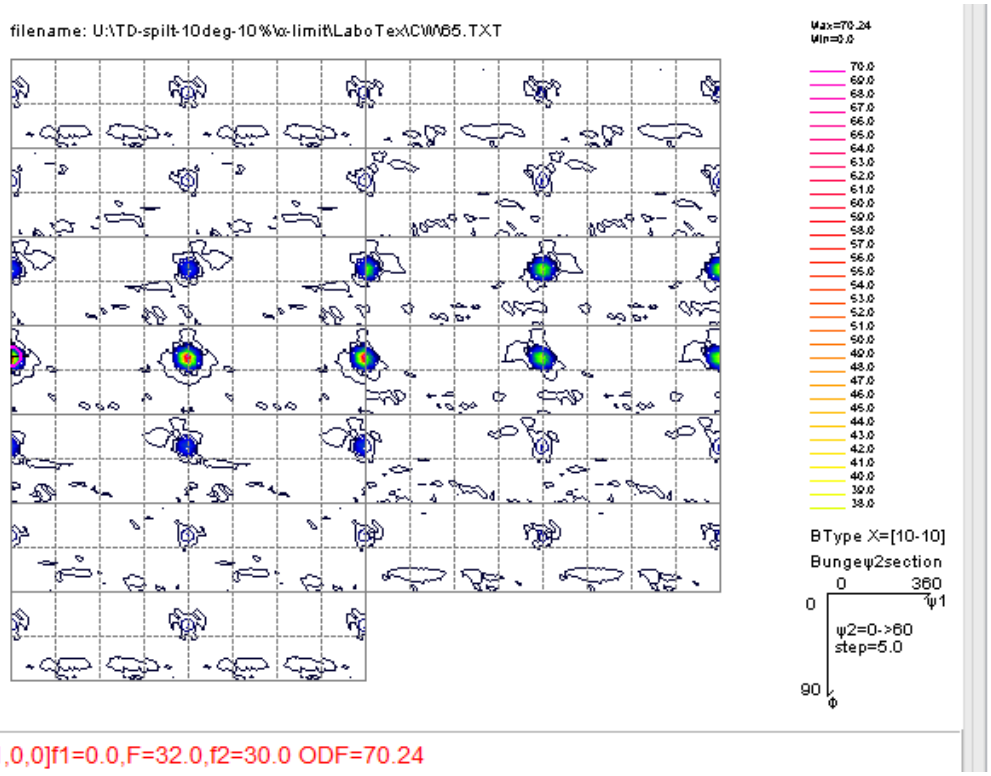


{hkl}<uvtw>,mtex70
{0001}<10-10>,0.82
{0001}<2-1-10>,0.82
{-12-10}<10-10>,0.89
{01-10}<2-1-10>,1.19
{-12-10}<0001>,0.89
{01-10}<0001>,1.02
{-12-15}<10-10>,3.98
{01-13}<2-1-10>,6.51
{-12-14}<10-10>,2.52
{02-25}<2-1-10>,6.7
{-12-18}<4-843>,1.22
{01-14}<0-221>,0.9
{-12-16}<1-211>,0.85
{01-13}<0-332>,0.92

