

## brass、copper 方位に関する極点図範囲の影響

### TexTools の場合

Brass,copper の完全極点図{111},{100},{110}を作成し、極点図の範囲が ODF 解析結果に及ぼす結果を確認した。

| $\alpha$ 範囲 | ODF  | {111} | {100} | {110} | error(%) | brassVF(%) | copperVF(%) | {111} <sub>a=0</sub> |
|-------------|------|-------|-------|-------|----------|------------|-------------|----------------------|
| 0-90        | 28.9 | 4.2   | 3.7   | 4.5   | 2.59     | 12.88      | 13.12       | 0.6152               |
| 0-85        | 10.8 | 2.7   | 2.3   | 2.6   | 2.70     | 11.97      | 12.33       | 0.6533               |
| 0-80        | 10.9 | 2.7   | 2.3   | 2.6   | 3.19     | 12.01      | 12.30       | 0.6400               |
| 0-75        | 10.6 | 2.7   | 2.3   | 2.6   | 3.57     | 12.01      | 12.26       | 0.6455               |
| 0-70        | 10.4 | 2.7   | 2.3   | 2.6   | 3.40     | 11.94      | 12.30       | 0.6459               |
| 0-65        | 10.5 | 2.7   | 2.3   | 2.6   | 3.04     | 11.90      | 12.19       | 0.6790               |
| 0-60        | 10.8 | 2.7   | 2.3   | 2.6   | 2.87     | 11.91      | 12.02       | 0.6762               |
| 0-55        | 10.6 | 2.6   | 2.4   | 2.5   | 2.97     | 11.56      | 11.80       | 0.7171               |
| 0-50        | 9.9  | 2.5   | 2.4   | 2.5   | 5.09     | 11.27      | 11.35       | 0.8947               |
| 0-45        | 9.4  | 2.4   | 2.4   | 2.5   | 4.35     | 10.38      | 10.71       | 1.2081               |
| 0-40        | 8.8  | 2.3   | 2.4   | 2.4   | 3.86     | 10.03      | 10.31       | 0.9072               |
| 0-35        | 7.9  | 2.4   | 2.3   | 2.4   | 4.67     | 9.39       | 10.19       | 0.8731               |
| 0-30        | 6.8  | 2.2   | 1.9   | 2.3   | 2.63     | 7.28       | 9.26        | 0.9307               |

$\alpha$  範囲を制限すると、完全極点図の ODF 値が半分になるが、結晶方位は正確得られる。

制限が 1/2 になると、ODF 値が急激に下がる。

ODF 最大密度が下がると比例してバックグラウンドレベルがあがる。

結果として ADC 法の場合、 $\alpha$  範囲がある程度確保されていれば正確な定量が出来る。

この解析は brass,copper に対して行った結果であり、全ての方位に関する結果ではない。

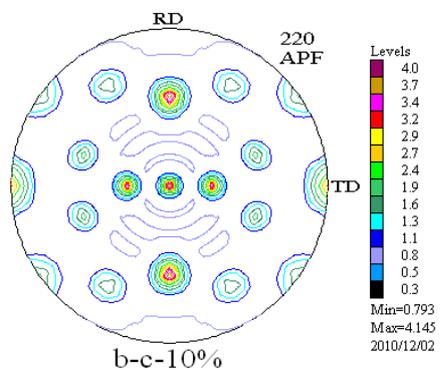
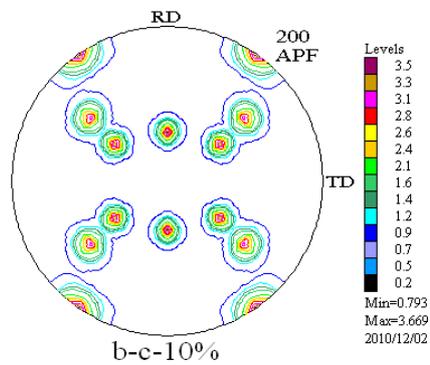
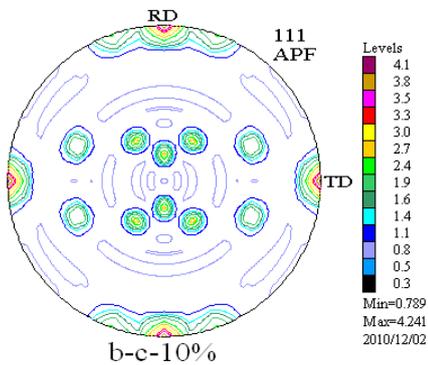
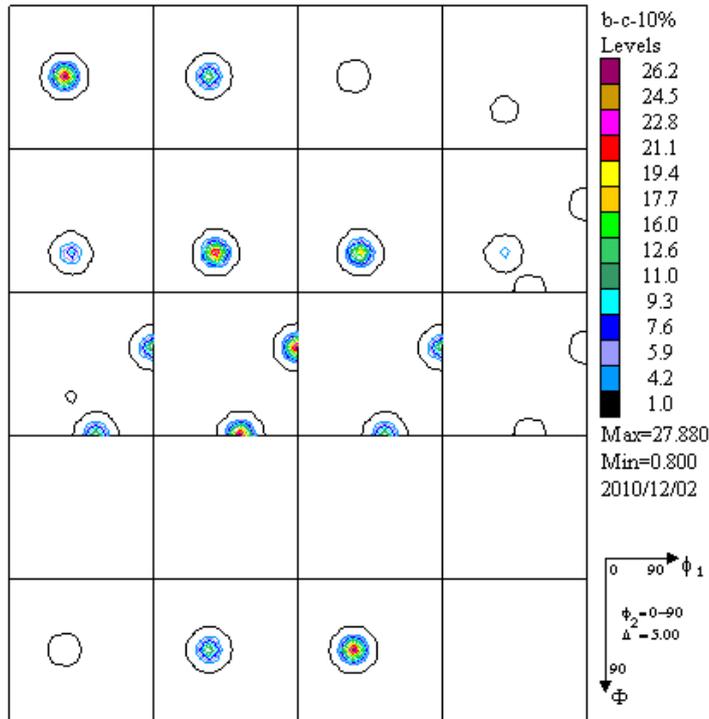
2010年12月02日

He k p e r T e x

方法、

LaboTexで結晶方位を作成、極点図をExportして、PFtoODFでTexToolsの入力制限を行い、TexToolsのODF解析結果のErrorで判断する。

LaboTexの結晶方位は、brass, copper 10%とする。



|                       |        |          |                 |
|-----------------------|--------|----------|-----------------|
| 111-b-c-10%.TPF       | 3 KB   | TPF ファイル | 2010/12/02 8:24 |
| 200-b-c-10%.TPF       | 3 KB   | TPF ファイル | 2010/12/02 8:24 |
| 220-b-c-10%.TPF       | 3 KB   | TPF ファイル | 2010/12/02 8:25 |
| b-c-10%ODF-Export.TXT | 275 KB | テキスト文書   | 2010/12/02 8:24 |

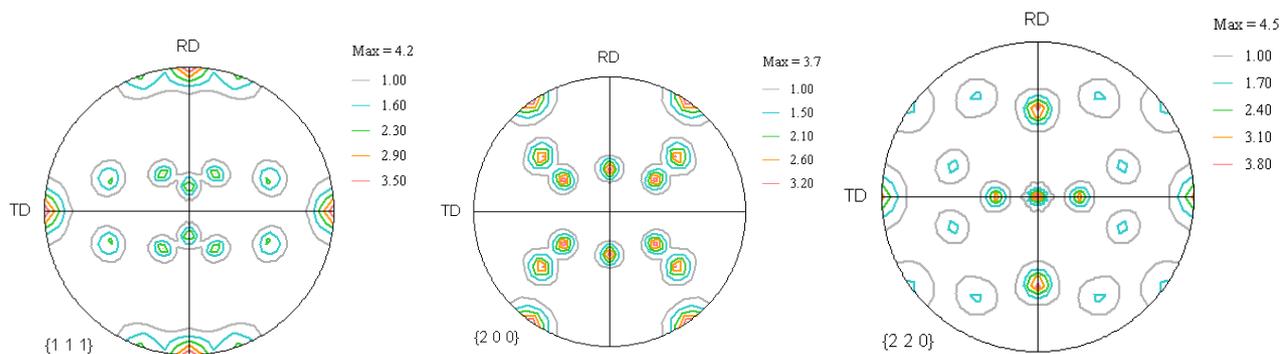
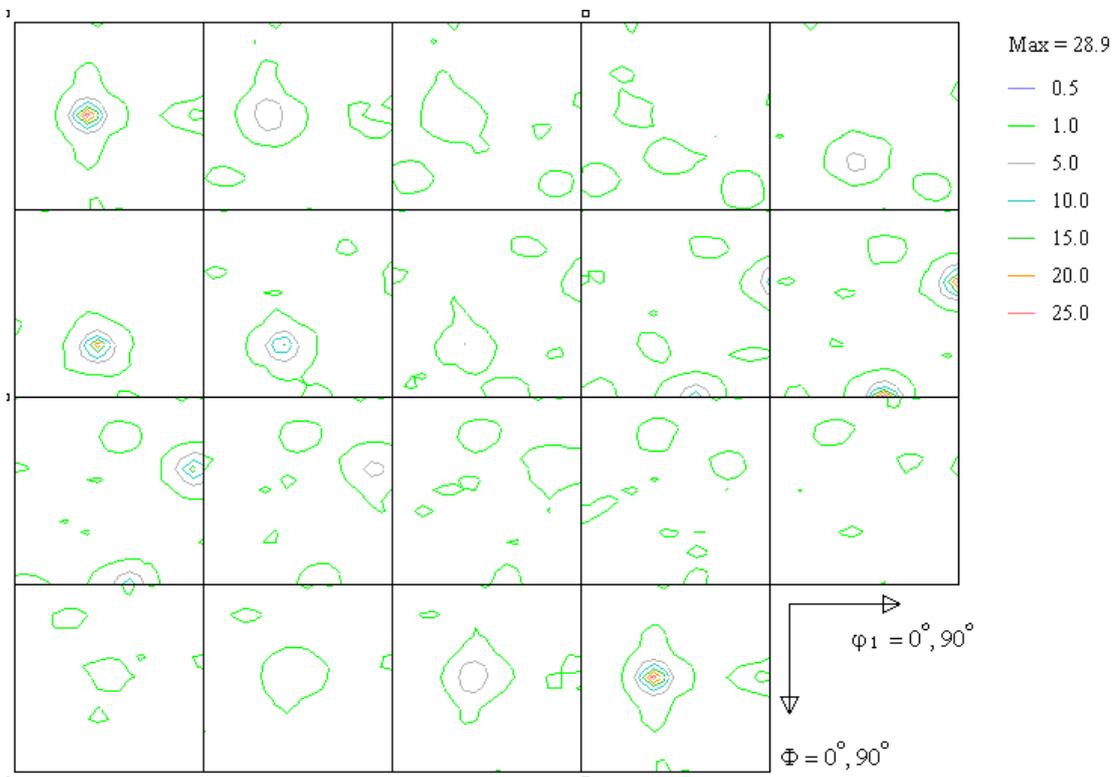
PFtoODF 3に入力するために、TXT2フォーマットに変換

