Schmid因子計算の確認Ｔｏｏｌ

単結晶測定反射極点図１面から複数の極点図生成
結晶方位回転確認
回転方位のｅｕｌｅｒ角度計算
ＢＣＣ，ＦＣＣ，ＨＣＰシュミット因子計算

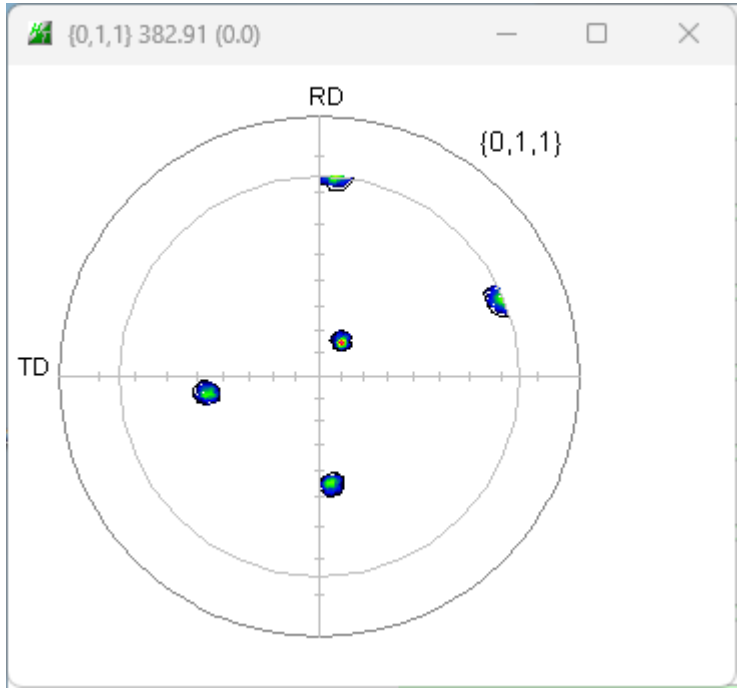
2023/05/05

単結晶のＳｃｈｍｉｄ因子

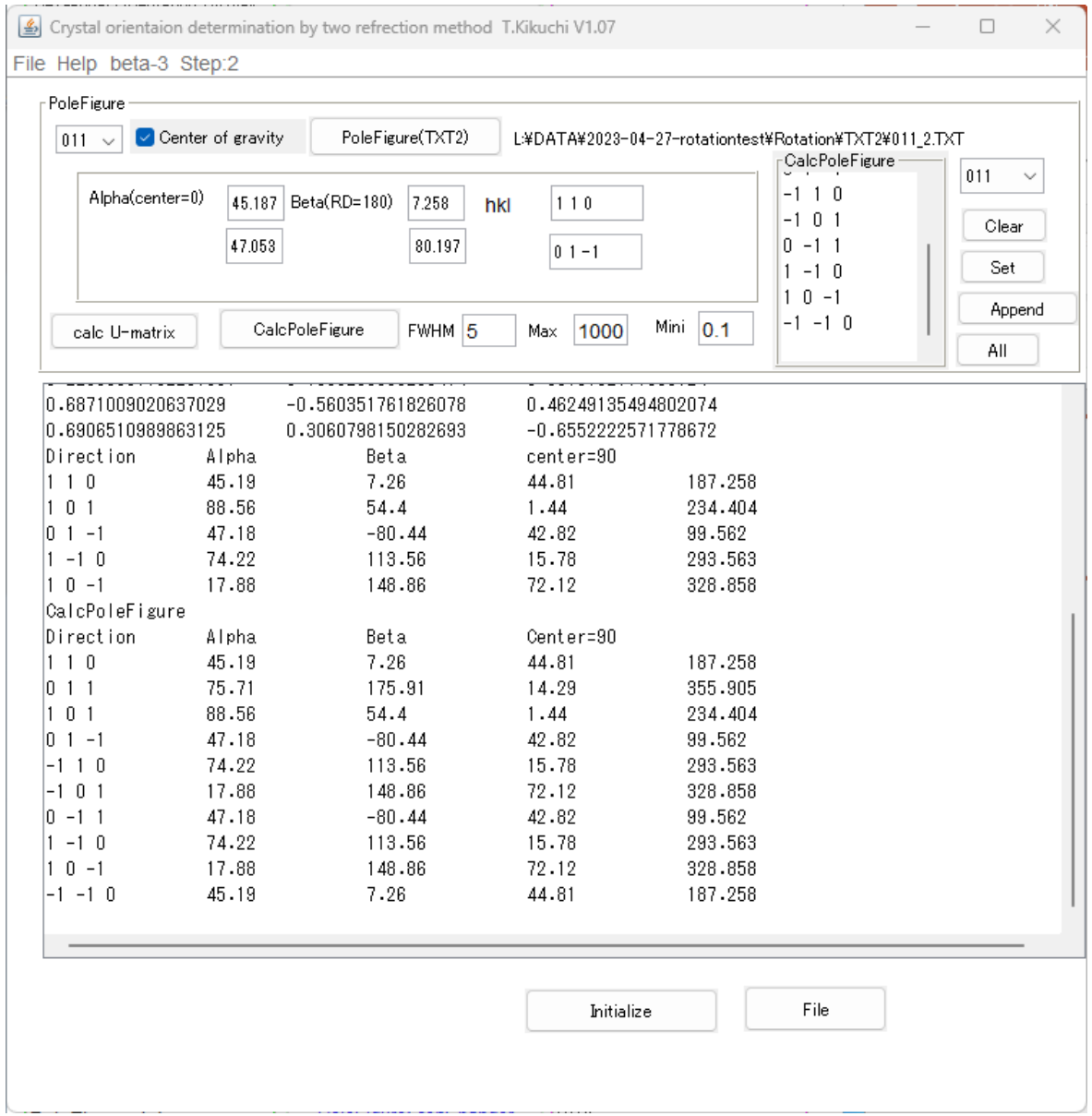
{220}面の極点測定（step=2.5deg）

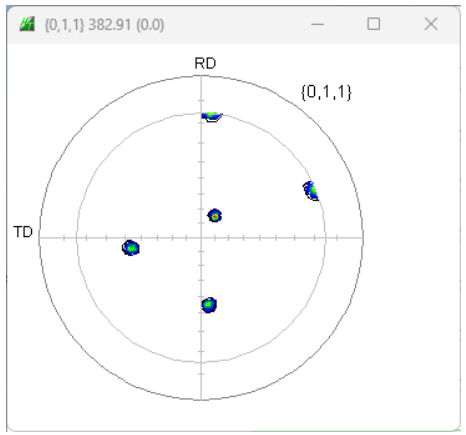