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=6.51

α 範囲が 0->65 の場合

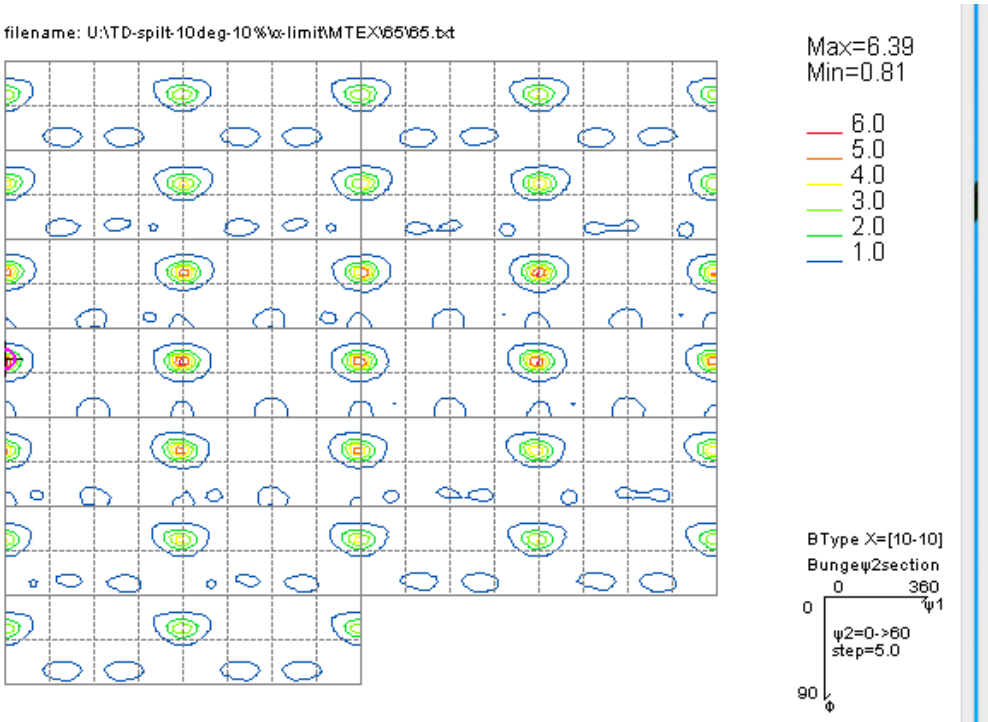
LaboTex



{hkl}<uvtw>,labo65
{0001}<10-10>,0.78
{0001}<2-1-10>,0.9
{-12-10}<10-10>,0.94
{01-10}<2-1-10>,1.39
{-12-10}<0001>,0.25
{01-10}<0001>,0.95
{-12-15}<10-10>,3.02
{01-13}<2-1-10>,70.24
{-12-14}<10-10>,1.78
{02-25}<2-1-10>,60.36
{-12-18}<4-843>,0.83
{01-14}<0-221>,0.9
{-12-16}<1-211>,0.88
{01-13}<0-332>,0.93