|                    |       |          |                 |
|--------------------|-------|----------|-----------------|
| 111-b-c-10%.TPF    | 3 KB  | TPF ファイル | 2010/12/02 8:24 |
| 200-b-c-10%.TPF    | 3 KB  | TPF ファイル | 2010/12/02 8:24 |
| 220-b-c-10%.TPF    | 3 KB  | TPF ファイル | 2010/12/02 8:25 |
| 200_5.0deg-rp2.TXT | 22 KB | テキスト文書   | 2010/12/02 8:27 |
| 111_5.0deg-rp2.TXT | 23 KB | テキスト文書   | 2010/12/02 8:27 |
| 220_5.0deg-rp2.TXT | 23 KB | テキスト文書   | 2010/12/02 8:28 |

このTXT2フォーマットデータは完全極点図である。

完全極点図をPF to ODF 3に読み込み、極点図の範囲制限しながらTexToolsの処理結果を評価

| PF Data |                    | SelectFile(TXT(b,intens),TXT2(a,b,intens)) | h,k,l | 2Theta | Alfa Area | AlfaS | AlfaE | Select                              |
|---------|--------------------|--|-------|--------|-----------|-------|-------|-------------------------------------|
|         | 111_5.0deg-rp2.TXT |  | 1,1,1 | 00     | 00->90.0  | 00    | 90.0  | <input checked="" type="checkbox"/> |
|         | 200_5.0deg-rp2.TXT |  | 2,0,0 | 00     | 00->90.0  | 00    | 90.0  | <input checked="" type="checkbox"/> |
|         | 220_5.0deg-rp2.TXT |  | 2,2,0 | 00     | 00->90.0  | 00    | 90.0  | <input checked="" type="checkbox"/> |



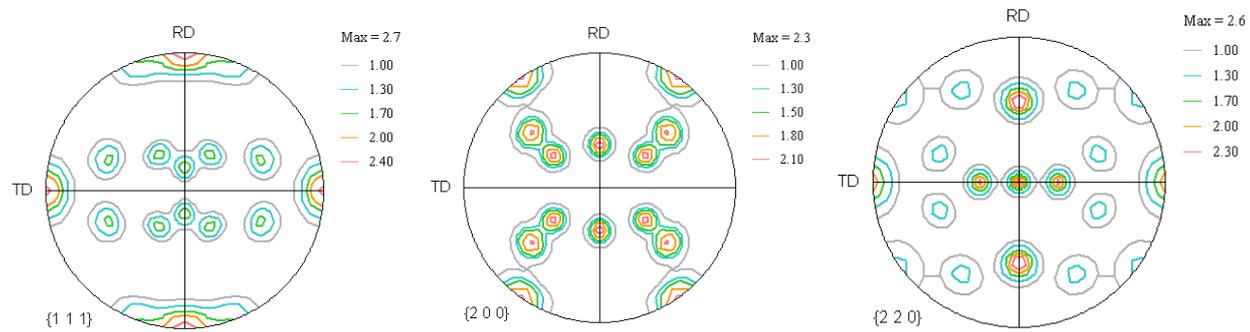
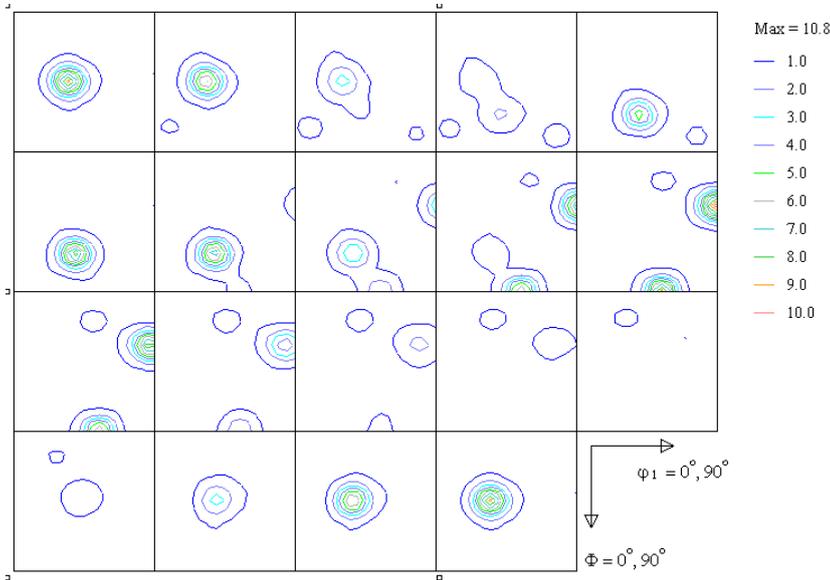
HODFのエラー

$\chi^2$   
 15      15↓  
 0.0100   0.0259↓  
 0.0↓  
 0.6152   0.6034   0.6322   0.7509   0.7943   0.7809   0.8792   0.9914   1.0203   0.9870  
 1.0000   0.0014   0.0700   0.7000   0.7040   0.7500   0.0000   0.0004   0.0150   0.0000  
 15 degree ValueFraction

|               |   |
|---------------|---|
| ODF File Name | M:\TexToolsの入力データ\評価\0-90\0-90.HODF                               |
| Result:       | Cube=1.67%Goss=1.77%Brass=12.88%S=11.57%Copper=13.12%R-Cube=1.87% |

0-85の場合

| PF Data |                   | SelectFile(TXT(b,intens),TXT2(a,b,intens)) | h,k,l | 2Theta | Alfa Area | AlfaS | AlfaE | Select                              |
|---------|-------------------|--|-------|--------|-----------|-------|-------|-------------------------------------|
|         | 111_50deg-rp2.TXT |  | 1,1,1 | 00     | 00->90.0  | 00    | 85    | <input checked="" type="checkbox"/> |
|         | 200_50deg-rp2.TXT |  | 2,0,0 | 00     | 00->90.0  | 00    | 85    | <input checked="" type="checkbox"/> |
|         | 220_50deg-rp2.TXT |  | 2,2,0 | 00     | 00->90.0  | 00    | 85    | <input checked="" type="checkbox"/> |