反射極点図{011}から{001},{011},{111}　の完全極点図を作成

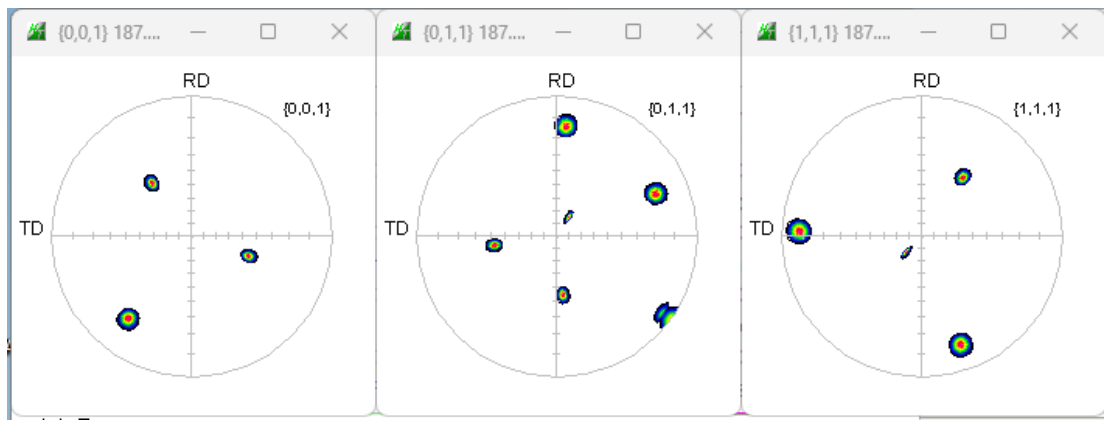
ODF解析により方位解析



{001},{011},{111}極点図作成

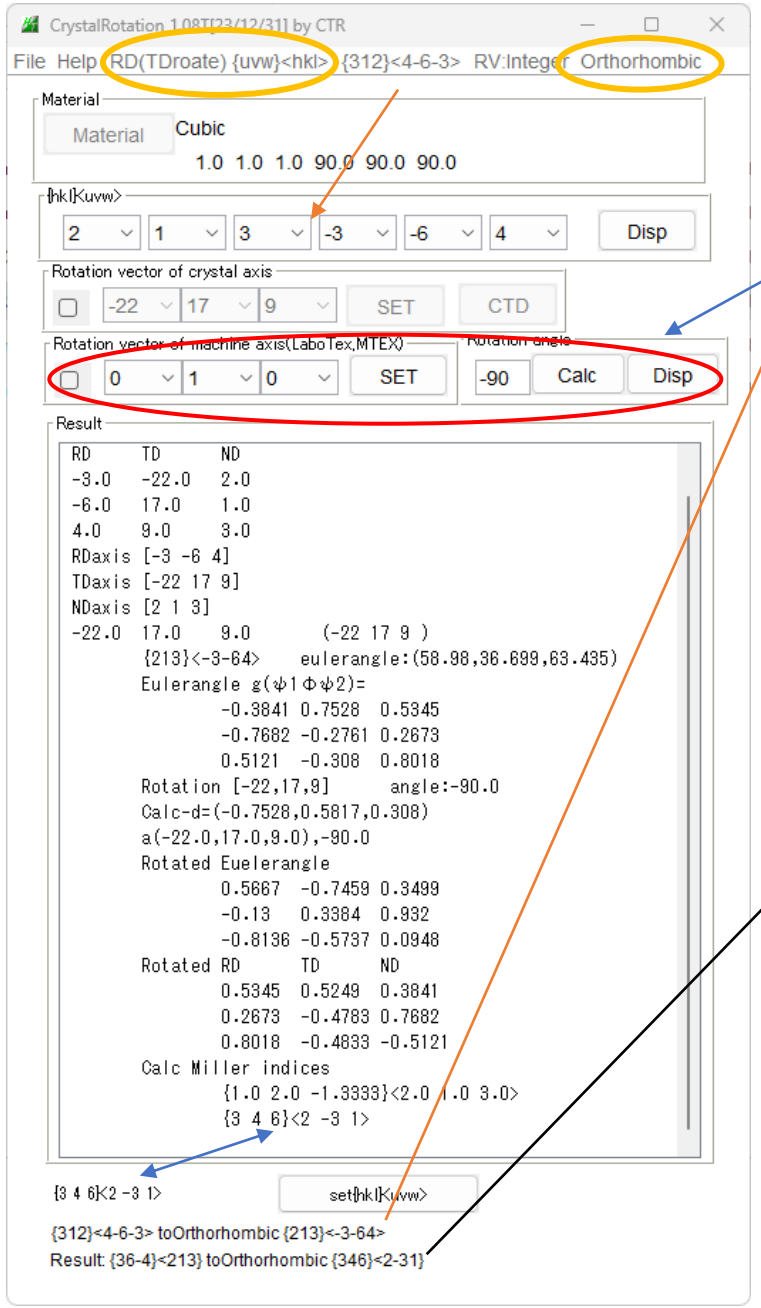






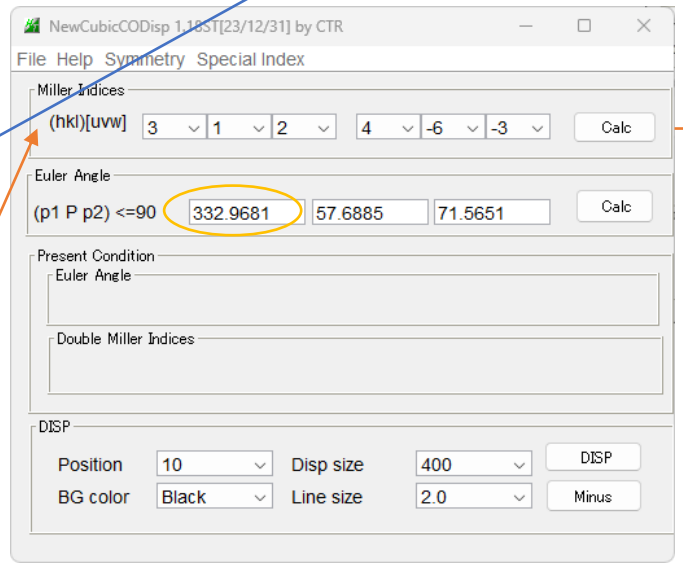
ODFにより方位解析
反射極点図１面から方位解析が可能

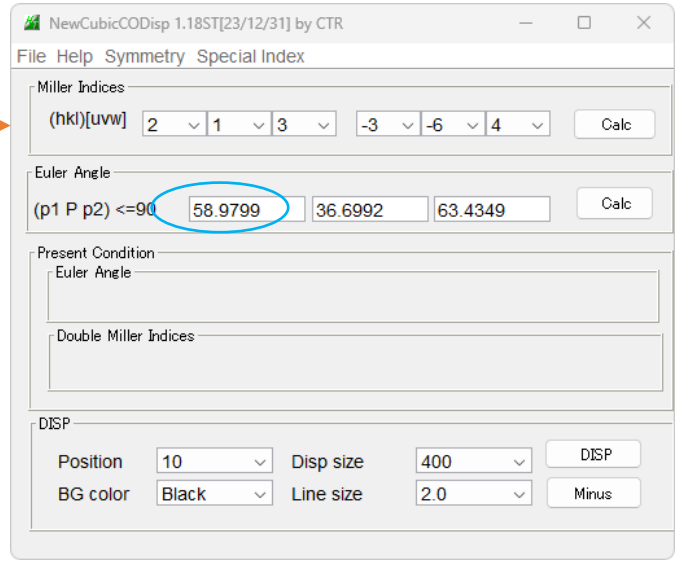
回転

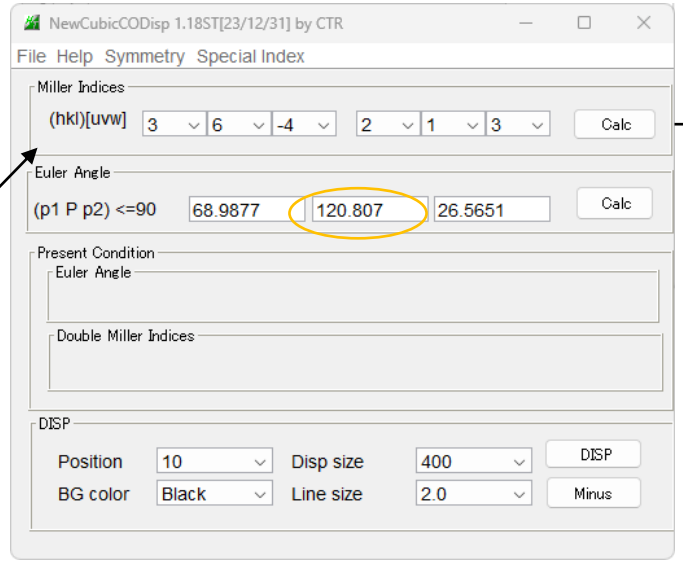


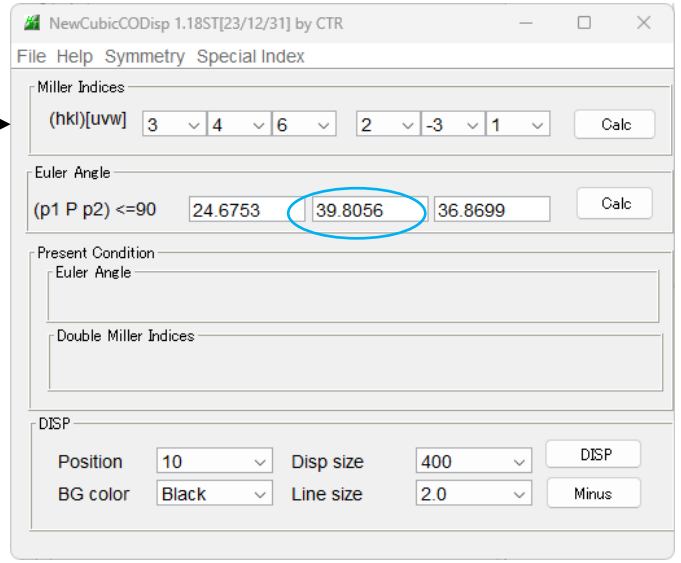
回転方向を選択し方位入力

入力方位{312}<4-6-3>に対しOrthorhombic変換{213}<-3-64>
TD軸[-22 17 9]90度回転、{36-4}<213>を得て、Orthorhombic変換で{346}<2-31>を得る



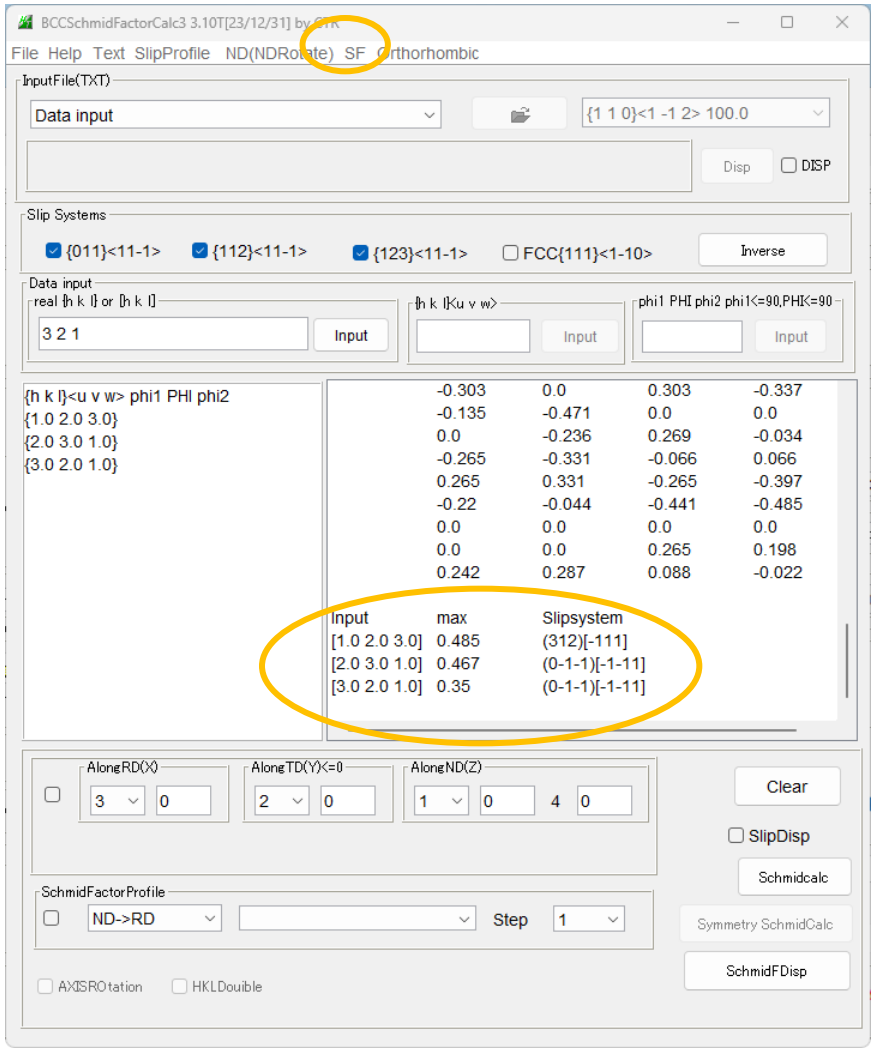


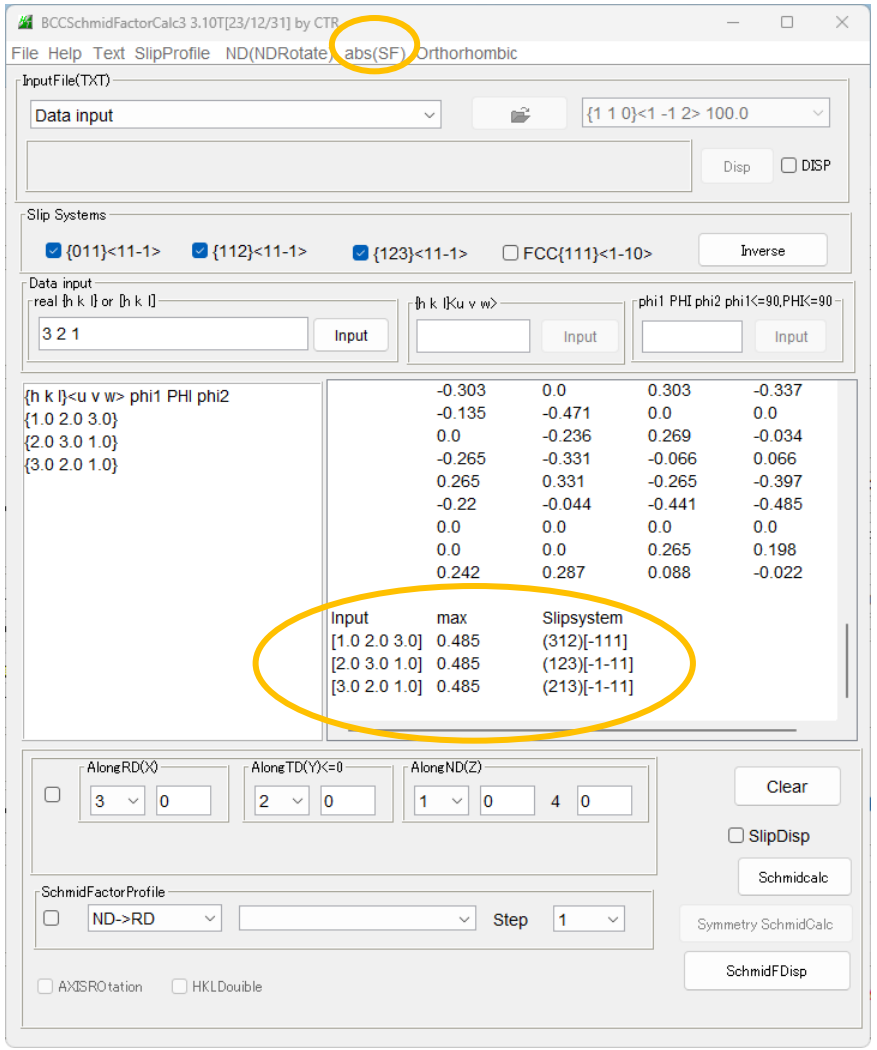




{hkl}<uvw>をTD軸回転で{uvw}<hkl>を得る

方向によりSchmid因子は異なるが絶対値で一致する

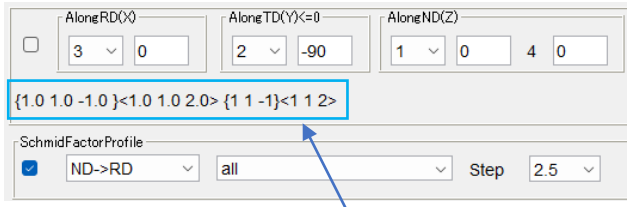




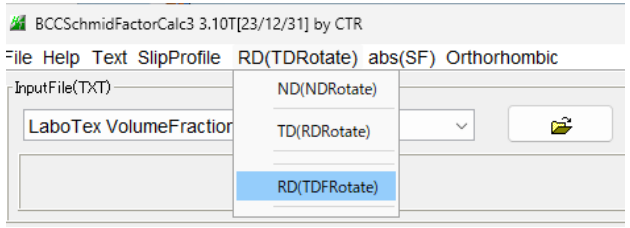
絶対値は対称方位を含む絶対値シュミット因子最大値が計算される

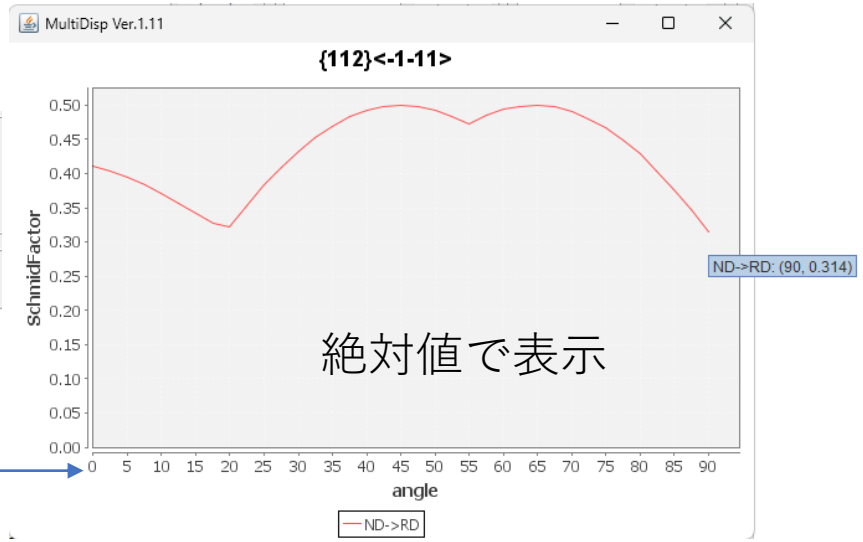
回転

{1 1 2}<-1 -1 1> 100.0
RDaxis [-1 -1 1]
TDaxis [-1 1 0]
NDaxis [1 1 2]

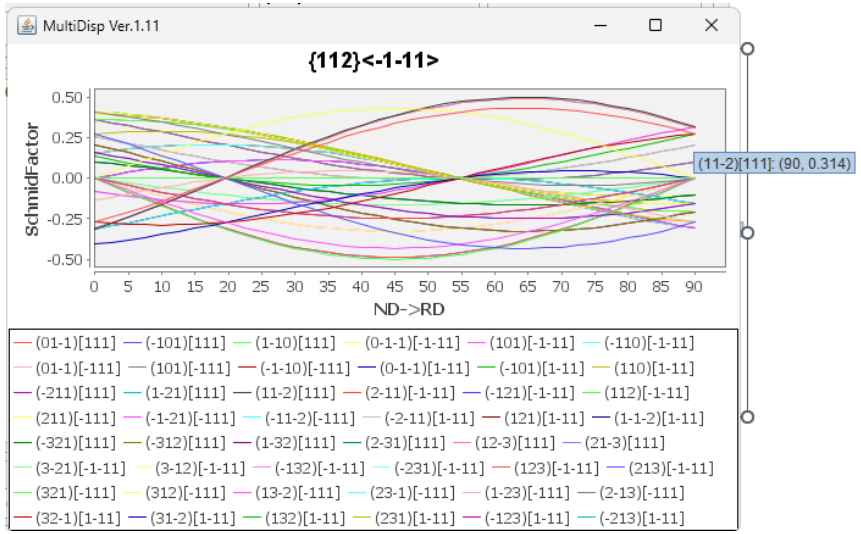


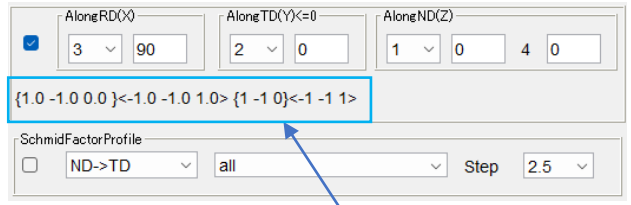
RD方向は{uvw}<hkl>
TD-axisで回転



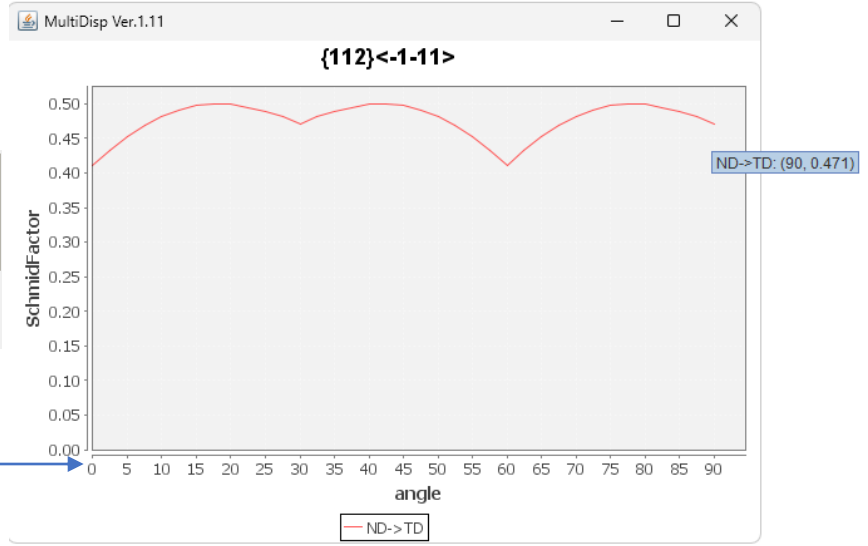


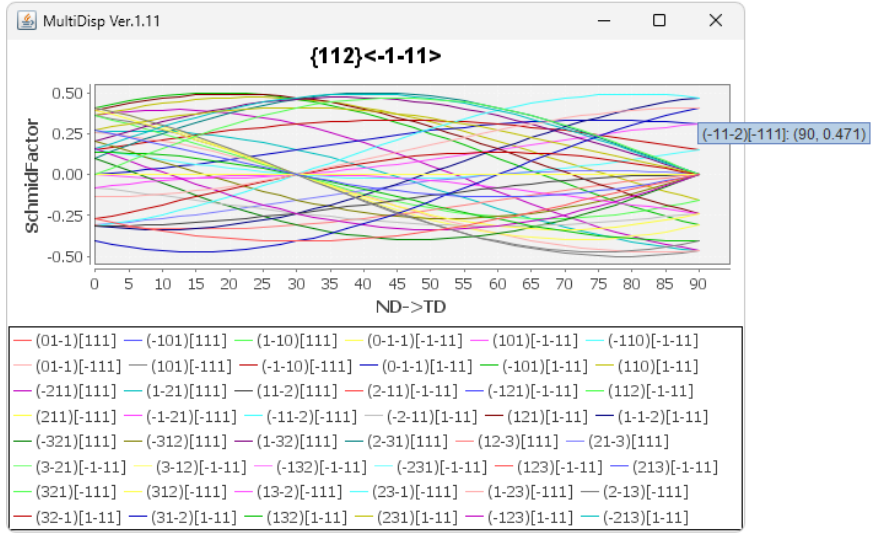
表示は絶対値ではなくﾌﾟﾗｽﾏｲﾅｽの最大値で表現



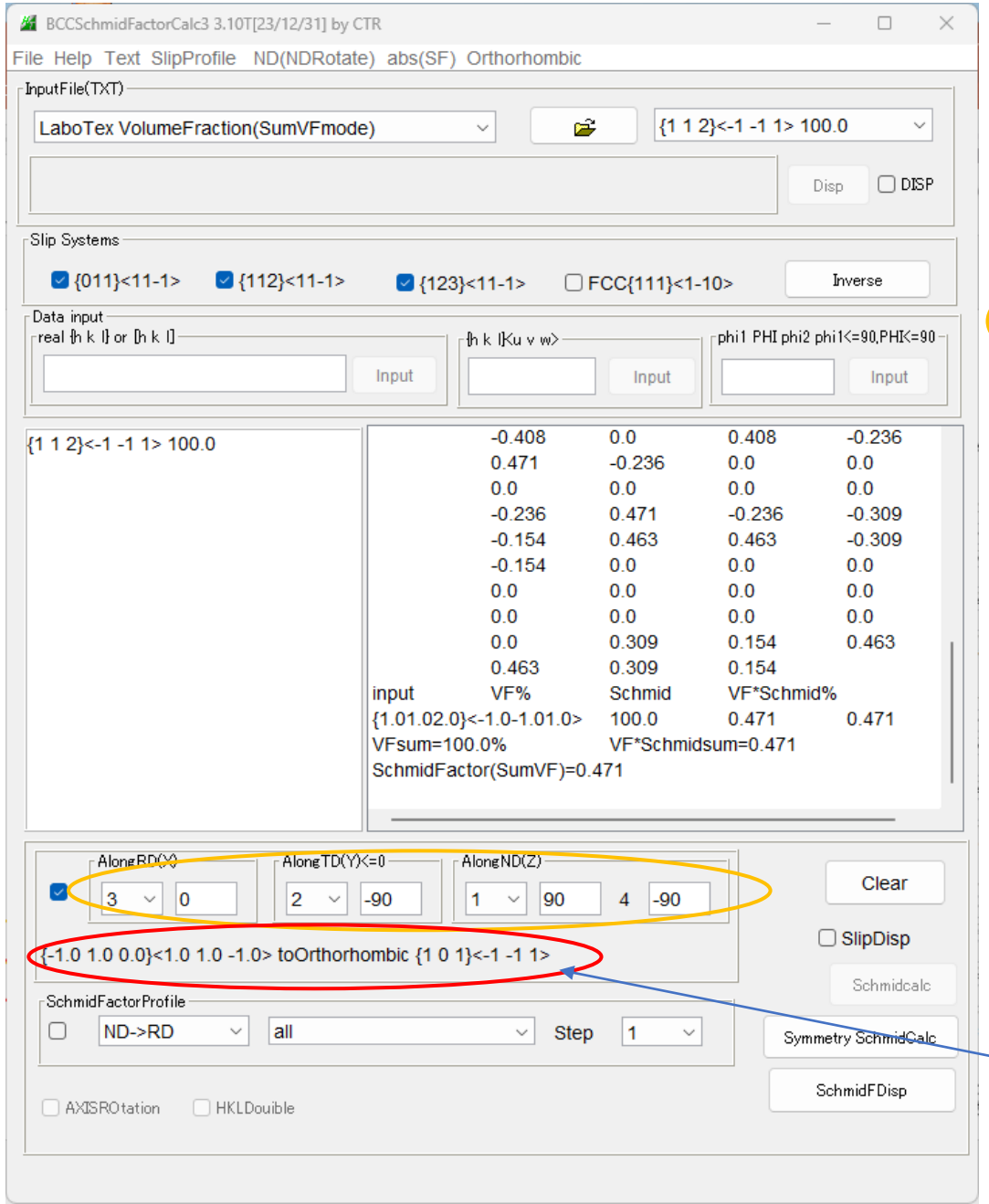


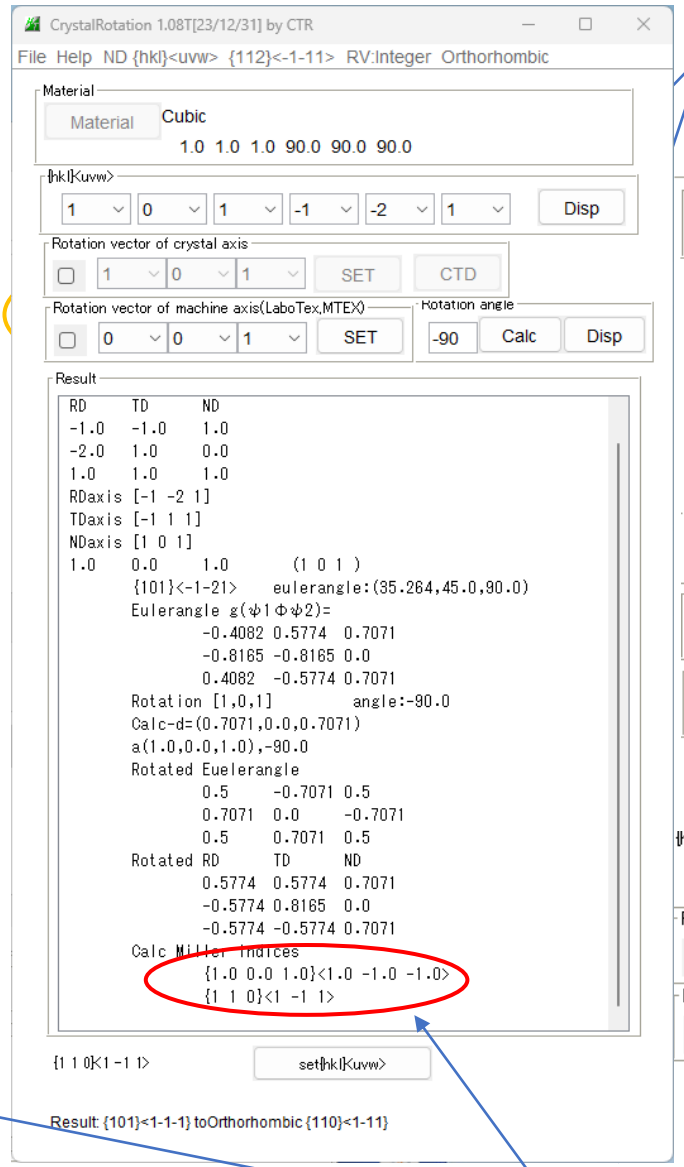
TD方向は{TD}<uvw>
RD-axisで回転



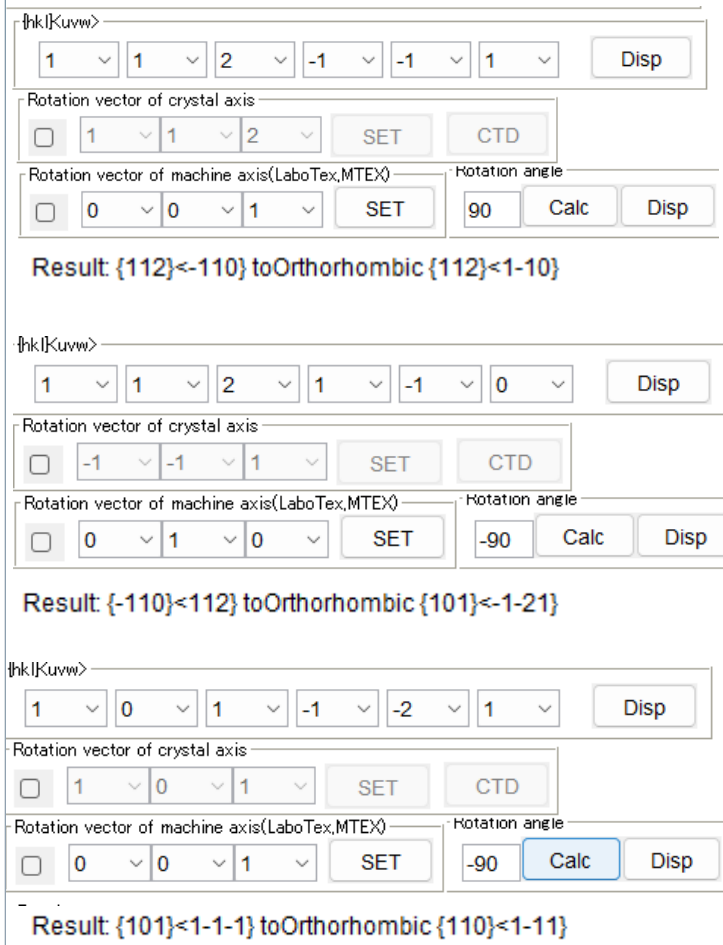


連続回転　　{112}<-1-11>をND(90)、TD(-90)、ND(-90)で{-110}<-11-1>が計算され、SF=0.471を得る





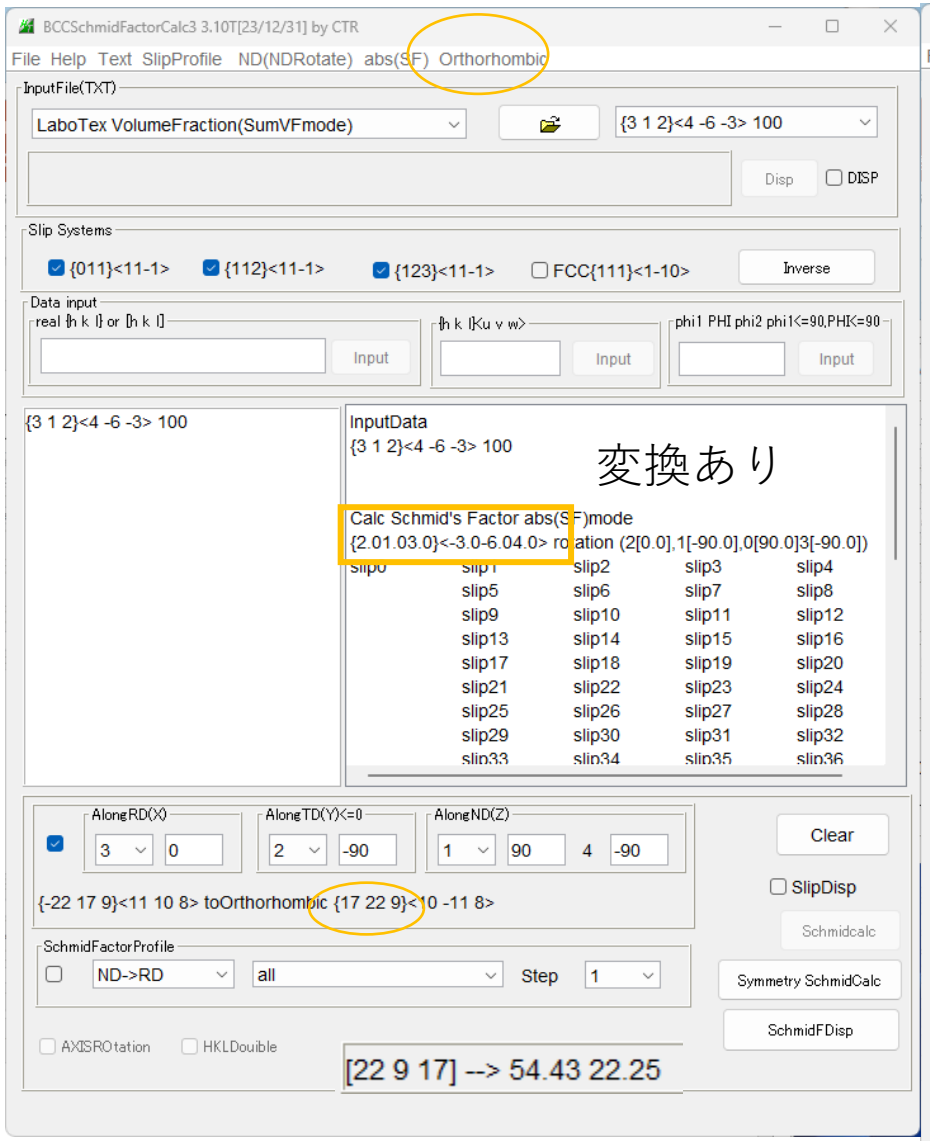
繰り返し

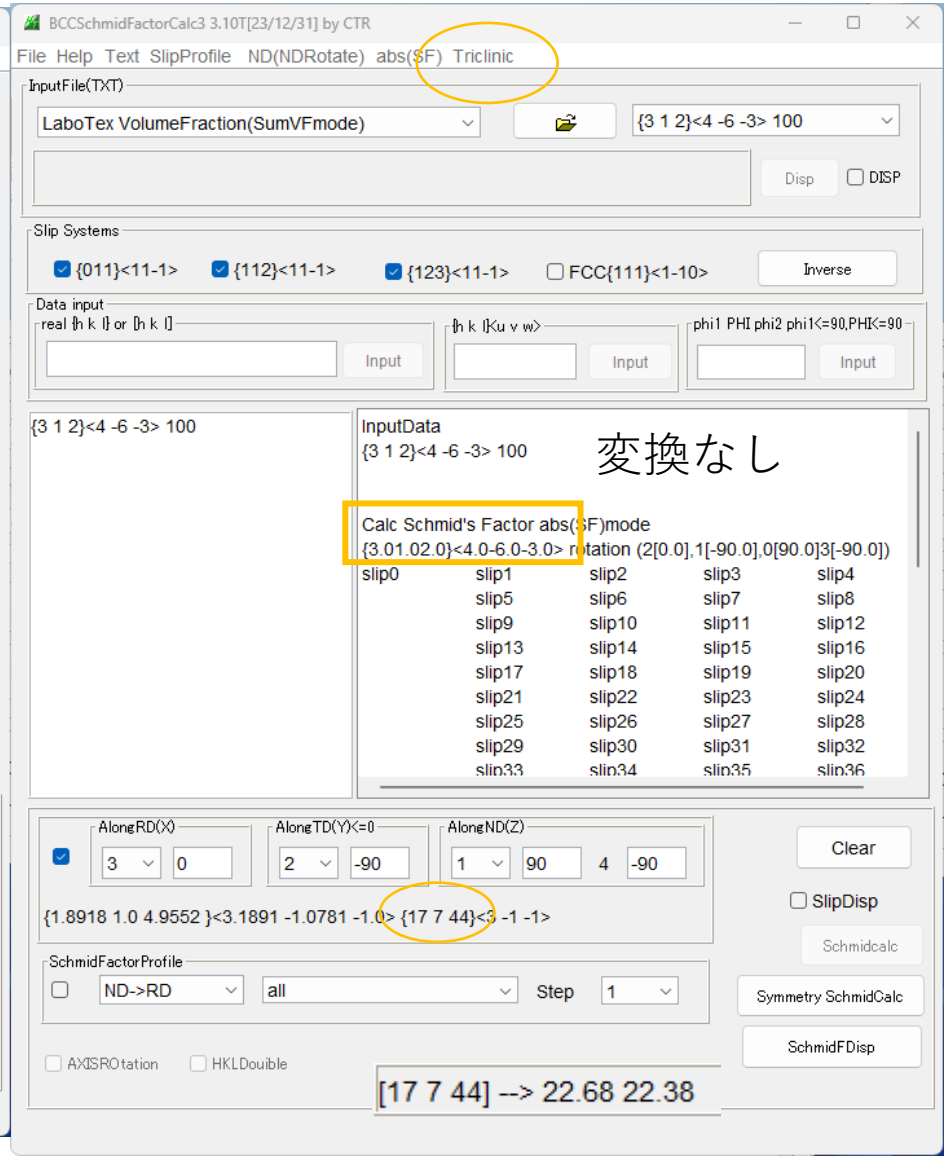


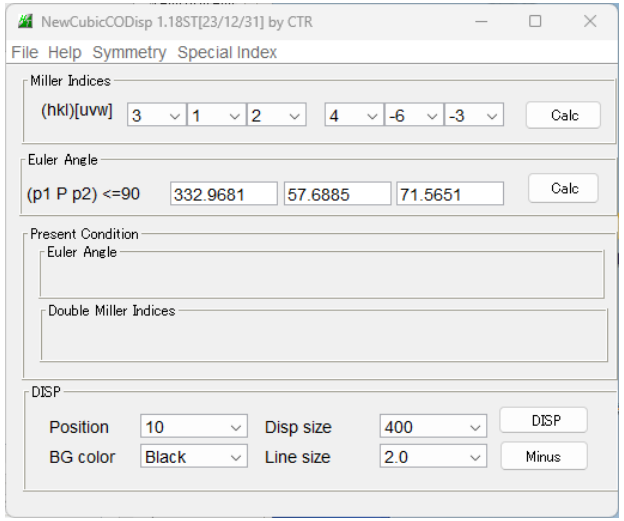
CrystalRotationは回転毎に整数化、Orthorhombicチェックが行われているが、
BccSchmidFactorCalcは実数のままで計算し、最後に整数化Orthorhombicチェック

Orthorhombic↔Triclinc

Orthorhombic(90,90,90)　Triclinc(360,90,90)



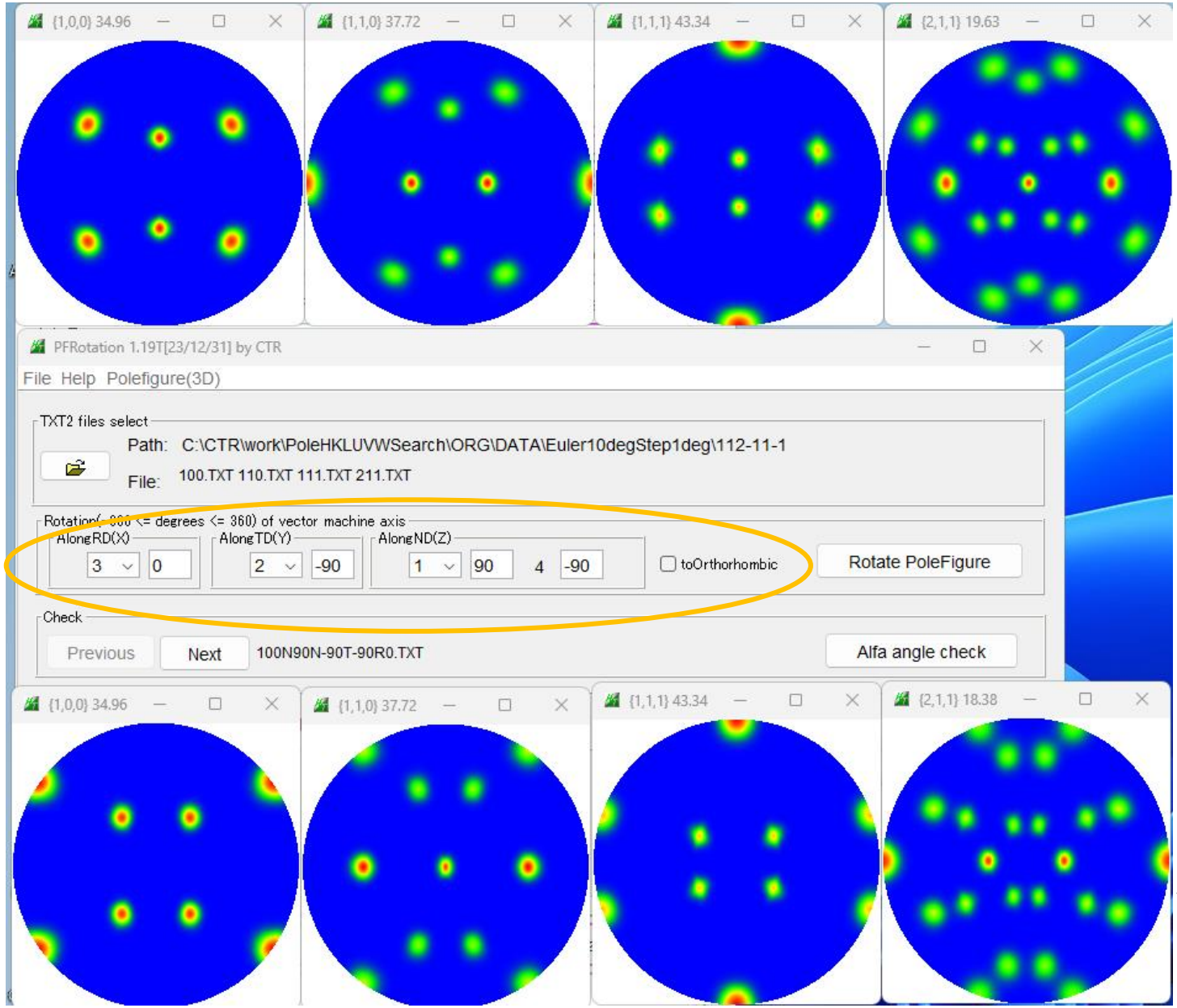




{2.01.03.0}<-3.0-6.04.0>　100.0　0.477
VFsum=100.0%　VF*Schmidsum=0.477
SchmidFactor(SumVF)=0.477

{3.01.02.0}<4.0-6.0-3.0>　100.0　0.494
VFsum=100.0%　VF*Schmidsum=0.494
SchmidFactor(SumVF)=0.494

連続回転をPFRotationで確認



{112}<111>

ND 90度回転
TD –90度回転
ND -90度回転
を連続した結果

{110}<111>