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=70.24

MTEX

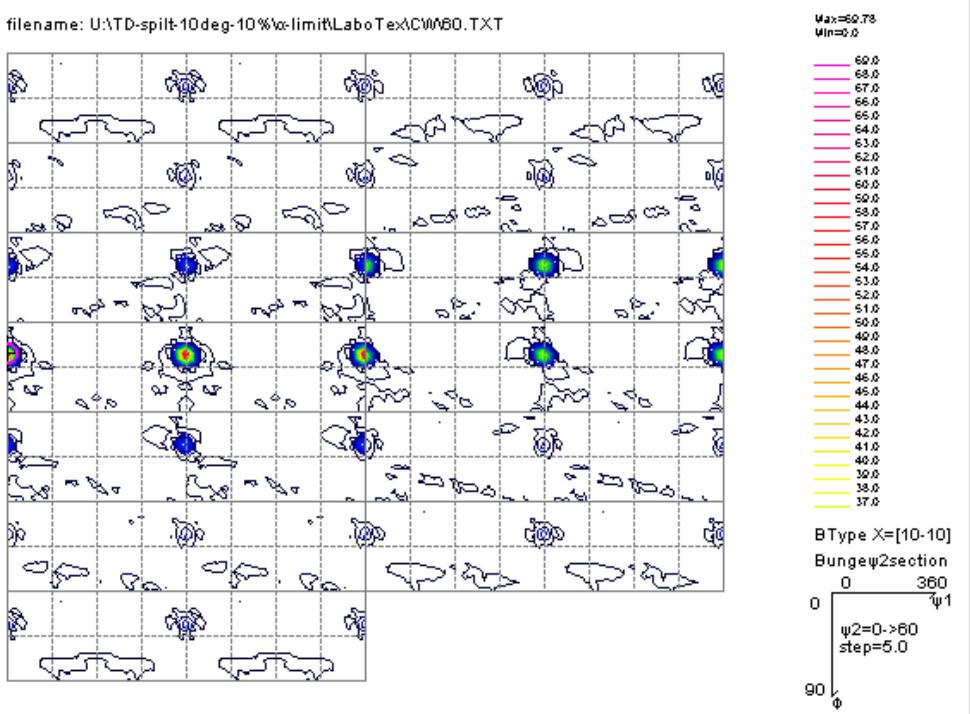


{hkl}<uvtw>,mtex65
{0001}<10-10>,0.81
{0001}<2-1-10>,0.81
{-12-10}<10-10>,0.88
{01-10}<2-1-10>,1.13
{-12-10}<0001>,0.88
{01-10}<0001>,1.03
{-12-15}<10-10>,4.02
{01-13}<2-1-10>,6.21
{-12-14}<10-10>,2.54
{02-25}<2-1-10>,6.39
{-12-18}<4-843>,1.22
{01-14}<0-221>,0.89
{-12-16}<1-211>,0.84
{01-13}<0-332>,0.9

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=6.21

α範囲が 0->60 の場合

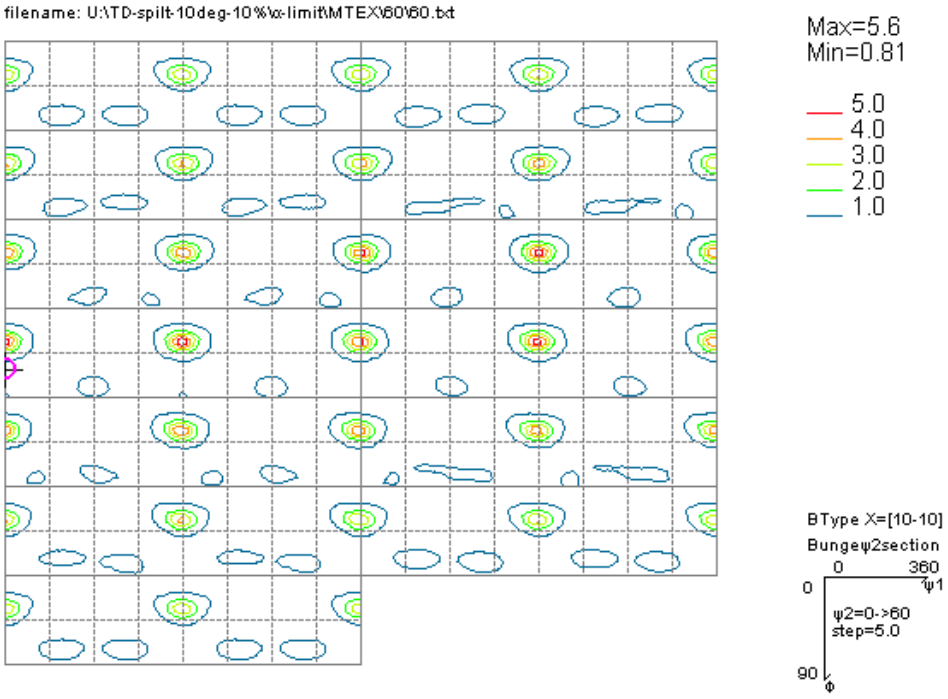
LaboTex



{hkl}<uvtw>,labo60
{0001}<10-10>,0.8
{0001}<2-1-10>,0.86
{-12-10}<10-10>,0.86
{01-10}<2-1-10>,1.04
{-12-10}<0001>,0.27
{01-10}<0001>,0.95
{-12-15}<10-10>,3.57
{01-13}<2-1-10>,69.78
{-12-14}<10-10>,1.72
{02-25}<2-1-10>,56.93
{-12-18}<4-843>,0.99
{01-14}<0-221>,0.92
{-12-16}<1-211>,0.93
{01-13}<0-332>,0.91

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=69.78

MTEX



{hkl}<uvtw>,mtex60
{0001}<10-10>,0.82
{0001}<2-1-10>,0.81
{-12-10}<10-10>,0.89
{01-10}<2-1-10>,1.01
{-12-10}<0001>,0.89
{01-10}<0001>,0.99
{-12-15}<10-10>,3.97
{01-13}<2-1-10>,5.45
{-12-14}<10-10>,2.52
{02-25}<2-1-10>,5.6
{-12-18}<4-843>,1.23
{01-14}<0-221>,0.86
{-12-16}<1-211>,0.85
{01-13}<0-332>,0.87