HODF

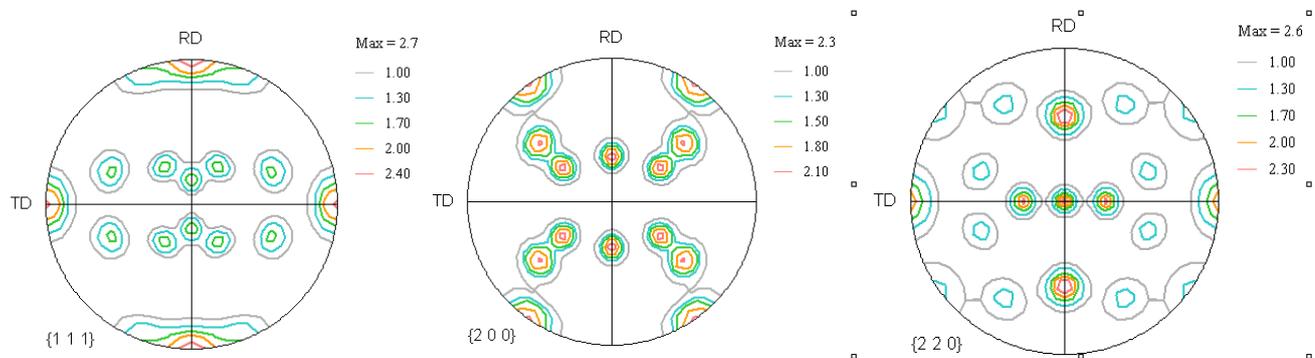
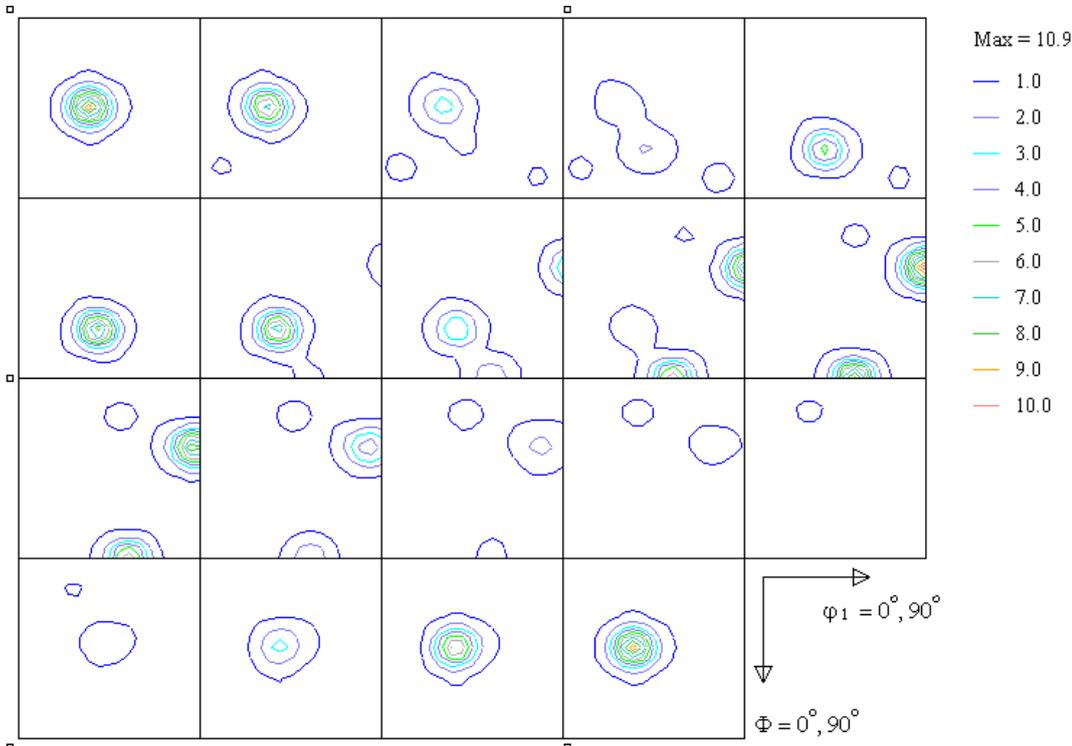
入力極点図と再計算極点図の差の割合

|        |         |        |        |        |        |        |        |        |        |  |
|--------|---------|--------|--------|--------|--------|--------|--------|--------|--------|--|
| 15     | 15↓     |        |        |        |        |        |        |        |        |  |
| 0.0100 | 0.0270↓ |        |        |        |        |        |        |        |        |  |
| 0.0↓   |         |        |        |        |        |        |        |        |        |  |
| 0.6537 | 0.6764  | 0.7355 | 0.8094 | 0.8455 | 0.8240 | 0.7893 | 0.7835 | 0.8291 | 0.8991 |  |

15 degree ValueFraction

|               |   |
|---------------|---|
| ODF File Name | M:\TexToolsの入力データ評価#0-85#0-85.HODF                                |
| Result:       | Cube=1.73%Goss=1.77%Brass=11.97%S=12.63%Copper=12.33%R-Cube=1.83% |

| PF Data                                     |                    | h,k,l | 2Theta | Alfa Area | AlfaS | AlfaE | Select                              |
|---|--------------------|-------|--------|-----------|-------|-------|-------------------------------------|
| SelectFile(TXT(b,intens),TXT2(a,b,intens.)) | 111_5.0deg-rp2.TXT | 1,1,1 | 0.0    | 0.0->90.0 | 0.0   | 80    | <input checked="" type="checkbox"/> |
|   | 200_5.0deg-rp2.TXT | 2,0,0 | 0.0    | 0.0->90.0 | 0.0   | 80    | <input checked="" type="checkbox"/> |
|   | 220_5.0deg-rp2.TXT | 2,2,0 | 0.0    | 0.0->90.0 | 0.0   | 80    | <input checked="" type="checkbox"/> |



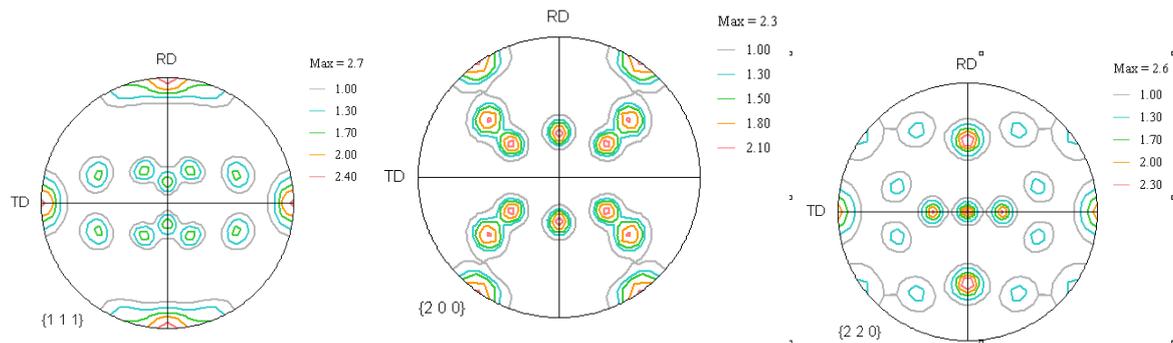
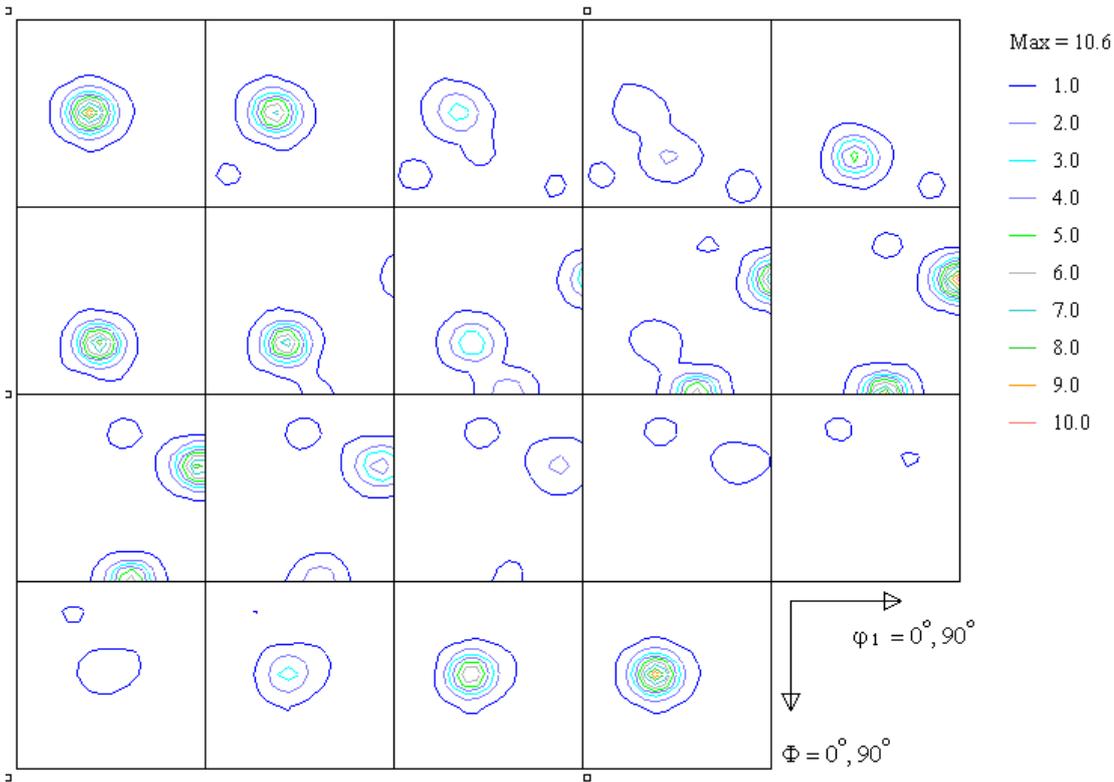
HODF

15 15↓  
 0.0100 0.0319↓  
 0.0↓  
 0.6400 0.6646 0.7332 0.8236 0.8822 0.8804 0.8471 0.8243 0.8292 0.8473  
 0.0555 0.0540 0.0407 0.0255 0.0040 0.7510 0.7000 0.0010 0.0000

15 degree ValueFraction

|               |   |
|---------------|---|
| ODF File Name | M:\TexToolsの入力データ評価#0-80#0-80.HODF                                |
| Result:       | Cube=1.75%Goss=1.78%Brass=12.01%S=12.58%Copper=12.30%R-Cube=1.79% |

| PF Data                                    |                    | h,k,l | 2Theta | Alfa Area | AlfaS | AlfaE | Select                              |
|--|--------------------|-------|--------|-----------|-------|-------|-------------------------------------|
| SelectFile(TXT(b,intens),TXT2(a,b,intens)) |                    |       |        |           |       |       |                                     |
|  | 111_5.0deg-rp2.TXT | 1,1,1 | 0.0    | 0.0->90.0 | 0.0   | 75    | <input checked="" type="checkbox"/> |
|  | 200_5.0deg-rp2.TXT | 2,0,0 | 0.0    | 0.0->90.0 | 0.0   | 75    | <input checked="" type="checkbox"/> |
|  | 220_5.0deg-rp2.TXT | 2,2,0 | 0.0    | 0.0->90.0 | 0.0   | 75    | <input checked="" type="checkbox"/> |



HODF

```

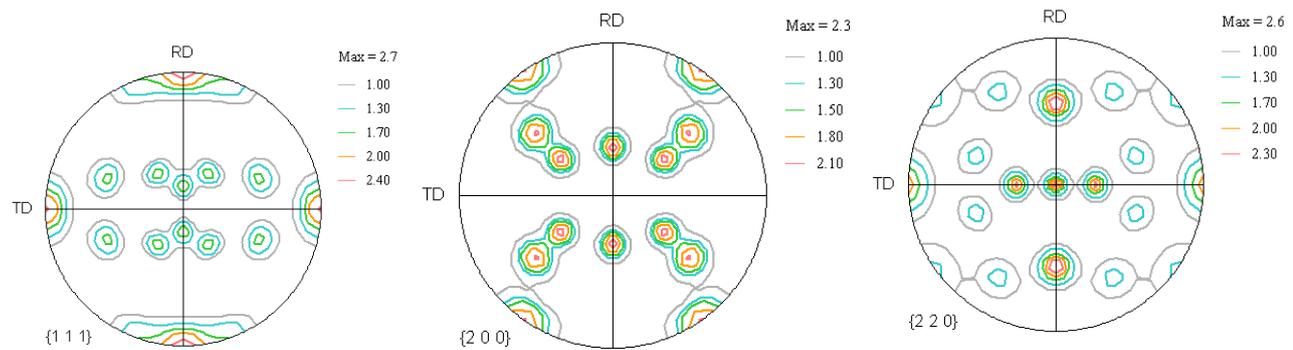
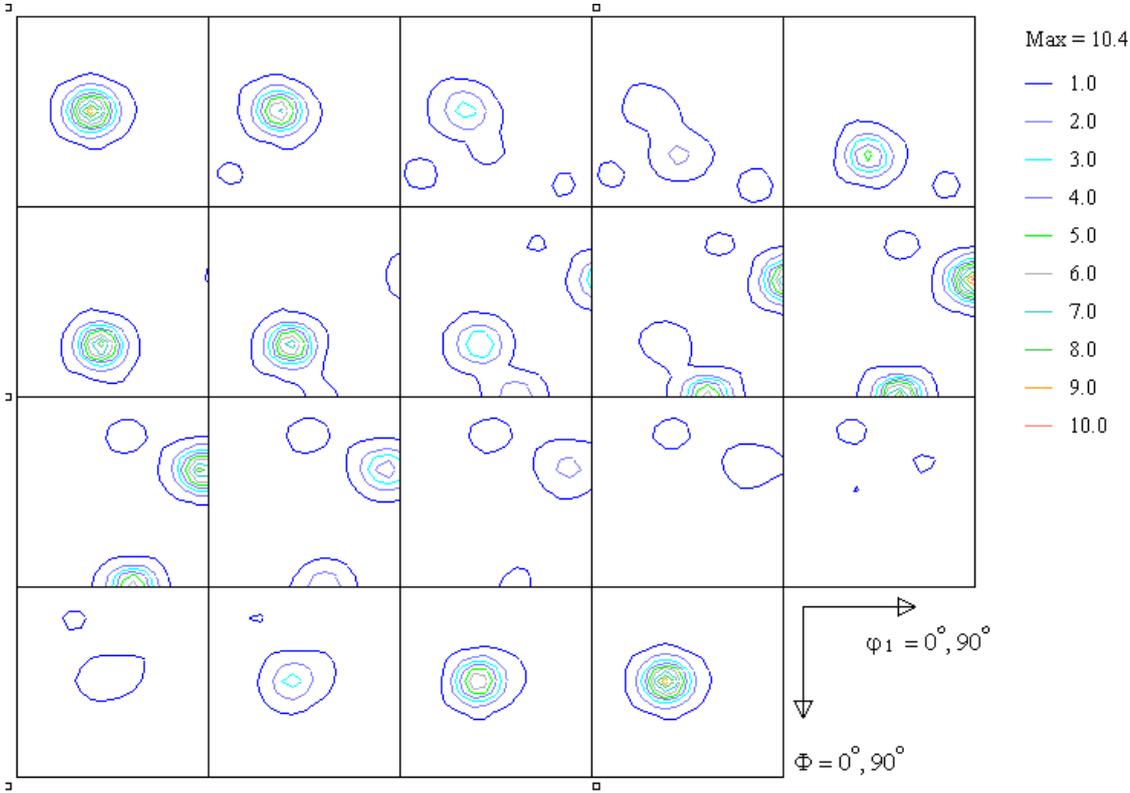
15      15↓
0.0100  0.0357↓
0.0↓
0.6455  0.6696  0.7370  0.8239  0.8775  0.8691  0.8313  0.8084  0.8157  0.8385
    
```

15 degree ValueFraction

ODF File Name: M:\TexToolsの入力データ評価#0-75#0-75.HODF

Result: Cube=1.76%Goss=1.76%Brass=12.01%S=12.58% Copper=12.26%R-Cube=1.78%

| PF Data |                    | SelectFile(TXT(b,intens),TXT2(a,b,intens)) | h,k,l | 2Theta | Alfa Area | AlfaS | AlfaE | Select                              |
|---------|--------------------|--|-------|--------|-----------|-------|-------|-------------------------------------|
|         | 111_5.0deg-rp2.TXT |  | 1,1,1 | 0.0    | 0.0->90.0 | 0.0   | 70    | <input checked="" type="checkbox"/> |
|         | 200_5.0deg-rp2.TXT |  | 2,0,0 | 0.0    | 0.0->90.0 | 0.0   | 70    | <input checked="" type="checkbox"/> |
|         | 220_5.0deg-rp2.TXT |  | 2,2,0 | 0.0    | 0.0->90.0 | 0.0   | 70    | <input checked="" type="checkbox"/> |



HODF

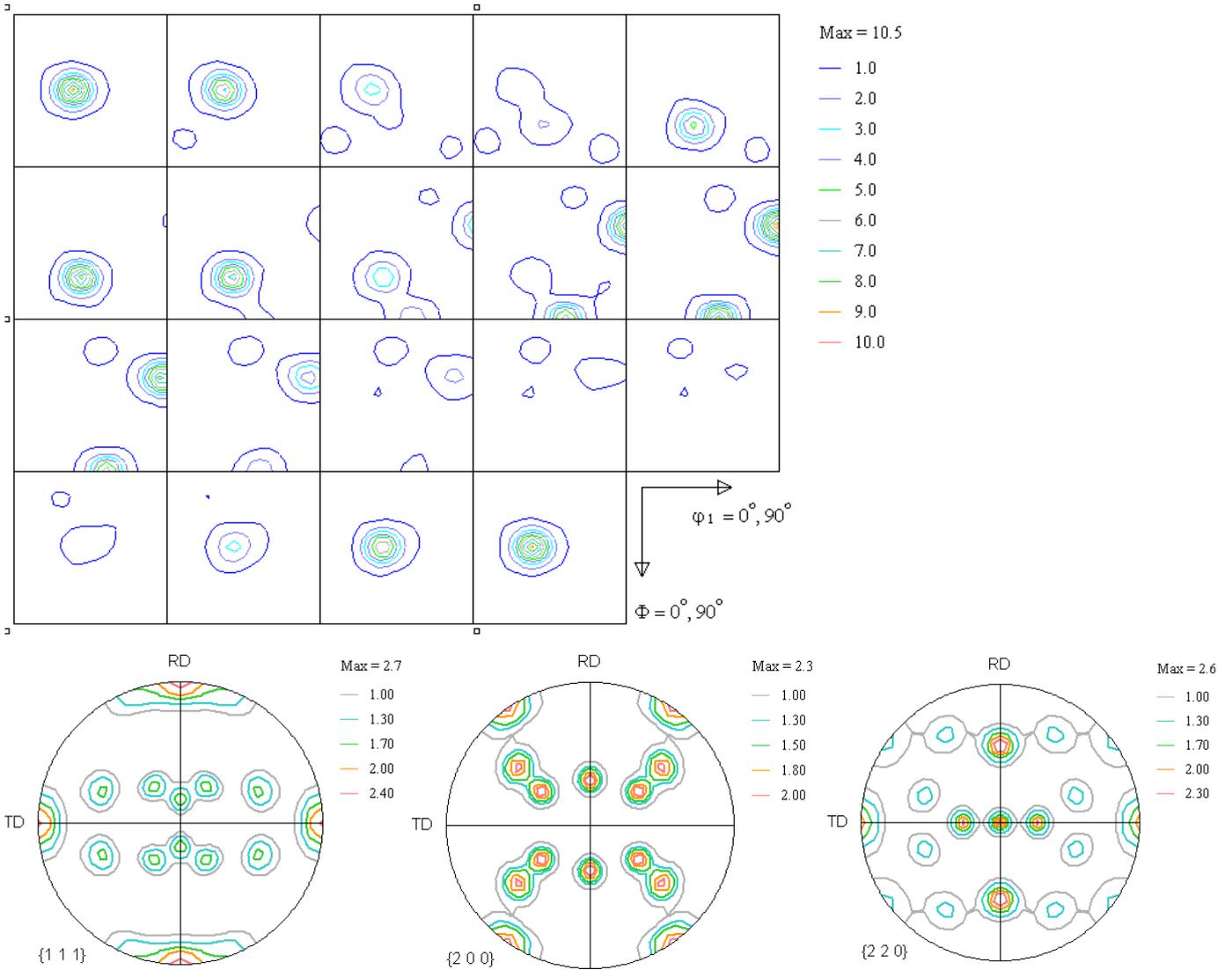
15      15↓  
 0.0100   0.0340↓  
 0.0↓  
 0.6459   0.6696   0.7347   0.8163   0.8651   0.8568   0.8241   0.8077   0.8188   0.8395  
 0.8442   0.8205   0.8221   0.8217   0.7062   0.7512   0.7120   0.7018   0.8001   0.8395