(0,1,1)[1,0,0]f1=0.0,F=61.9,f2=30.0 ODF=0.93

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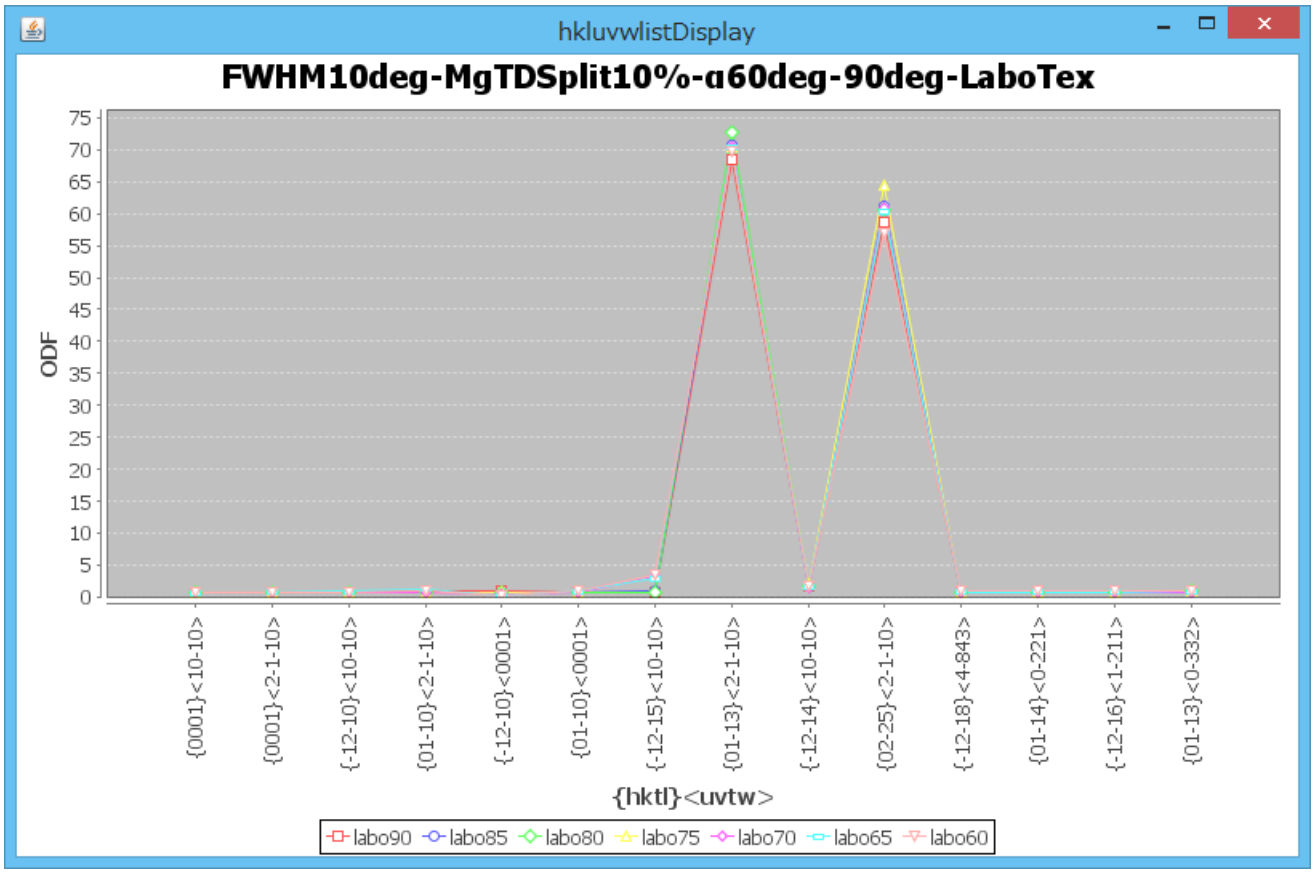