15 degree ValueFraction

ODF File Name    M:\TexToolsの入力データ評価\0-70\0-70.HODF

Result:    Cube=1.77%Goss=1.73%Brass=11.94%S=12.54%Copper=12.30%R-Cube=1.77%

| PF Data |                    | SelectFile(TXT(b,intens),TXT2(a,b,intens)) | h,k,l | 2Theta | Alfa Area | AlfaS | AlfaE | Select                              |
|---------|--------------------|--|-------|--------|-----------|-------|-------|-------------------------------------|
|         | 111_5.0deg-rp2.TXT |  | 1,1,1 | 00     | 0.0->90.0 | 0.0   | 65    | <input checked="" type="checkbox"/> |
|         | 200_5.0deg-rp2.TXT |  | 2,0,0 | 00     | 0.0->90.0 | 0.0   | 65    | <input checked="" type="checkbox"/> |
|         | 220_5.0deg-rp2.TXT |  | 2,2,0 | 00     | 0.0->90.0 | 0.0   | 65    | <input checked="" type="checkbox"/> |



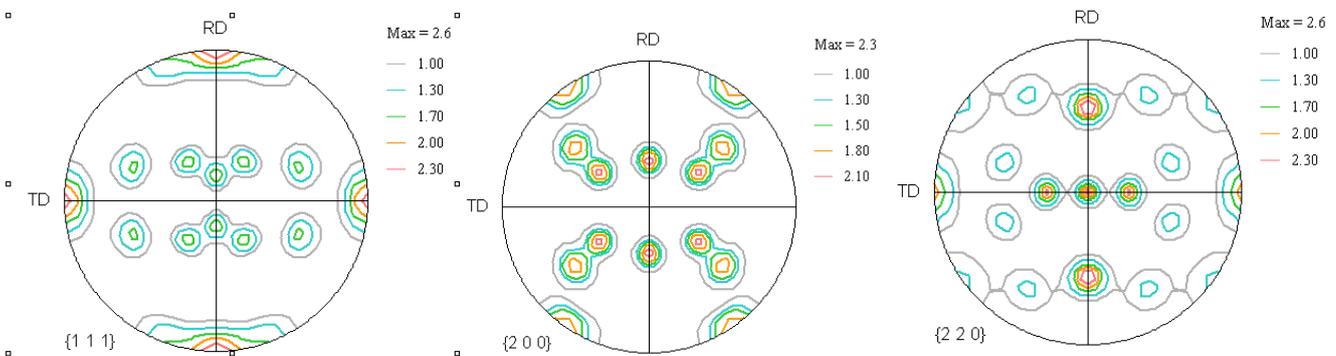
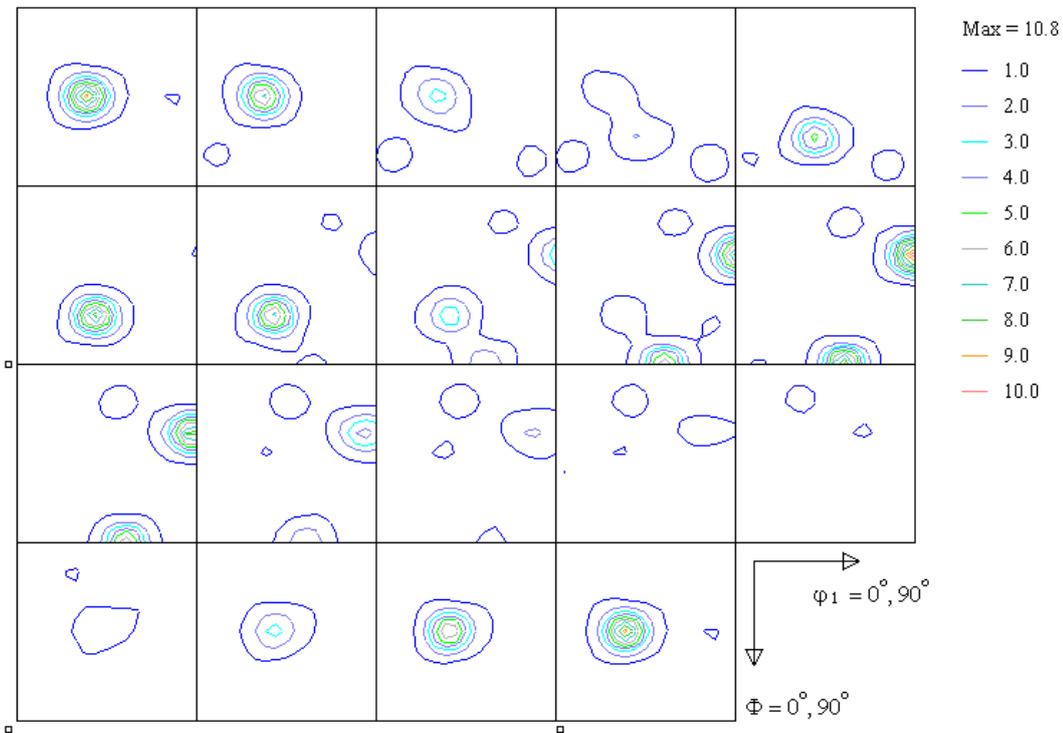
HODF

15 15↓  
 0.0100 0.0304↓  
 0.0↓  
 0.6790 0.6944 0.7420 0.8118 0.8626 0.8619 0.8321 0.8120 0.8180 0.8337  
 0.0040 0.0000 0.0001 0.0040 0.0004 0.7055 0.7070 0.7150 0.7117

15 degree ValueFraction

|               |   |
|---------------|---|
| ODF File Name | M:\TexToolsの入力データ\評価値#0-65#0-65.HODF                              |
| Result:       | Cube=1.78%Goss=1.73%Brass=11.90%S=12.47%Copper=12.19%R-Cube=1.77% |

| PF Data |                   | SelectFile(TXT(b,intens),TXT2(a,b,intens.)) | h,k,l | 2Theta | Alfa Area | AlfaS | AlfaE | Select                              |
|---------|-------------------|---|-------|--------|-----------|-------|-------|-------------------------------------|
|         | 111_50deg-rp2.TXT |   | 1,1,1 | 00     | 0.0->90.0 | 0.0   | 60    | <input checked="" type="checkbox"/> |
|         | 200_50deg-rp2.TXT |   | 2,0,0 | 00     | 0.0->90.0 | 0.0   | 60    | <input checked="" type="checkbox"/> |
|         | 220_50deg-rp2.TXT |   | 2,2,0 | 00     | 0.0->90.0 | 0.0   | 60    | <input checked="" type="checkbox"/> |



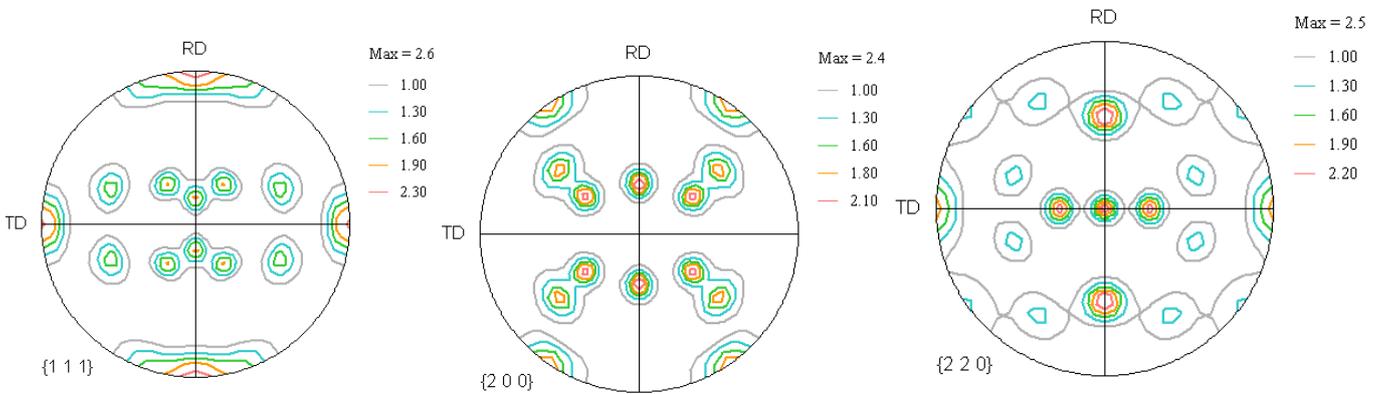
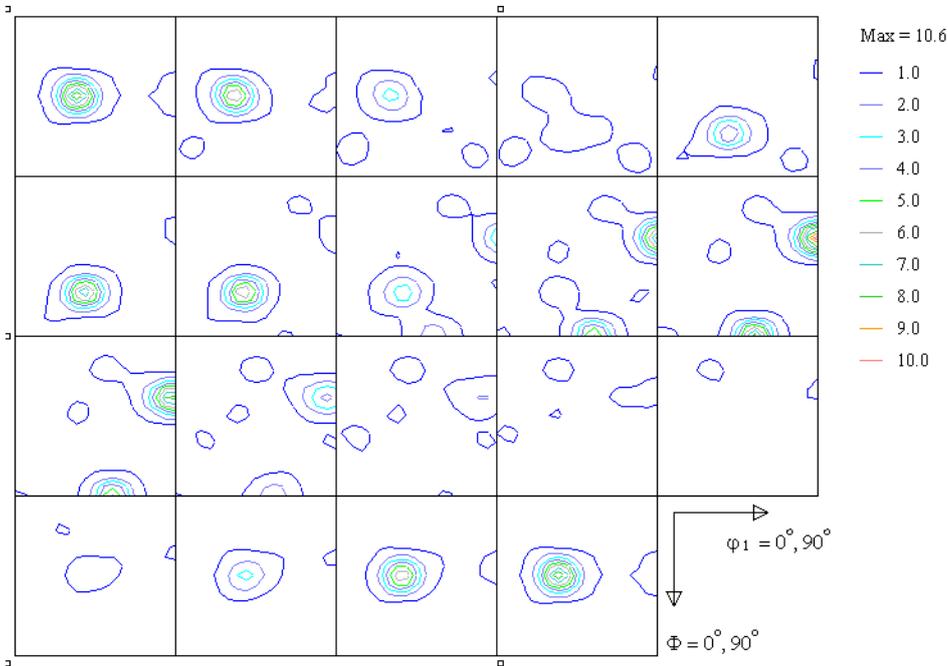
HODF

$\downarrow$   
 15      15↓  
 0.0100   0.0287↓  
 0.0↓  
 0.6762   0.6929   0.7443   0.8193   0.8744   0.8723   0.8348   0.8071   0.8055   0.8187  
 0.0250   0.0200   0.0202   0.0200   0.0100   0.7072   0.7072   0.7172   0.7150  
 15 degree ValueFraction

ODF File Name: M:\TexToolsの入力データ評価#0-60#0-60.HODF

Result: Cube=1.80%Goss=1.73%Brass=11.91%S=12.39% Copper=12.02% R-Cube=1.74%

| SelectFile(TXT(b,intens),TXT2(a,b,intens)) |                   | h,k,l | 2Theta | Alfa Area | AlfaS | AlfaE | Select                              |
|--|-------------------|-------|--------|-----------|-------|-------|-------------------------------------|
|  | 111_50deg-rp2.TXT | 1,1,1 | 00     | 0.0->90.0 | 0.0   | 55    | <input checked="" type="checkbox"/> |
|  | 200_50deg-rp2.TXT | 2,0,0 | 00     | 0.0->90.0 | 0.0   | 55    | <input checked="" type="checkbox"/> |
|  | 220_50deg-rp2.TXT | 2,2,0 | 00     | 0.0->90.0 | 0.0   | 55    | <input checked="" type="checkbox"/> |



HODF

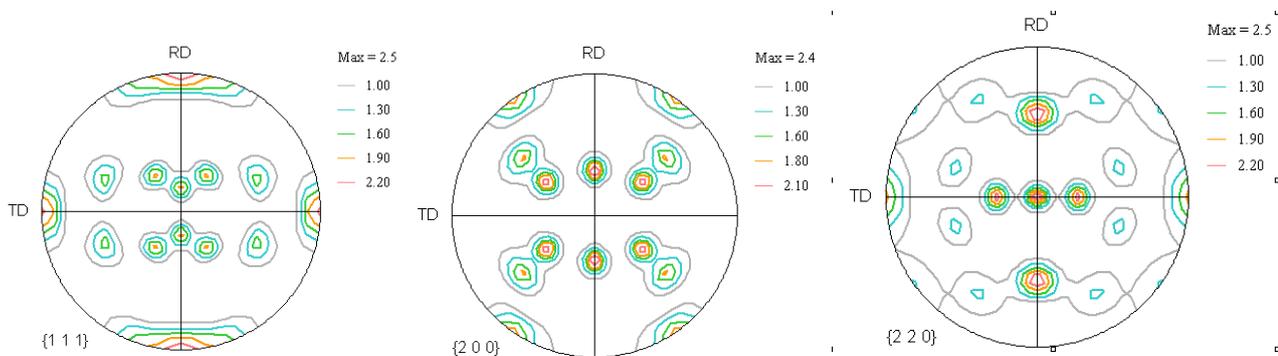
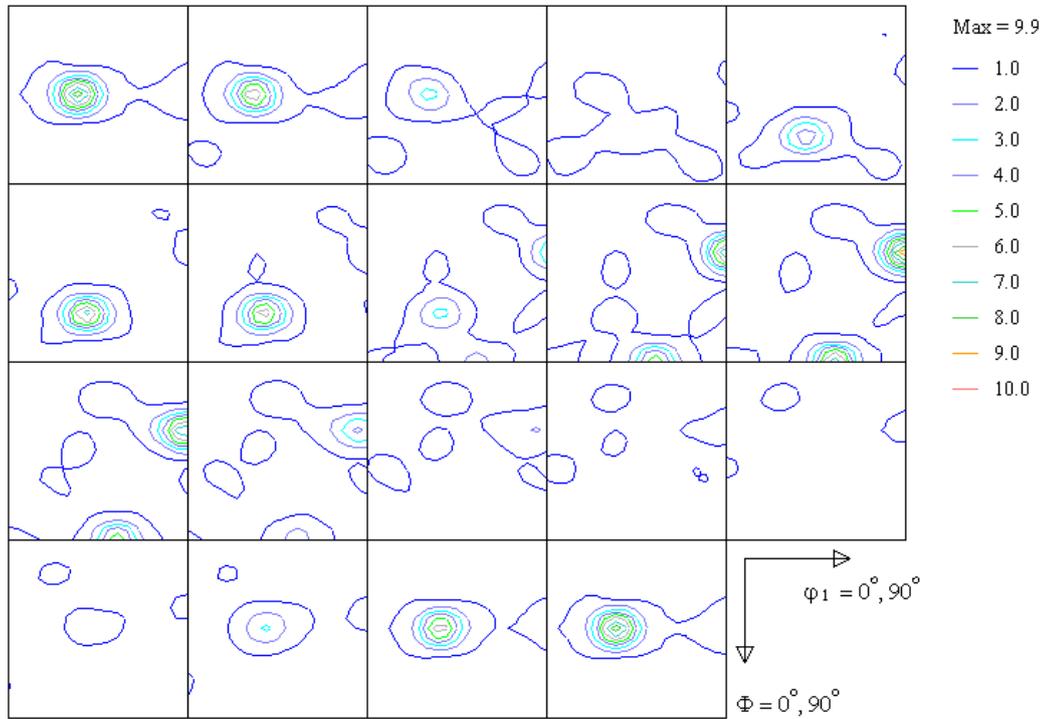
```

15      15↓
0.0100  0.0297↓
0.0↓
0.7171  0.7280  0.7700  0.8387  0.8874  0.8772  0.8355  0.8086  0.8063  0.8100
    
```

15 degree ValueFraction

|               |   |
|---------------|---|
| ODF File Name | M:\TexToolsの入力データ\評価\0-55\0-55.HODF                               |
| Result:       | Cube=1.86%Goss=1.81%Brass=11.56%S=12.41%Copper=11.80%R-Cube=1.71% |

| PF Data |                    | SelectFile(TXT(b,intens),TXT2(a,b,intens.)) | h,k,l | 2Theta | Alfa Area | AlfaS | AlfaE | Select                              |
|---------|--------------------|---|-------|--------|-----------|-------|-------|-------------------------------------|
|         | 111_5.0deg-rp2.TXT |   | 1,1,1 | 0.0    | 0.0->90.0 | 0.0   | 50    | <input checked="" type="checkbox"/> |
|         | 200_5.0deg-rp2.TXT |   | 2,0,0 | 0.0    | 0.0->90.0 | 0.0   | 50    | <input checked="" type="checkbox"/> |
|         | 220_5.0deg-rp2.TXT |   | 2,2,0 | 0.0    | 0.0->90.0 | 0.0   | 50    | <input checked="" type="checkbox"/> |