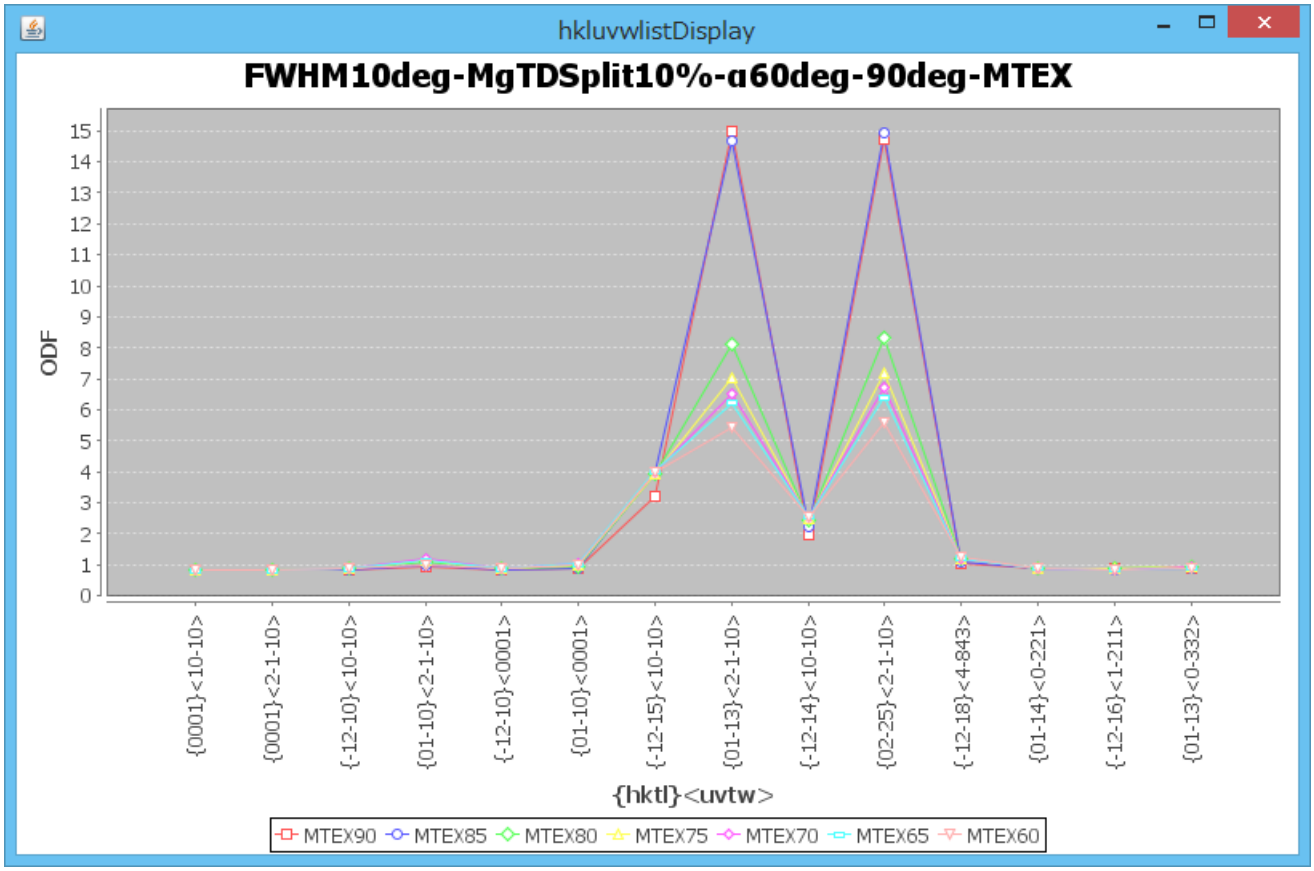


ＭＴＥＸ



ＭＴＥＸではα範囲が変わると、ＴＤＳｐｌｉｔの結晶方位密度が変化する。

ＦＷＨＭ＝２０ｄｅｇではほとんど変化は認められなかった。

ＭＴＥＸでは強い配向の場合、極点図の範囲に影響を受ける。

これはＨｅｒｍｏｎｉｃの特徴で、展開次数の変更が必要か？？？