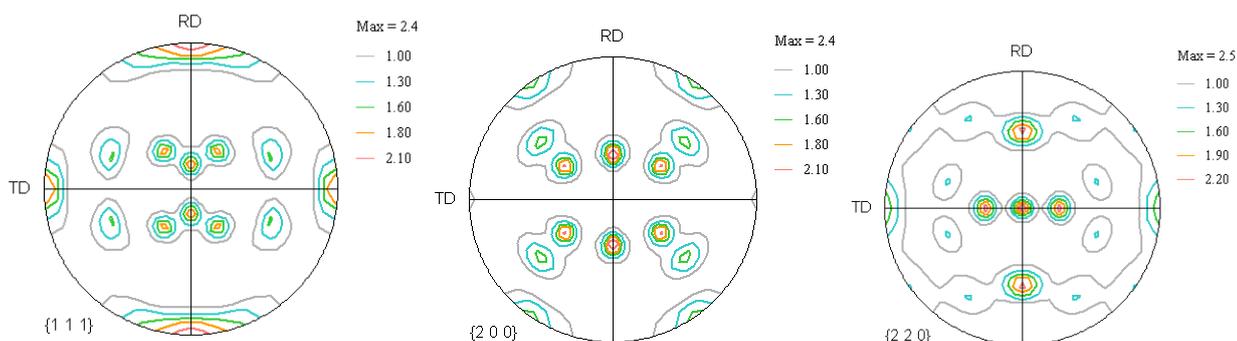
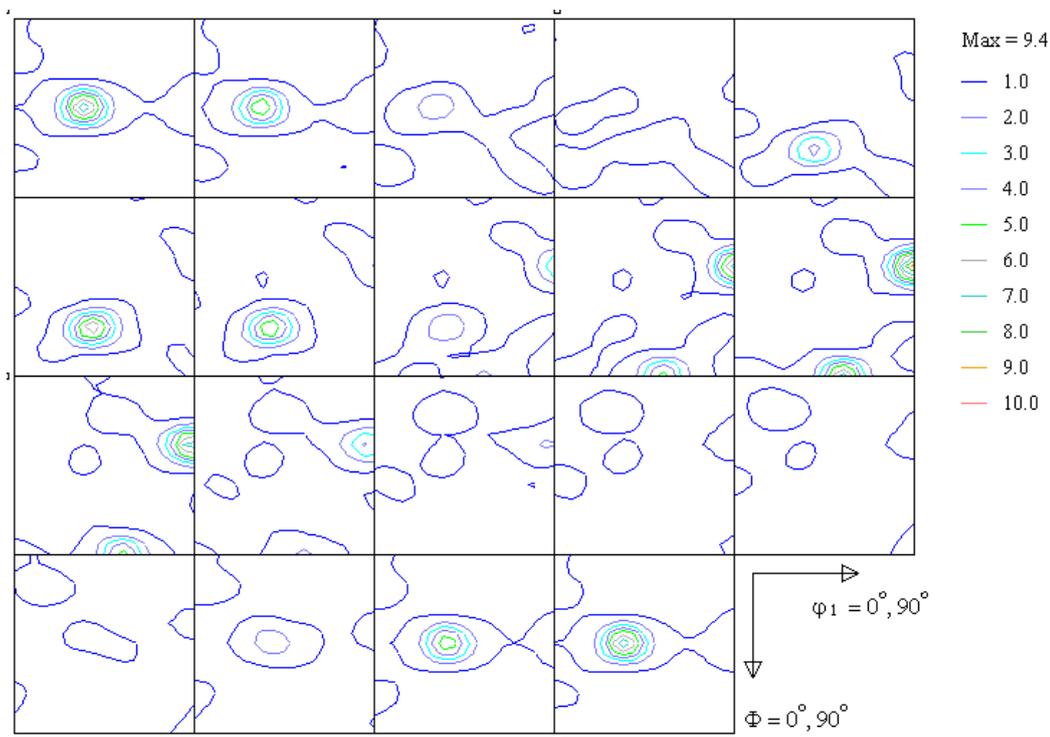
HODF

15      15↓  
 0.0100   0.0509↓  
 0.0↓  
 0.8947   0.8762   0.8442   0.8297   0.8247   0.8025   0.7637   0.7376   0.7450   0.7760  
 0.7801   0.7800   0.7750   0.7500   0.7000   0.7011   0.6140   0.6505   0.6701   0.7000  
 15 degree ValueFraction

ODF File Name    M:\TexToolsの入力データ評価\0-50\0-50.HODF

Result:            Cube=1.97%Goss=1.91%Brass=11.27%S=12.26%Copper=11.35%R-Cube=1.63%

| PF Data                                     |                   | h,k,l | 2Theta | Alfa Area | AlfaS | AlfaE | Select                              |
|---|-------------------|-------|--------|-----------|-------|-------|-------------------------------------|
| SelectFile(TXT(b,intens),TXT2(a,b,intens.)) |                   |       |        |           |       |       |                                     |
|   | 111_50deg-rp2.TXT | 1,1,1 | 00     | 00->900   | 0.0   | 45    | <input checked="" type="checkbox"/> |
|   | 200_50deg-rp2.TXT | 2,0,0 | 00     | 00->900   | 0.0   | 45    | <input checked="" type="checkbox"/> |
|   | 220_50deg-rp2.TXT | 2,2,0 | 00     | 00->900   | 0.0   | 45    | <input checked="" type="checkbox"/> |



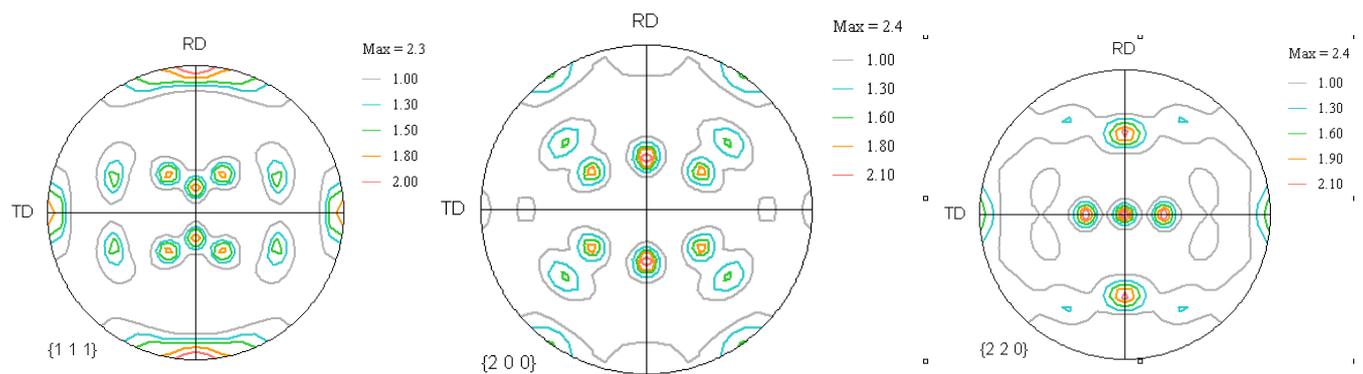
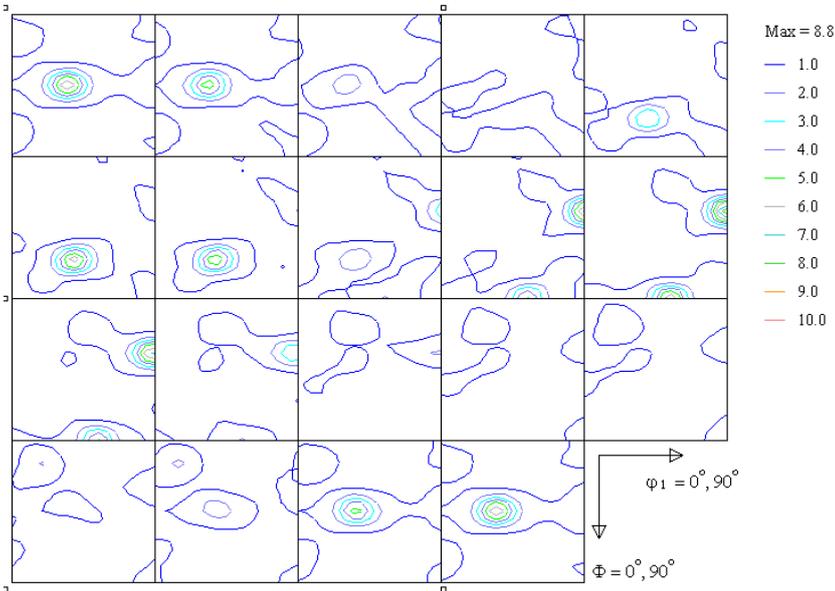
HODF

15      15↓  
 0.0100   0.0435↓  
 0.0↓  
 1.2081   1.1176   0.9293   0.7702   0.6970   0.6827   0.7148   0.7884   0.8755   0.9228

15 degree ValueFraction

|               |   |
|---------------|---|
| ODF File Name | M:\TexToolsの入力データ評価\0-45\0-45.HODF                                |
| Result:       | Cube=2.14%Goss=2.05%Brass=10.38%S=11.77%Copper=10.71%R-Cube=1.57% |

| PF Data |                    | SelectFile(TXT(b,intens),TXT2(a,b,intens)) | h,k,l | 2Theta   | Alfa Area | AlfaS | AlfaE                               | Select |
|---------|--------------------|--|-------|----------|-----------|-------|-------------------------------------|--------|
|         | 111_5.0deg-rp2.TXT | 1,1,1                                      | 0.0   | 0.0-90.0 | 0.0       | 40    | <input checked="" type="checkbox"/> |        |
|         | 200_5.0deg-rp2.TXT | 2,0,0                                      | 0.0   | 0.0-90.0 | 0.0       | 40    | <input checked="" type="checkbox"/> |        |
|         | 220_5.0deg-rp2.TXT | 2,2,0                                      | 0.0   | 0.0-90.0 | 0.0       | 40    | <input checked="" type="checkbox"/> |        |

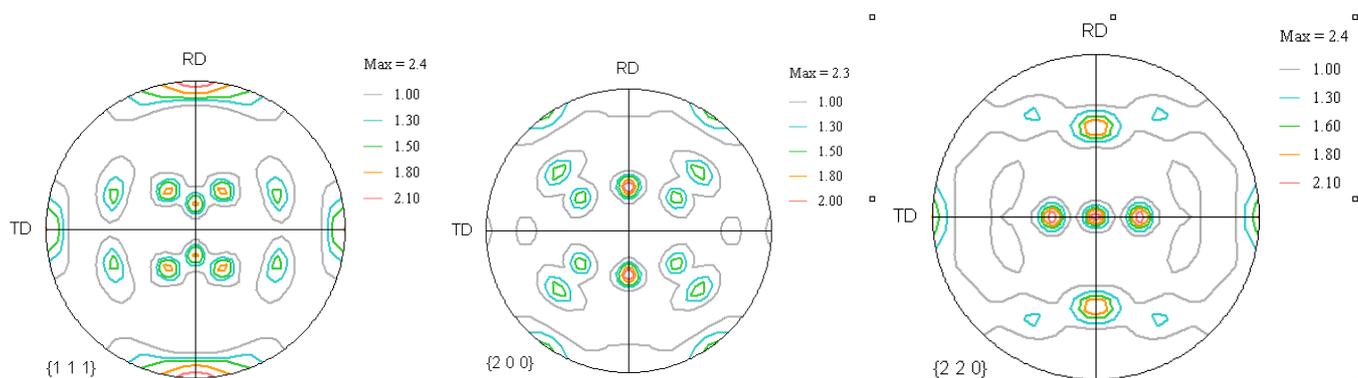
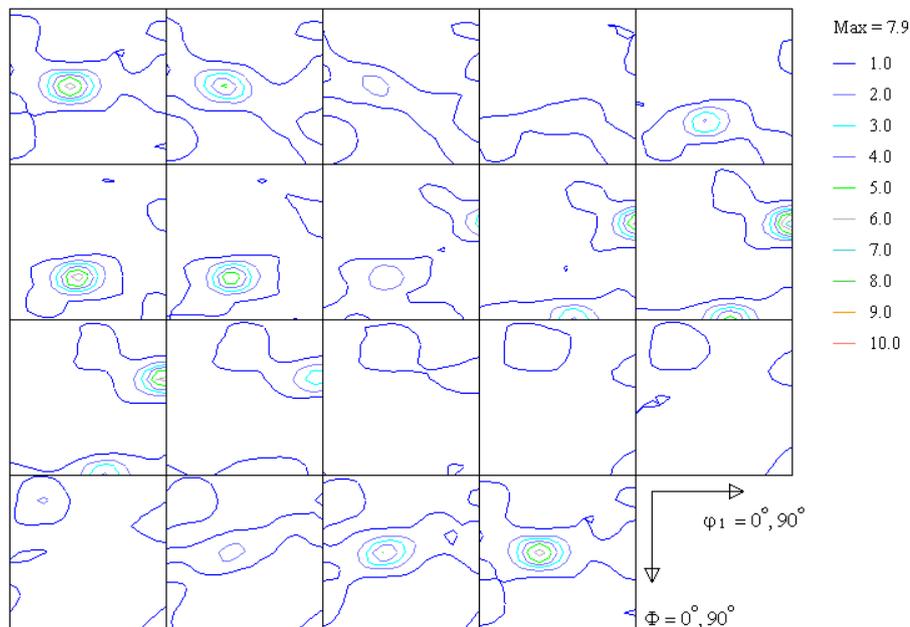


HODF

15      15↓  
 0.0100   0.0386↓  
 0.0↓  
 0.9072   0.8859   0.8361   0.8030   0.7863   0.7750   0.7642   0.7906   0.8672   0.9599  
 0.0000   0.0004   0.0070   0.0307   0.0000   0.0010   0.0547   1.1041   1.1077   .

|               |   |
|---------------|---|
| ODF File Name | M:\TexToolsの入力データ評価\0-40\0-40.HODF                                |
| Result:       | Cube=2.44%Goss=2.13%Brass=10.03%S=11.55%Copper=10.31%R-Cube=1.64% |

| PF Data |                    | SelectFile(TXT(b,intens),TXT2(a,b,intens.)) | h,k,l | 2Theta | Alfa Area | AlfaS | AlfaE | Select                              |
|---------|--------------------|---|-------|--------|-----------|-------|-------|-------------------------------------|
|         | 111_5.0deg-rp2.TXT |   | 1,1,1 | 0.0    | 0.0->90.0 | 0.0   | 35    | <input checked="" type="checkbox"/> |
|         | 200_5.0deg-rp2.TXT |   | 2,0,0 | 0.0    | 0.0->90.0 | 0.0   | 35    | <input checked="" type="checkbox"/> |
|         | 220_5.0deg-rp2.TXT |   | 2,2,0 | 0.0    | 0.0->90.0 | 0.0   | 35    | <input checked="" type="checkbox"/> |



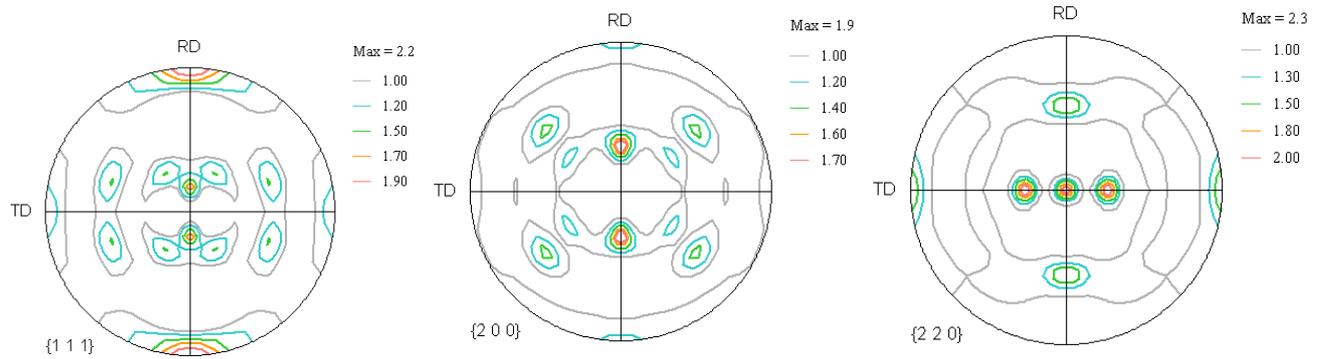
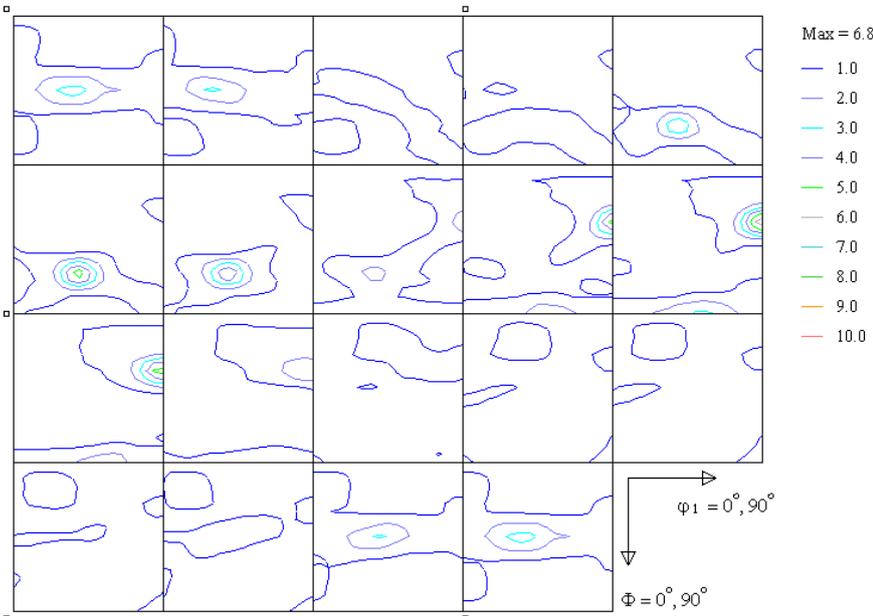
HODF

|        |         |        |        |        |        |        |        |        |        |
|--------|---------|--------|--------|--------|--------|--------|--------|--------|--------|
| 15     | 15↓     |        |        |        |        |        |        |        |        |
| 0.0100 | 0.0467↓ |        |        |        |        |        |        |        |        |
| 0.0↓   |         |        |        |        |        |        |        |        |        |
| 0.8731 | 0.8802  | 0.8938 | 0.9040 | 0.9039 | 0.8952 | 0.8869 | 0.8838 | 0.8886 | 0.8965 |

ODF File Name

Result:

| PF Data |                   | SelectFile(TXT(b,intens),TXT2(a,b,intens.)) | h,k,l | 2Theta    | Alfa Area | AlfaS | AlfaE                               | Select |
|---------|-------------------|---|-------|-----------|-----------|-------|-------------------------------------|--------|
|         | 111_50deg-rp2.TXT | 1,1,1                                       | 0.0   | 0.0->90.0 | 0.0       | 30    | <input checked="" type="checkbox"/> |        |
|         | 200_50deg-rp2.TXT | 2,0,0                                       | 0.0   | 0.0->90.0 | 0.0       | 30    | <input checked="" type="checkbox"/> |        |
|         | 220_50deg-rp2.TXT | 2,2,0                                       | 0.0   | 0.0->90.0 | 0.0       | 30    | <input checked="" type="checkbox"/> |        |



HODF

```

15      15↓
0.0100  0.0263↓
0.0↓
0.9307  0.9290  0.9253  0.9217  0.9200  0.9208  0.9226  0.9249  0.9281  0.9325
0.8888  0.8188  0.8187  0.8174  0.8158  0.8187  0.8188  0.8228  0.8277  .
    
```

ODF File Name

Result: