LaboTex

Version 3.0

The Texture Analysis Software for Windows
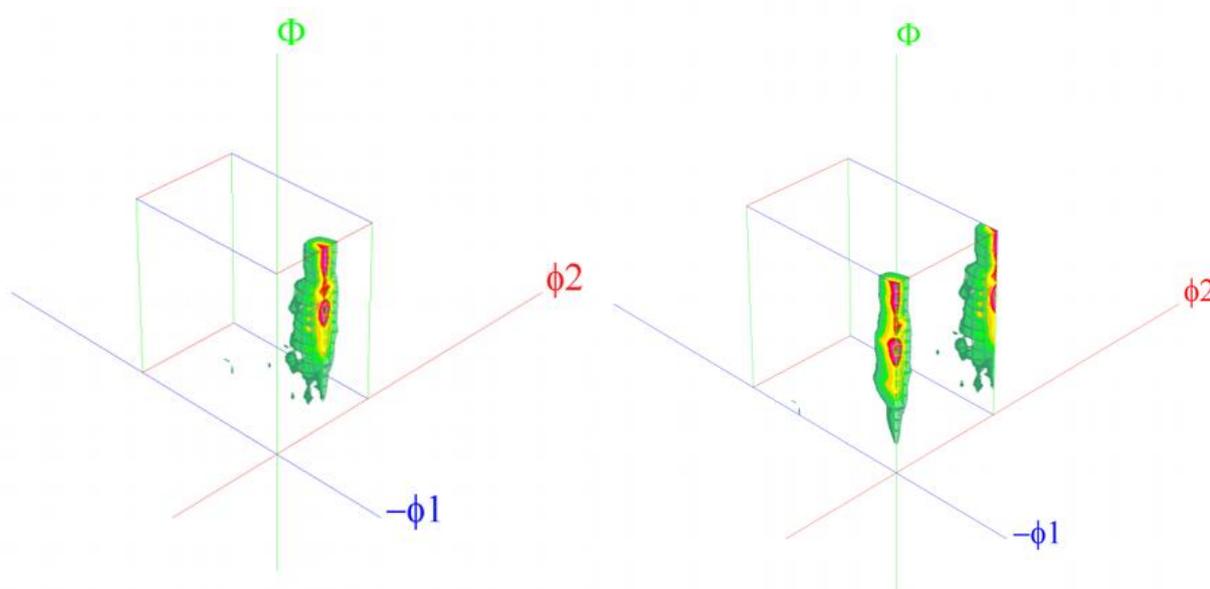
Piotr Ozga

Hexagonal Axes: Conventions & Conversions

Rel. 1.5

Contents

1. Hexagonal Notations

In Hexagonal System are used two notations:

1.1. Miller Notation (3 Axis Notation)
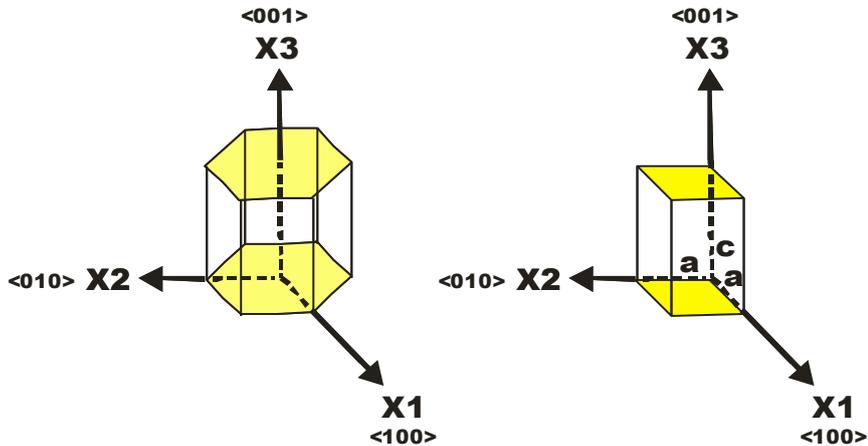
Plane in Miller Notation: {hkl}

Direction in Miller Notation <uvw>

If the direction <uvw> lies in the plane {hkl}, then:

$$hu + kv + lw = 0 \quad \text{(Weiss Zone Law – true in all crystal systems)}$$

In hexagonal system <uvw> direction in Miller Notation is not perpendicular to {uvw}plane as in cubic system.

For example: the {100} plane is perpendicular to direction <210> (not <100> as in cubic system).

1.2. Miller-Bravais Notation (4 Axis Notation)
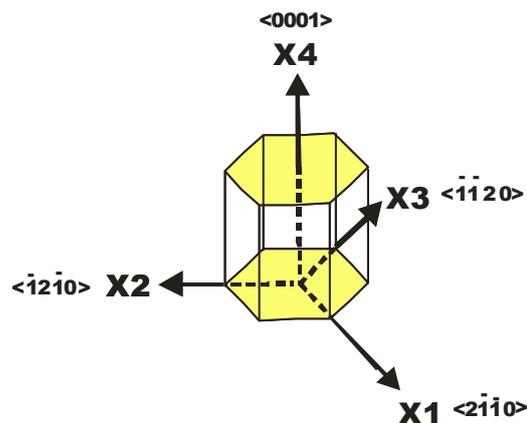
Plane in Miller-Bravais Notation: {HKTL}

Direction in Miller-Bravais Notation <UVTW>

T=-(H+K) (redundant information)

<UVTW> direction in Miller-Bravais Notation is perpendicular to {UVTW} plane (similar as in Miller Notation in cubic system).

2. Relations between Hexagonal Notations

Between Miller-Bravais indices and Miller indices are simple relations:

2.1. Calculation of Miller indices from Miller-Bravais indices

Direction <UVTW> to <uvw>:

u=U-T

v=V-T

w=W

for example: <2-1-10> is equal <100>;

Plane {UVTW} to {uvw}:

u=U

v=V

w=W

for example: {2-1-10}is equal {2-10};
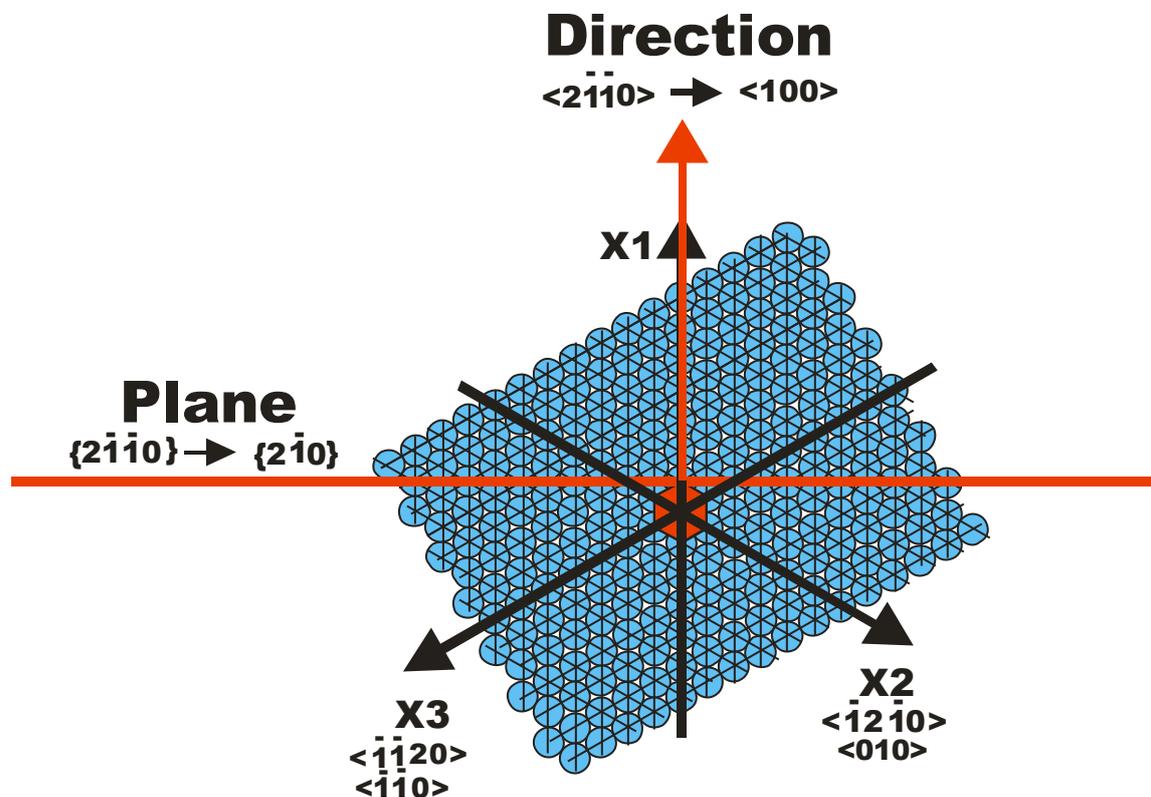
2.2. Calculation of Miller-Bravais indices from Miller indices

Direction <uvw> to <UVTW>

U=(2u-v)/3
V=(2v-u)/3
T=-(u+v)/3
W=w
for example:
<100> is equal <2-1-10>.
<210> is equal <10-10>

Plane {uvw} to {UVTW} :
U=u
V=v
T=-(u+v)
w=W
for example:
{2-10} is equal {2-1-10};
{10-10} ise equal {100}.
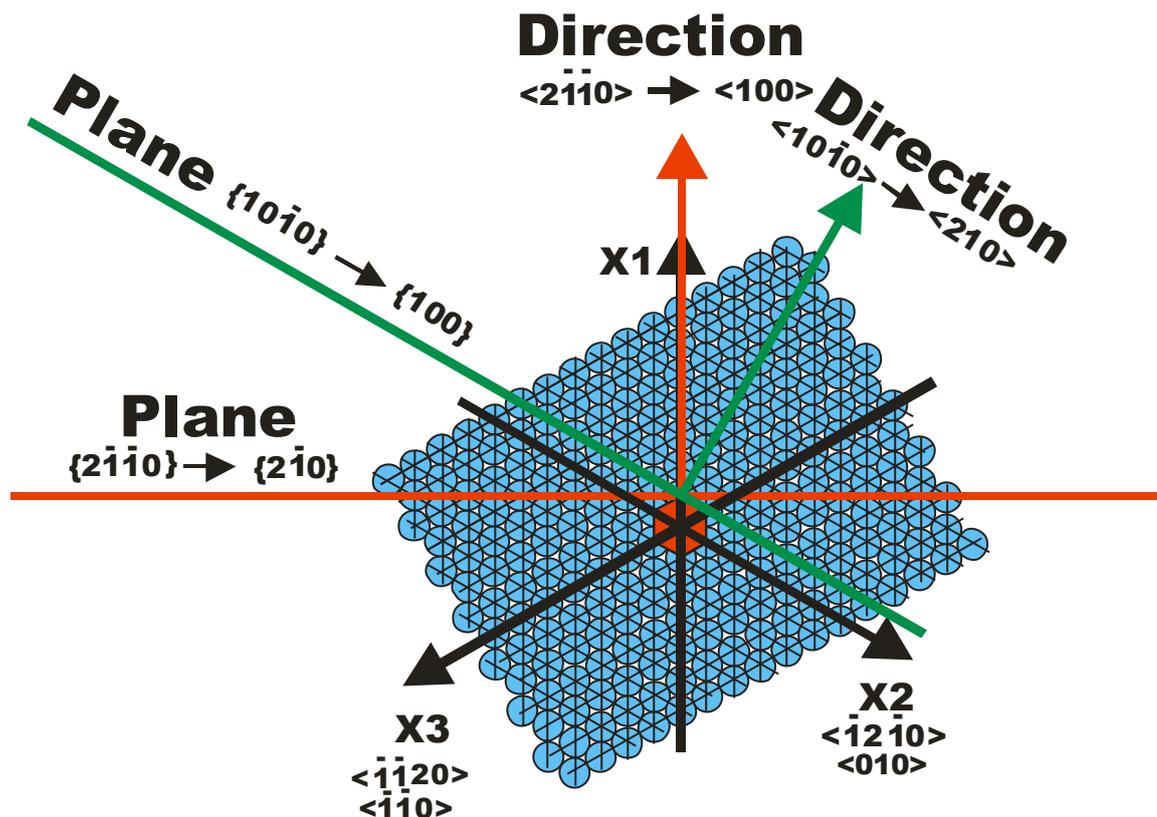

Example:
Conversion of orientation in Miller-Bravais indices {HKTL}<UVTW> to Miller indices {hkl}<uvw>:
Orientation {01-11}<2-1-10> ==> {011}<100>

3. Hexagonal Axes Conventions for Euler Angles

 User can use two hexagonal axes conventions for Euler Angles in LaboTex. The first convention is compatible with general LaboTex axes convention. The second convention is often used and it is not-compatible with general Labotex convention.

3.1. General Labotex Convention
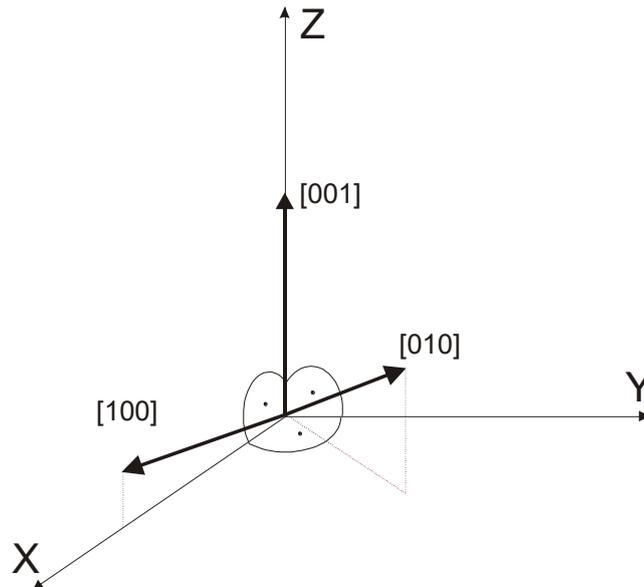
Crystal and sample coordinate systems. General LaboTex Axes and Angles Convention
(example for righ- handed coordinate systems)

LaboTex uses following general convention of the axes for fixing the crystal and sample coordinate system (see for figure above) :

1. X,Y,Z axis are perpendicular to each other,
2. [100] axis is in XZ plane,
3. Z axis is paralel to the [001] crystallographic axis,
4. Crystal coordinate system and sample coordinate system should be at the same order i.e. both right-handed or both left-handed,
5. Bunge definition of Euler angles.

where X,Y,Z - axes of the sample coordinate system,
        [100], [010],[001] - crystallographic axes.
LaboTex user can adjust convention in dialog "**LaboTex Options**".

3.2. First Hexagonal Convention

Sample and crystal systems position for Euler angle (0,0,0) in convention compatible with general LaboTex axes and angle convention are shown on the figures below:

Sample coordinate system

Crystal coordinate system

Normal Direction
001
Z

Rolling Direction
(Longitudinal Direction)
<100>
X

Transversal Direction
Y

<010>

SAMPLE

Sample Axis Definition
Euler Angles (0,0,0)

<001>
<0001>
X4/Z

X3
$<\bar{1}\bar{1}20>$
$<\bar{1}\bar{1}0>$

<010>
$<\bar{1}2\bar{1}0>$
X2

Y
$<0\bar{1}10>$
$<\bar{1}20>$

X
X1
$<2\bar{1}\bar{1}0>$
<100>

X

<100>

Y
$<\bar{1}\bar{2}0>$

<010>

$<2\bar{1}\bar{1}0>$
<100>
X

X1

$\{2\bar{1}\bar{1}0\}$

Y
$<0\bar{1}10>$
$<\bar{1}\bar{2}0>$

X2
$<\bar{1}2\bar{1}0>$
<010>

X3
$<\bar{1}\bar{1}20>$
$<\bar{1}\bar{1}0>$

7
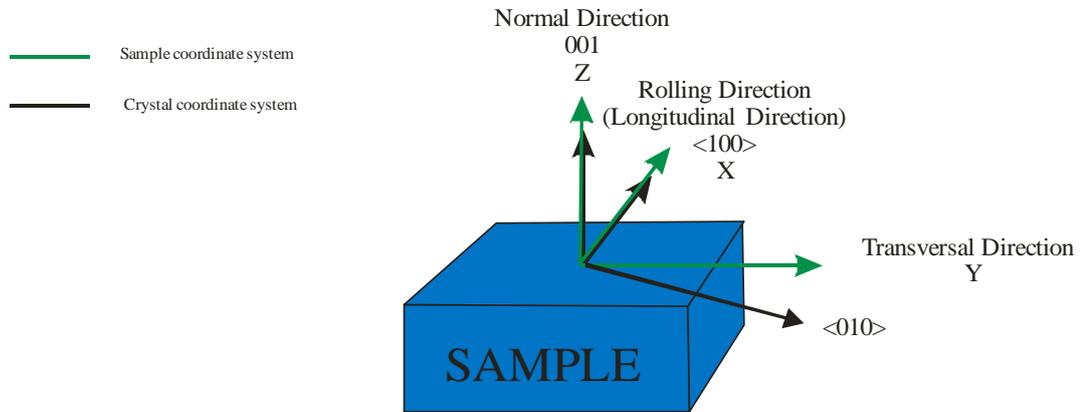
3.3. Second Hexagonal Convention

Sample and crystal systems position for Euler angle (0,0,0) in second hexagonal convention (convention non-compatible with general LaboTex axes and angle convention) are shown on the figures below:

Sample Axis Definition
Euler Angles (0,0,0)
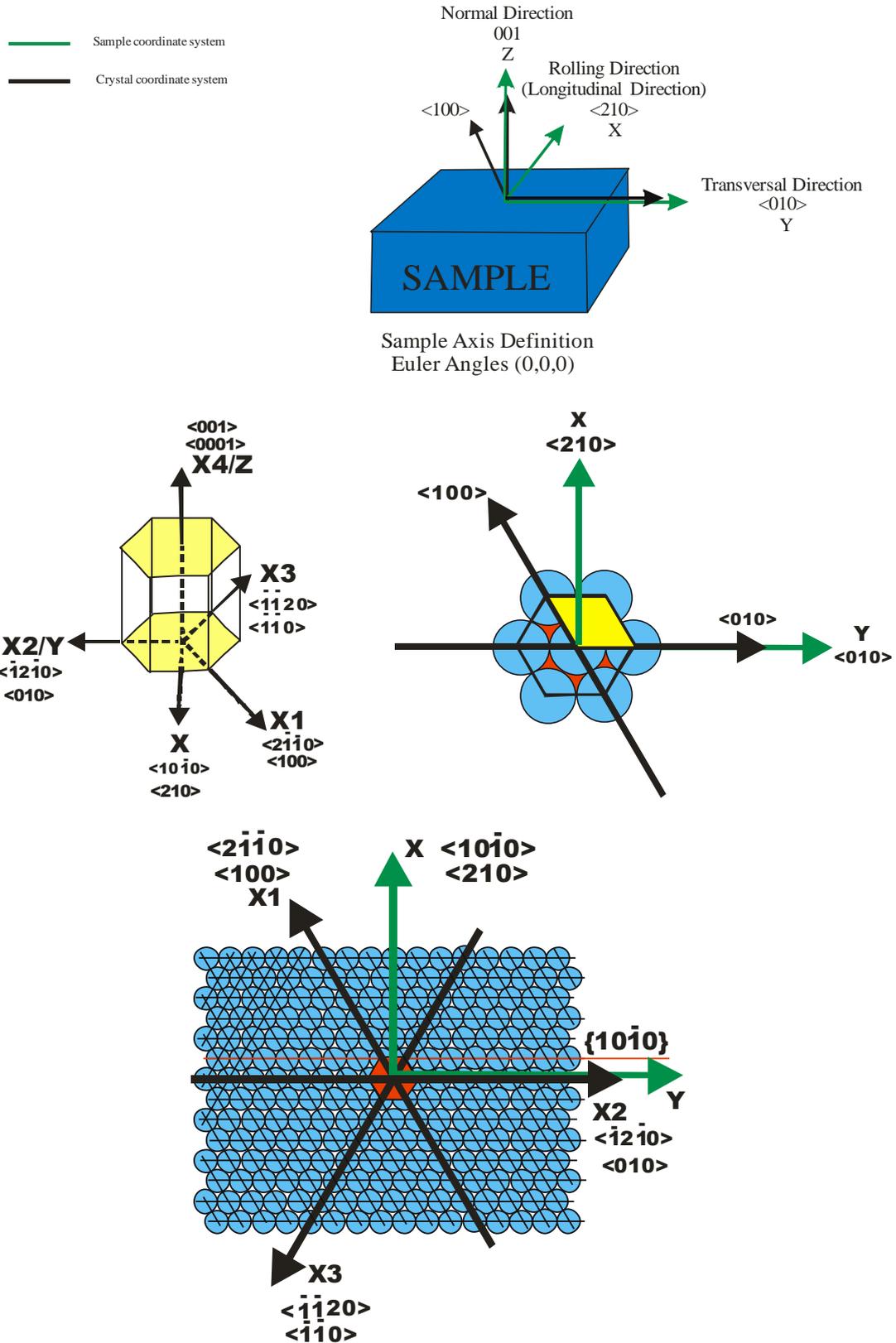
3.4. The Choice of Hexagonal Conventions in LaboTex

User can choose hexagonal convention in LaboTex using dialog 'Hexagonal Axes Convention". There is a special icon for this dialog on the main toolbar : [H] .
To display the ODF in convention compatible with general LaboTex convention, select the left radio button.

Below is shown the example of section of ODF with the marked positions of some orientations in this convention for hexagonal-close-packed (HCP) with an ideal c/a ≃ 1.63:

ODF - Section $\phi_2=0$
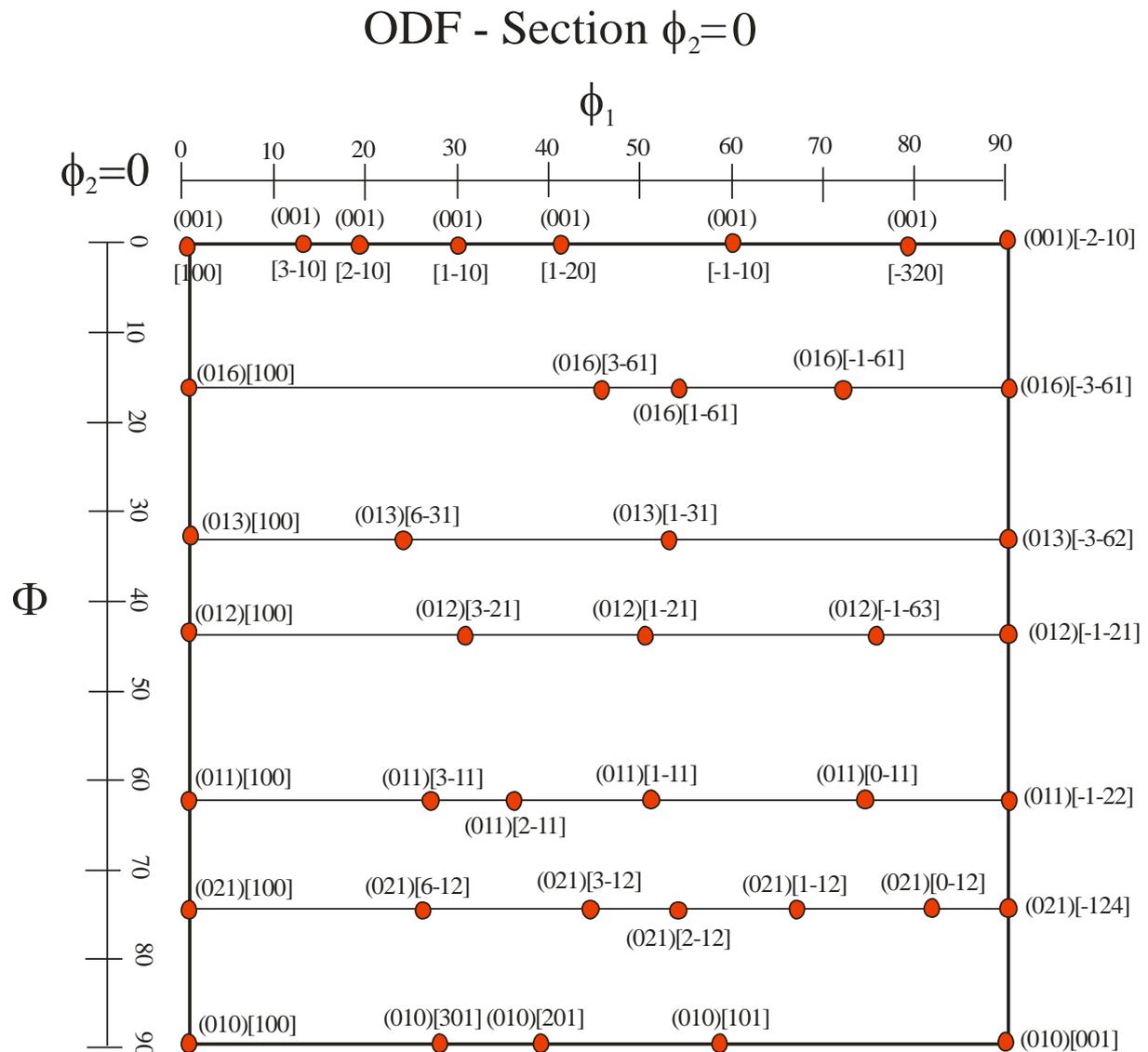
To display the ODF in convention non-compatible with general LaboTex convention, select the right radio button.
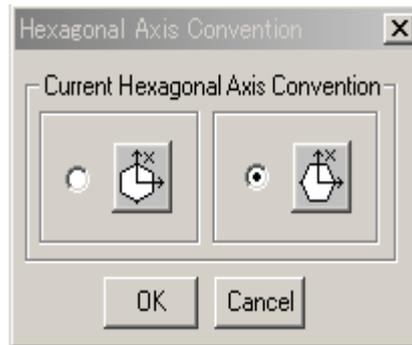
Below is shown the example of section of ODF (the same section as in previous example) with the marked positions of some orientations in non-LaboTex convention for hexagonal-close-packed (HCP) with an ideal c/a ≈ 1.63:

## ODF - Section $\phi_2=0$

ϕ_1

$\phi_2=0$

| 0 | 10 | 20 | 30 | 40 | 50 | 60 | 70 | 80 | 90 |

Φ

- 0: (001)[210], (001)[310], (001)[100], (001)[3-10], (001)[2-10], (001)[1-10], (001)[1-20], (001)[0-10]
- 20: (-12 10)[210], (12 10)[62-1], (-12 10)[2-92], (-12 10)[0-51]
- 30: (-126)[210], (-126)[811], (-126)[4-11], (-126)[2-21], (-126)[0-31]
- 40: (-124)[210], (-124)[611], (-124)[2-11], (-124)[2-32], (-124)[0-21]
- 55: (-122)[210], (-122)[621], (-122)[411], (-122)[4-13], (-122)[2-12], (-122)[0-11]
- 72: (-121)[210], (-121)[521], (-121)[311], (-121)[101], (-121)[0-12]
- 90: (-120)[210], (-120)[211], (-120)[212], (-120)[217], (-120)[001]

10
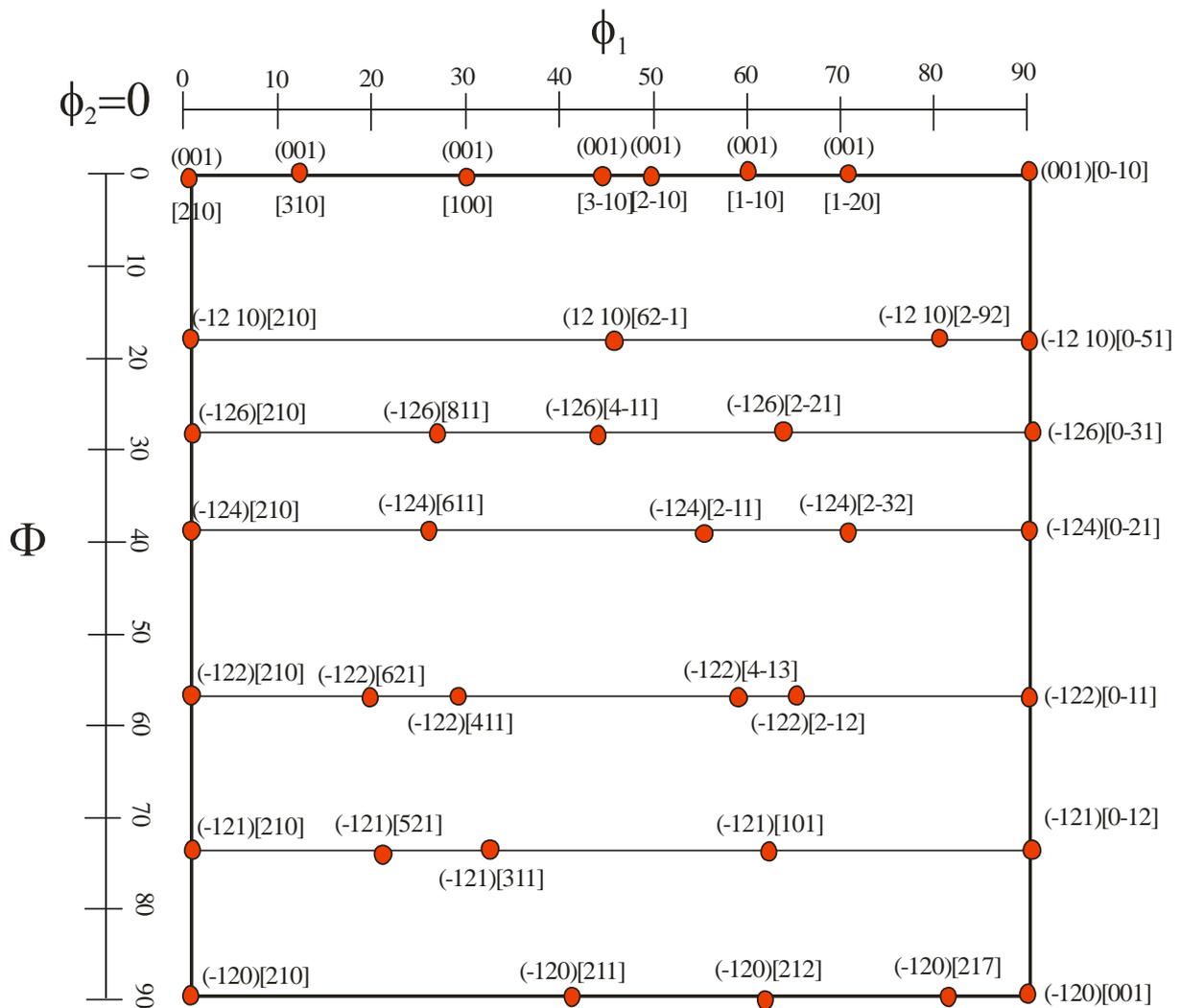
3.5. Example of ODFs for both conventions

Example of ODF of sample with strong {112}<1-10> texture component in the first hexagonal convention (component {112}<1-10> in Euler angles (0,58,30)):

i)   ODF projection ϕ_2;
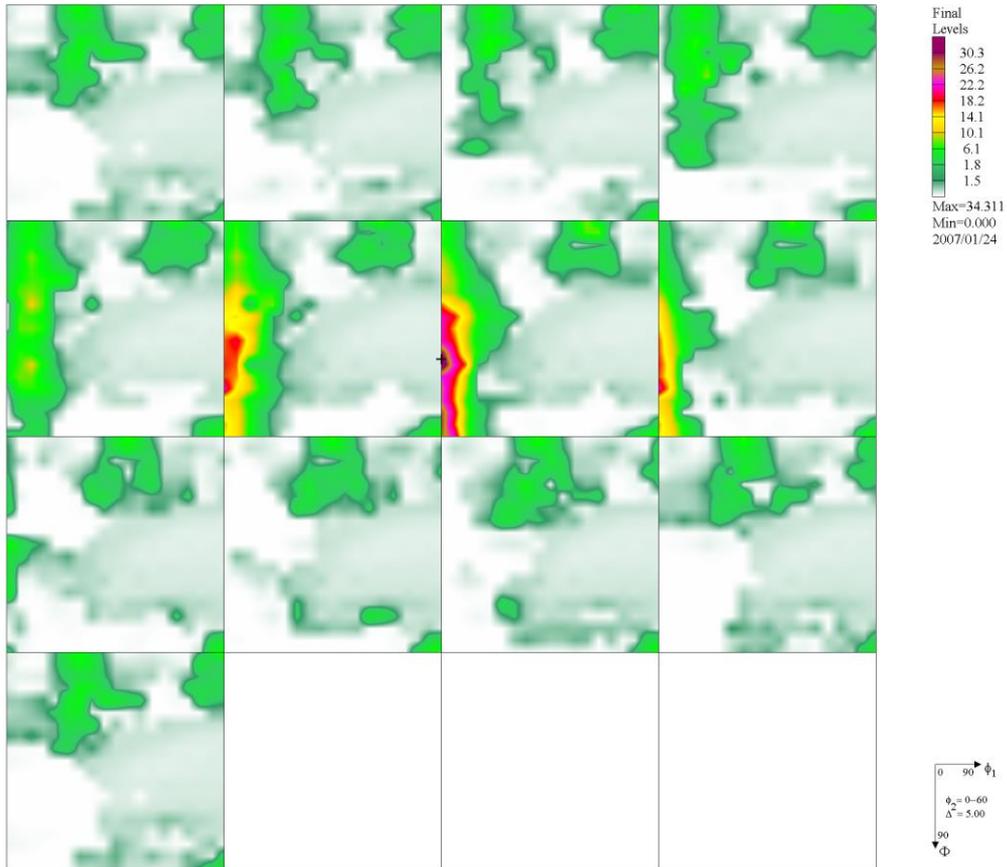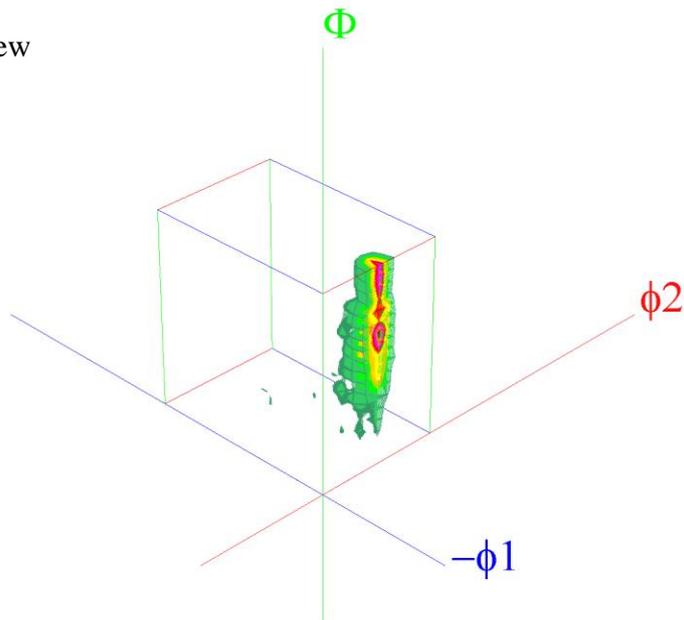
ii) ODF in the 3D view

Example of ODF of sample with strong {112}<1-10> texture component in the second hexagonal convention (component {112}<1-10> in Euler angles (0,58,0)):
i) ODF projection ϕ_2;
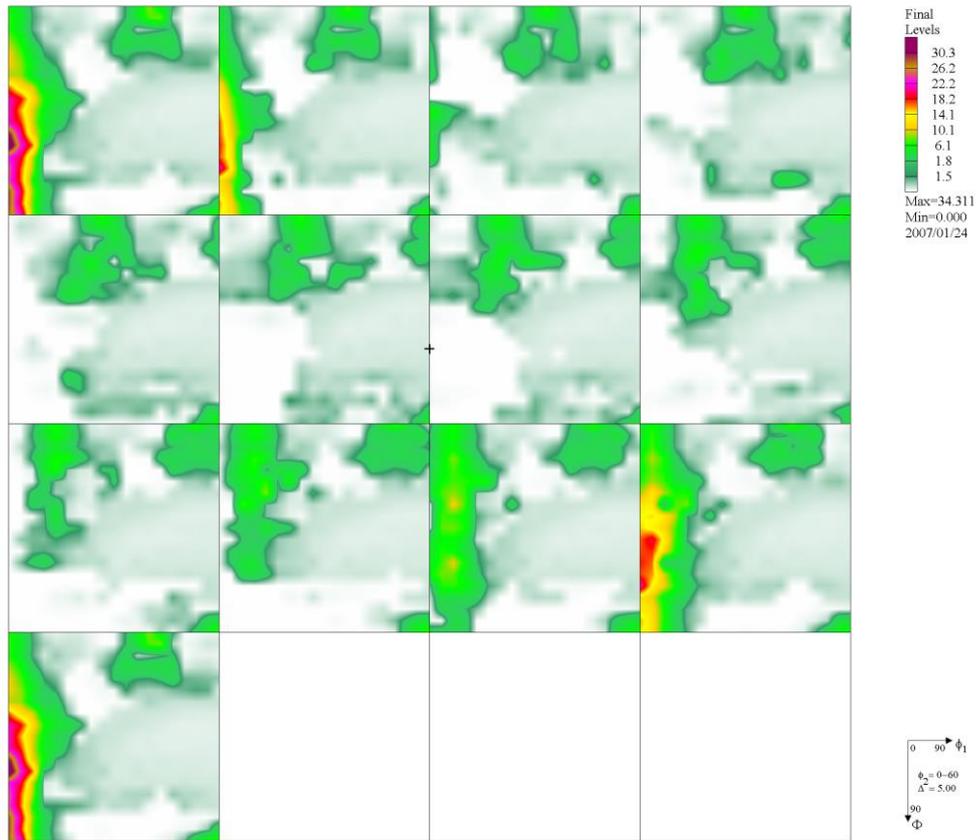
ii) ODF in the 3D view
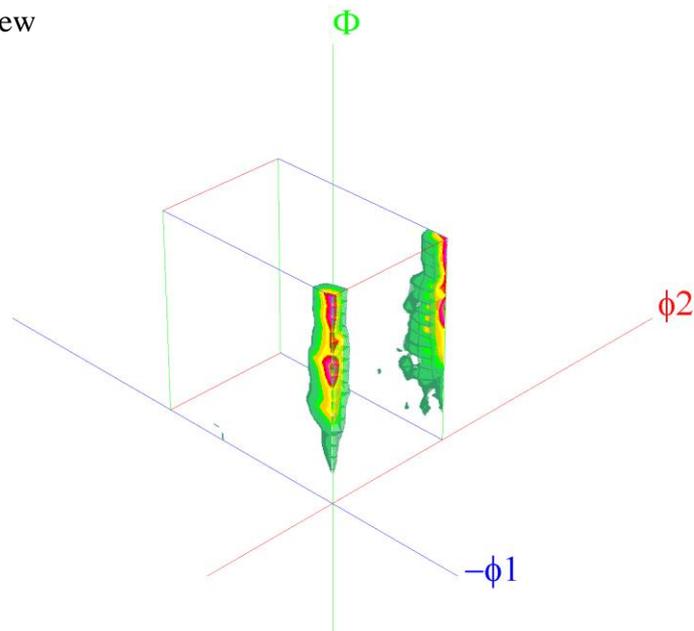
3.6. Single orientation data and hexagonal conventions

When you input single orientations data (file with set of orientations in Euler angles) you should choose convention for Euler angles in hexagonal crystal system (available from version 3.0.16). This choice is made in dialog „ODF Calculations from a Set of Single Orientations":
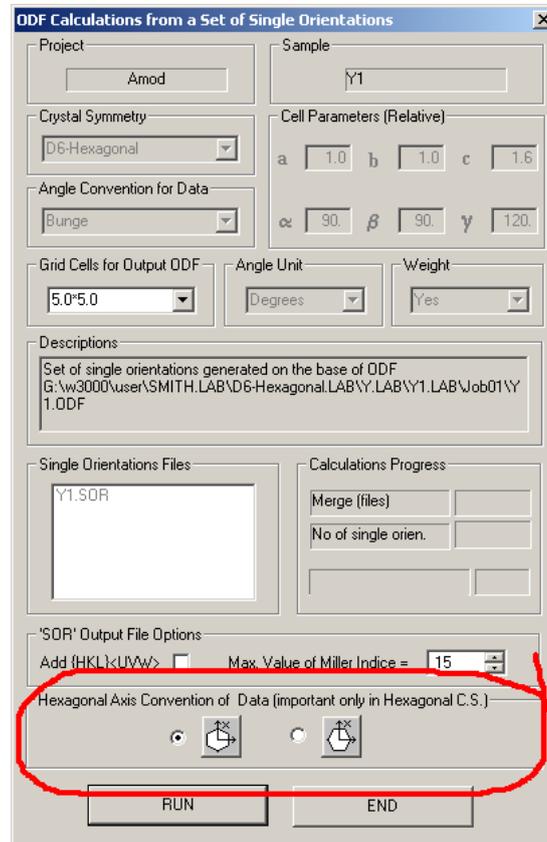
If you chose bad convention during input of data then LaboTex will show maximum in bad places on the ODF. Example below shows sections of ODFs with great participation of component {-124}<210> for both hexagonal conventions (section of ODF in the first convention is shown on the figure from the left and section of ODF in the second convention is shown on the figure from the right). The marks (in LaboTex mode: 'Analysis') indicate proper positions of orientation belong to {-124}<210> component (to change of hexagonal convention use a special icon from the main toolbar :).
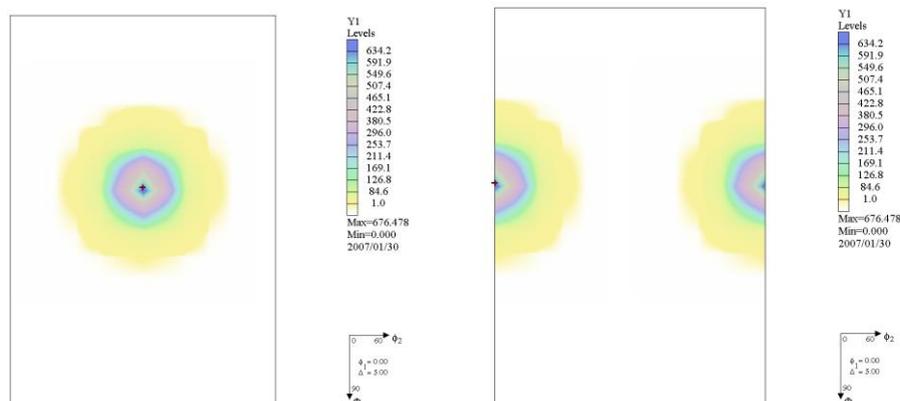
Example below shows sections of ODFs with great participation of component {-124}<210> which were input to LaboTex in bad convention. For both hexagonal conventions the marks indicate position of orientation belong to{-124}<210> component when maximum of ODF are moved to incorrect position (section of ODF in the first convention is shown on the figure from left and section of ODF in the second convention is shown on the figure from right).
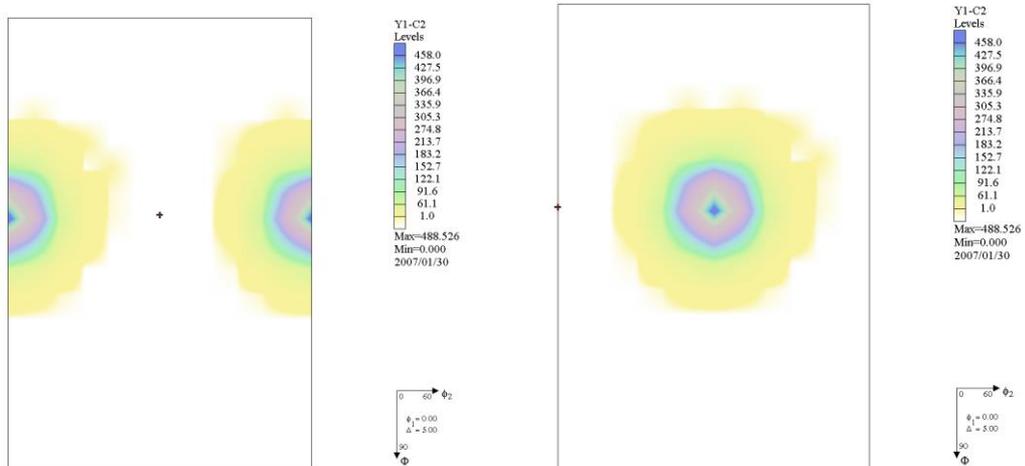
4.   Relation between cell parameters and components

In the hexagonal crystal system the positions of poles of orientation in the pole figures, inverse pole figures and in ODF are depend on cell parameters (c/a).

For example below are shown pole figures, inverse pole figures and ODF sections for strong component {-124}<210> and for c/a equal: 0.5 (left), 1.6 (central) and 10 (right):

Pole Figures

Inverse Pole Figures

X1

X2

X3
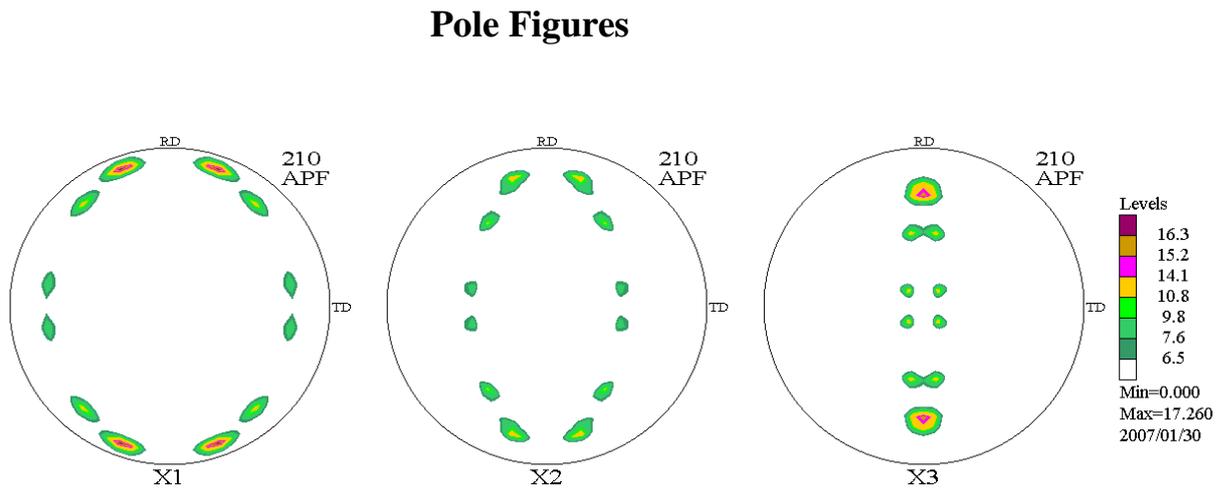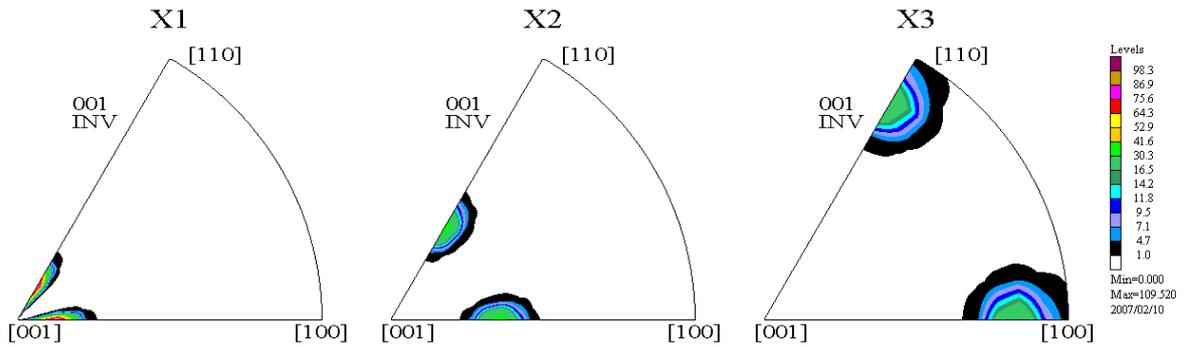
ODF sections
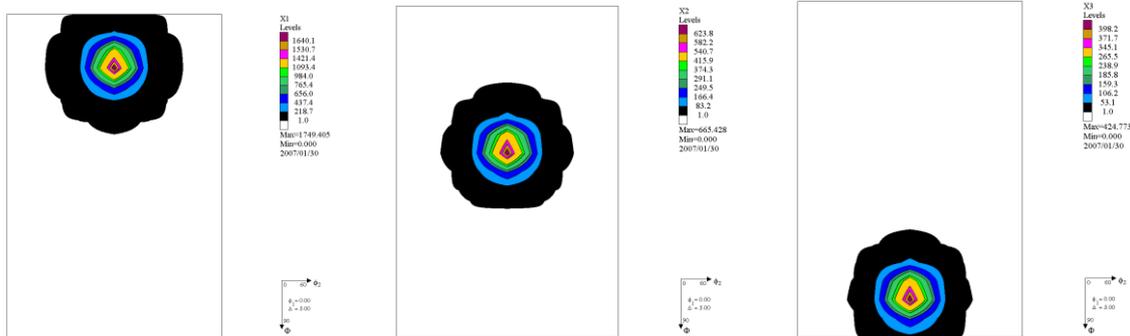
In hexagonal crystal system Euler angles for orientation {-124}<210> depend on cell parametres, hence when LaboTex shows poles for orientation given by Euler angles according to first pole figure i.e.{0,14,330} the others shows marks not in maxims (Euler angles for orientation {-124}<210> for second and third case of c/a are equal respectively {0,39,330} and {0,79,330}).
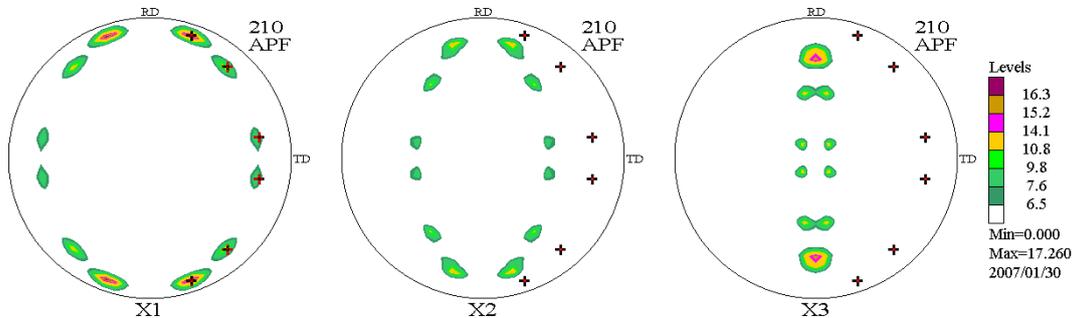
Euler angles are independent from cell parameters in case of some components, but positions of poles are moved on the pole figures with change of c/a.
Below is an example for component {100}<001> (c/a is equal: 0.5, 1.6 and 10 respectively):
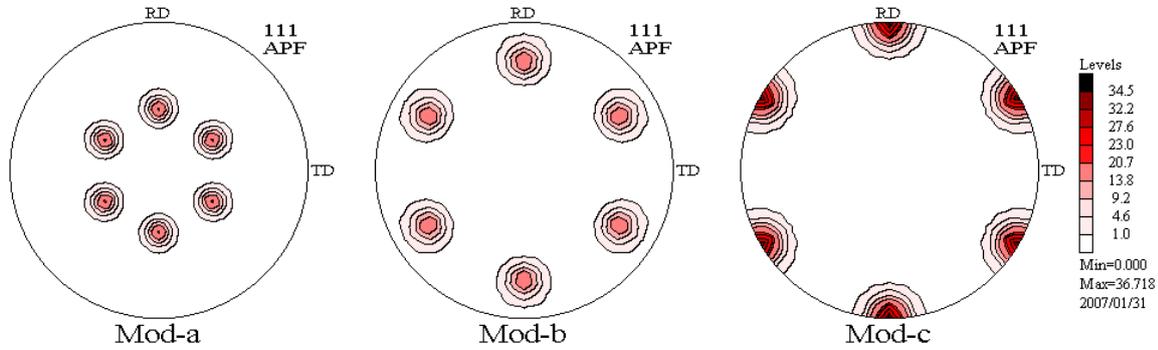
When you make in LaboTex simultaneously analysis of pole figures with different c/a then LaboTex marks poles of component {100}<001>.in maximum intensity for all pole figures with different c/a (Euler angles are independent from cell parameters):
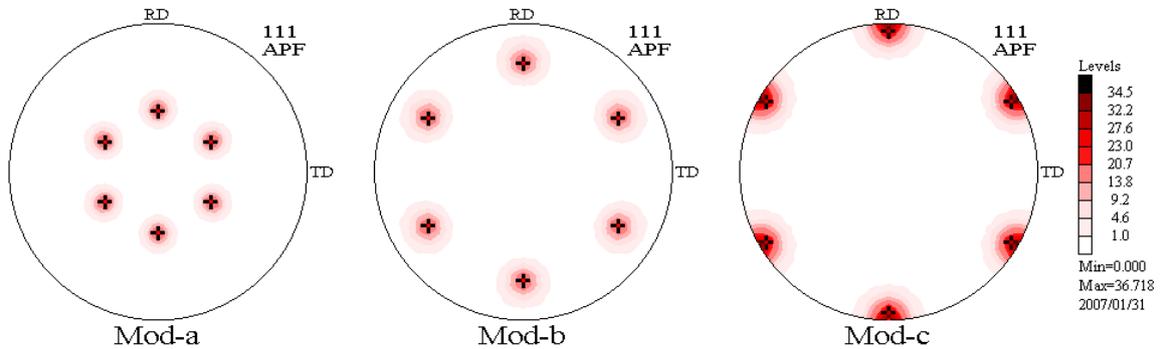
5.   Inverse pole figures in hexagonal system

The LaboTex displays complete and partial inverse pole figures. The partial pole figures are the unit triangles displayed in the range determined by directions <0001> , <2-1-10> and <11-20> (Miller-Bravais notation) or <001>, <100> and <110> (Miller notation).

Unit triangle (main area) is chosen from six symmetrically equivalent areas of full inverse pole figure as it is shown on the figures below for clockwise and counter clockwise axes systems:
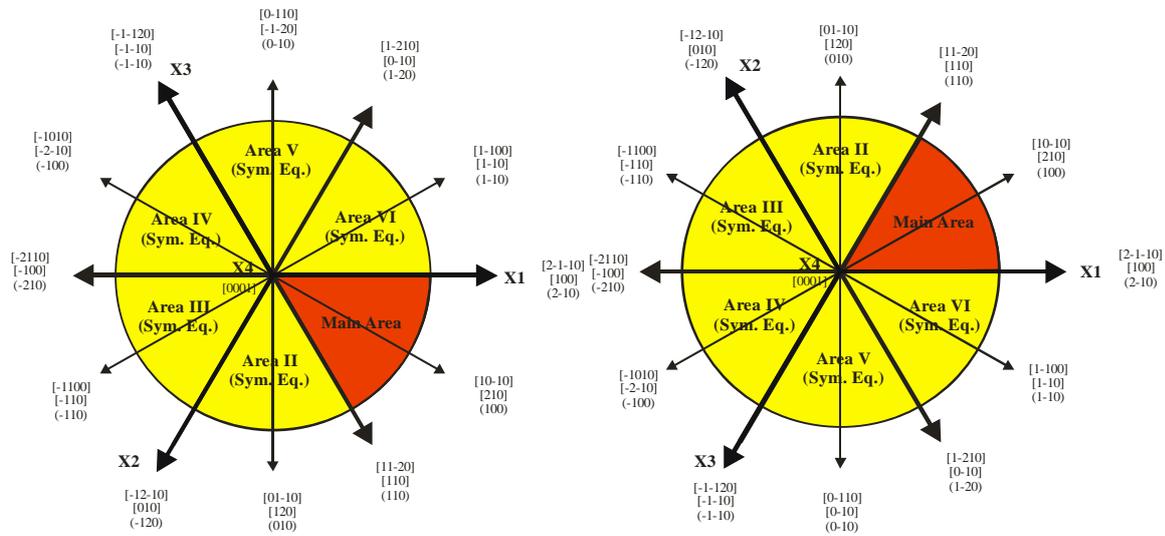
Below you can see examples of complete (full) and partial inverse pole figures for hexagonal crystal system (example calculated for strong component {-124}<210>, c/a=1.6):
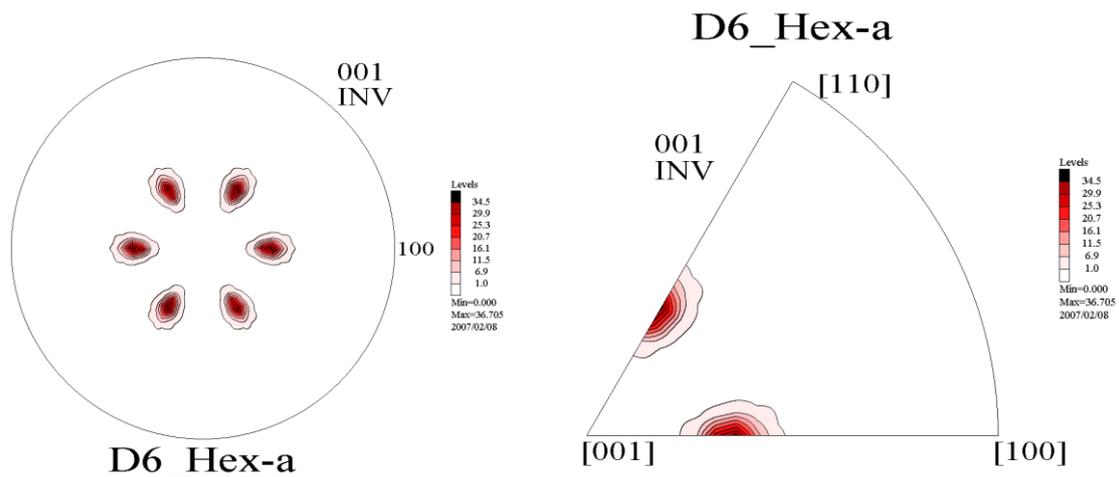

In some works the unit triangle is presented in smaller region than presented above i.e. only 30 degrees instead 60 degrees

LaboTex can calculate inverse pole figures for many directions defined on the basis of sample coordinate. Directions <XYZ> are determined on the similar rule as crystallographic <UVW>, whereat units for axes X,Y and Z are the same. The most important are inverse pole figure calculated for directions parallel to directions of sample coordinate system (XYZ):
- <100> i.e. direction along Reference/Rolling Direction (RD, X axis)
- <010> i.e. direction along Transverse (TD, Y axis)
- <001> i.e. direction along Normal direction (ND, Z axsis)

LaboTex calculates these inverse pole figures during ODF calculation. User can calculate inverse pole figures for other directions using special dialog which is accessible from menu item or from main toolbar.

LaboTex shows (XYZ) direction in the left side of inverse pole figure (it is marked red line):
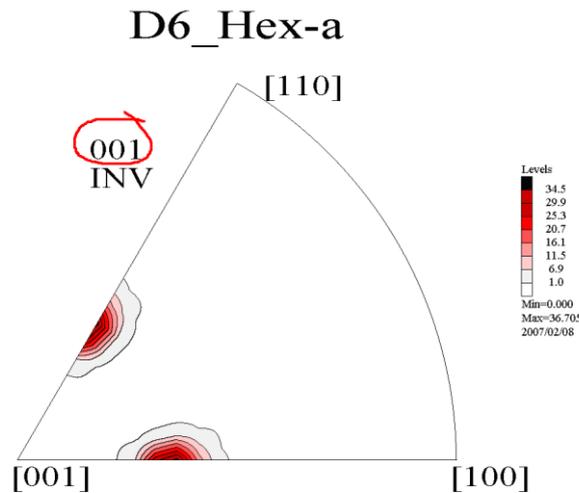

Intensity of inverse pole figure depend on numbers of crystal planes {hkl} perpendicular to chosen sample direction (<XYZ>). On the inverse pole figure the plane is represented by direction perpendicular for this plane.

For example: from definition of {hkl}<uvw>, {hkl} is a crystallographic plane parallel with the plane of the rolling (or other reference plane XY), <uvw> is a crystallographic direction in this plane and parallel with the rolling direction. Hence in hexagonal system, if preferred orientation is {hkl}<uvw> then plane {hkl}should be dominating on the inverse pole figure which shows distribution of directions parallel to normal direction (001, ND). As it is shown on the figure below, in the case of orientation {001}<100> the maximum of the plane {001} should observe (basal plane is marked by yellow color) .
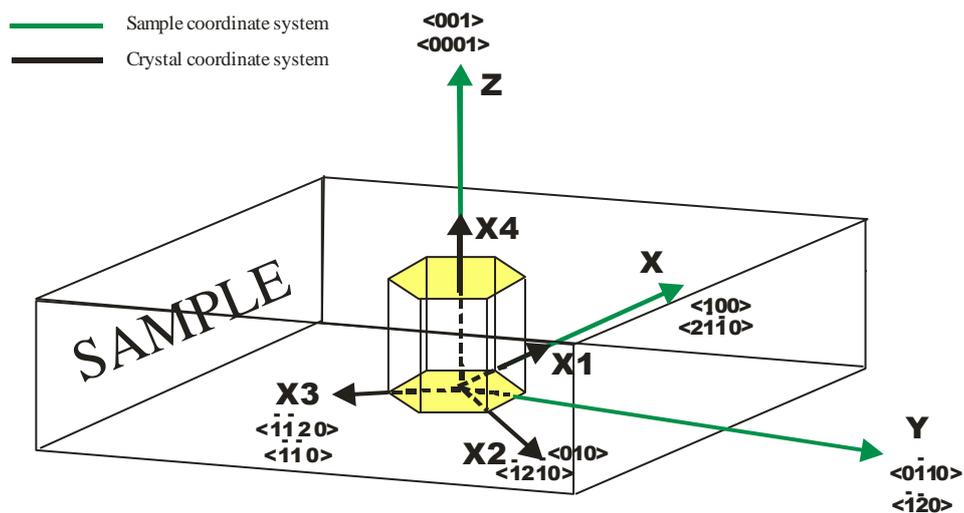
Orientation {001}<100>

Below, you can see this maximum on the inverse pole figure which were calculated for model which have 100% volume fraction of {001}<100> component and FWHM equal 10 degrees:
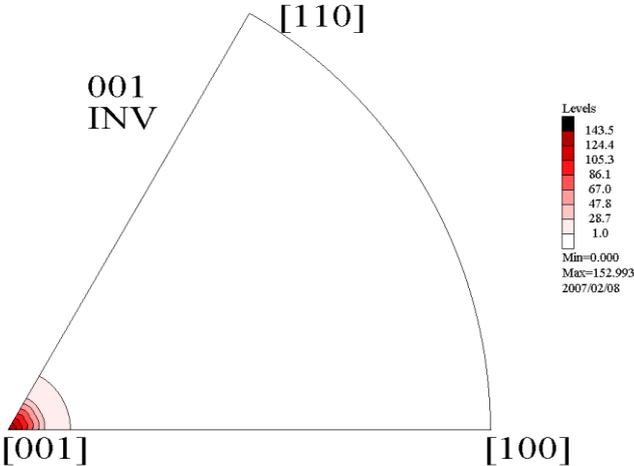

Pole figures (001), (100) and (110) for orientation {001}<100> show position of basal planes {0001}, first order prism planes {10-10} and second order prism planes {2-1-10}:
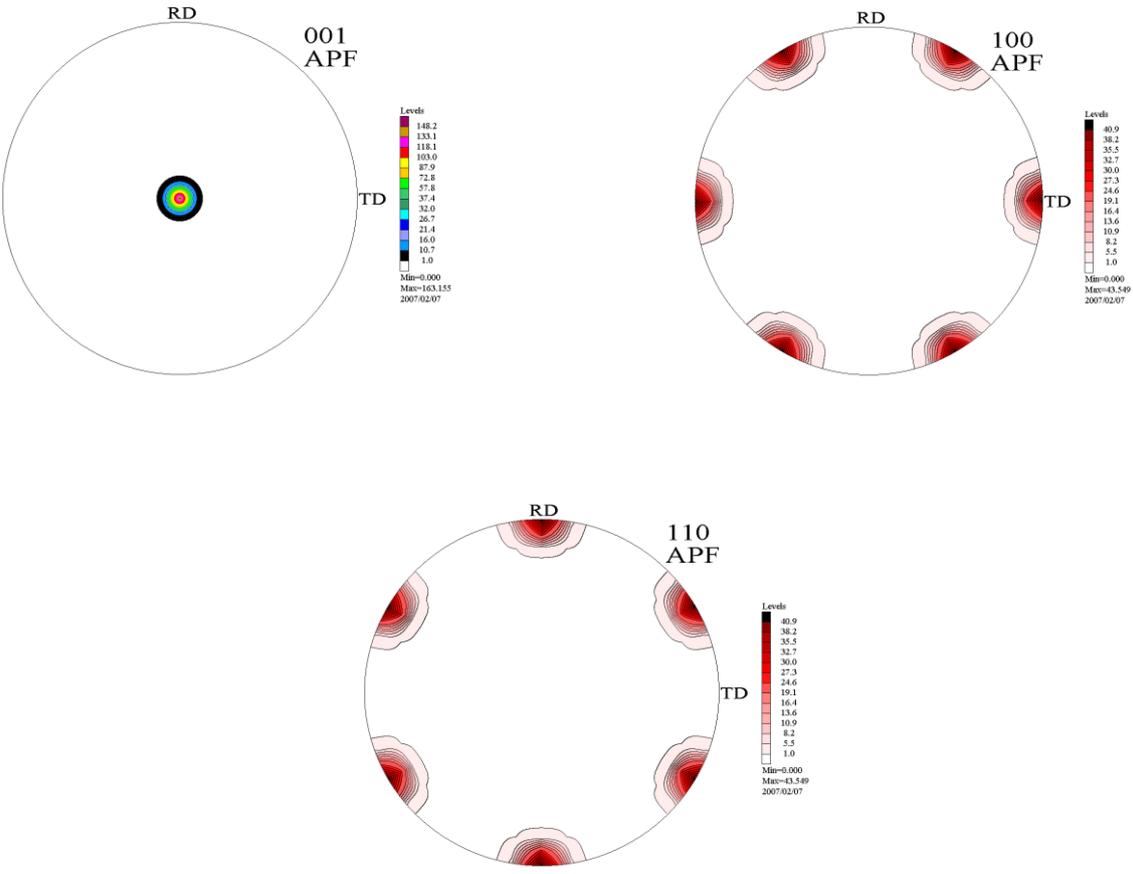
In case of inverse pole figures for RD and TD directions (XYZ=<100> and XYZ=<010>) we can observe the different positions of maximum for orientation {001}<100>. The plane perpendicular to X axis is {2-1-10}:
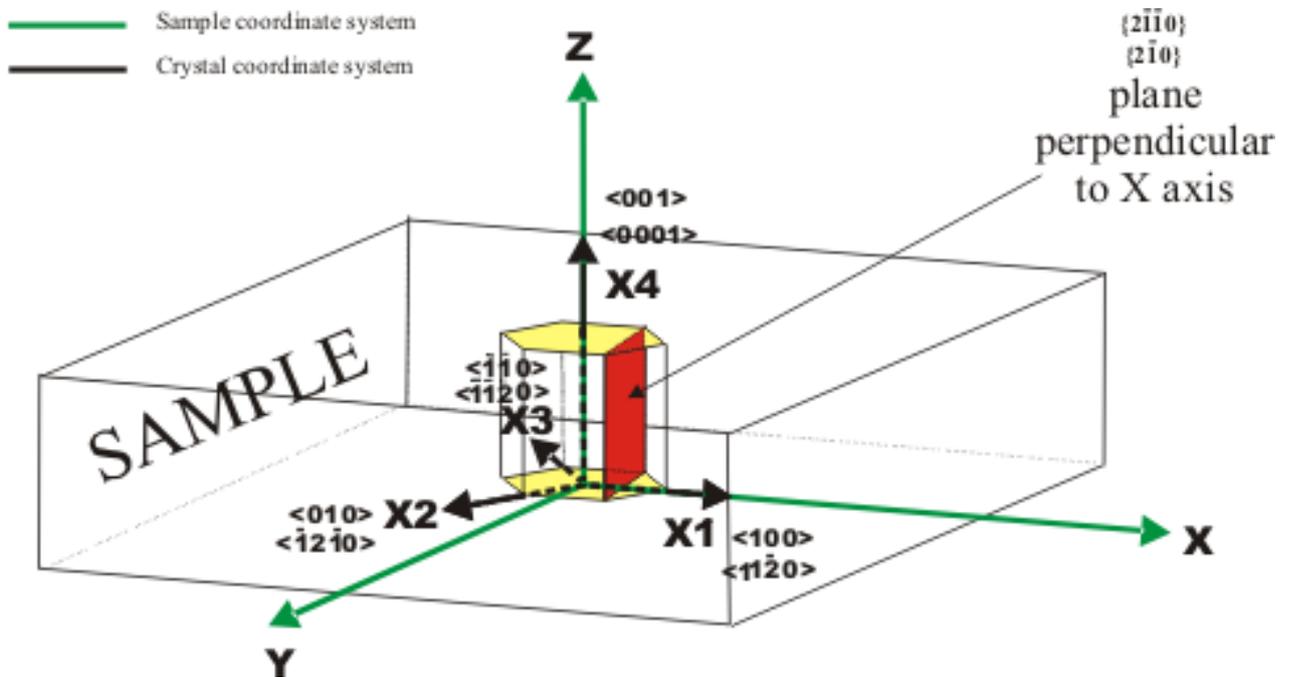
hence the maximum intensity is observed for direction equal [100] as also on symmetrically equivalent direction [110]:
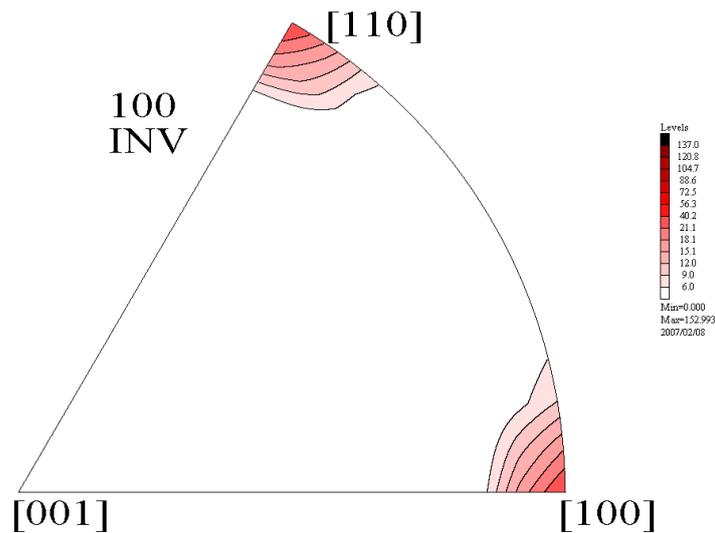
Below you can see that when you choose Y (i.e. (010) or TD) direction for inverse pole figure then the planes type {010}(the plane (010) is marked on the red in the figure) is perpendicular to this direction for orientation {001}<100>.
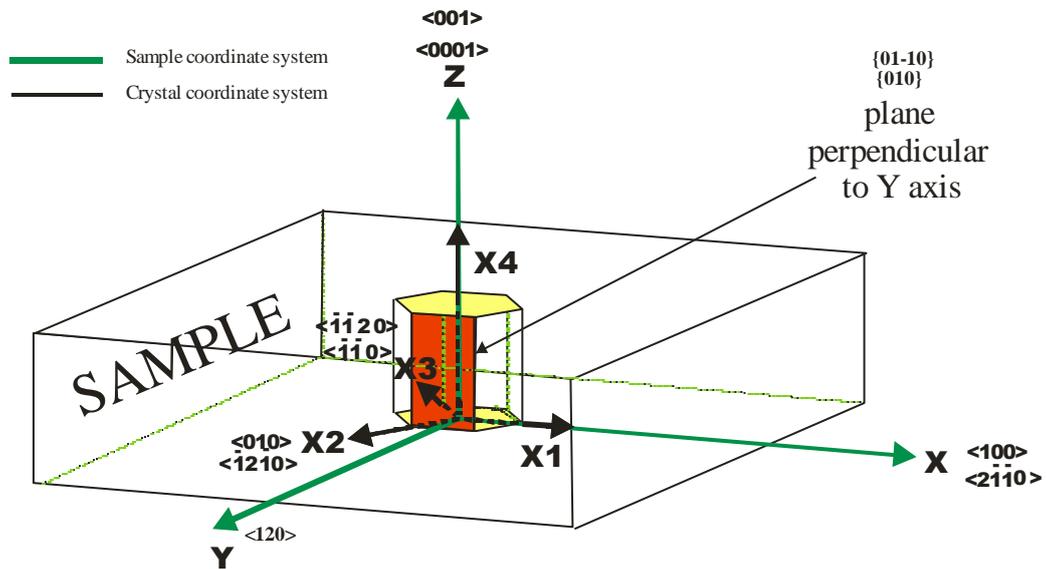
The perpendicular direction <120> will represent this plane on the inverse pole figure. Because direction <120> doesn't belong to the unit triangle (main, fundamental area) the equivalent direction <210> from unit triangle is choosen:
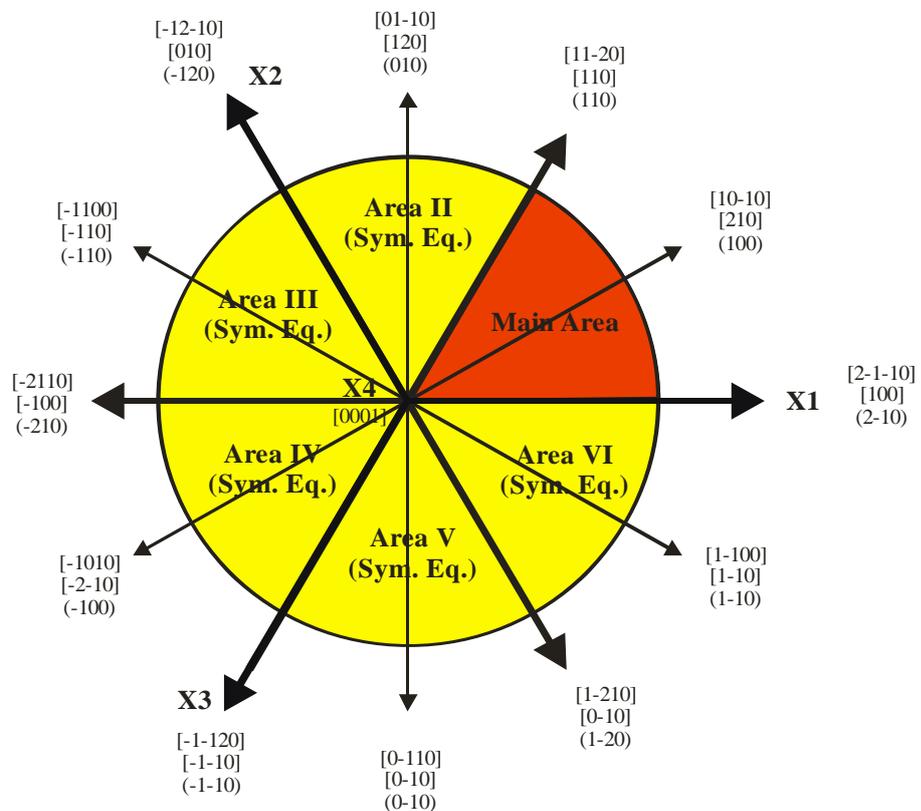
Below you can see the inverse pole figure for TD direction with maximum for direction <210> (<10-10>) determined by the planes: {100} or {10-10}.
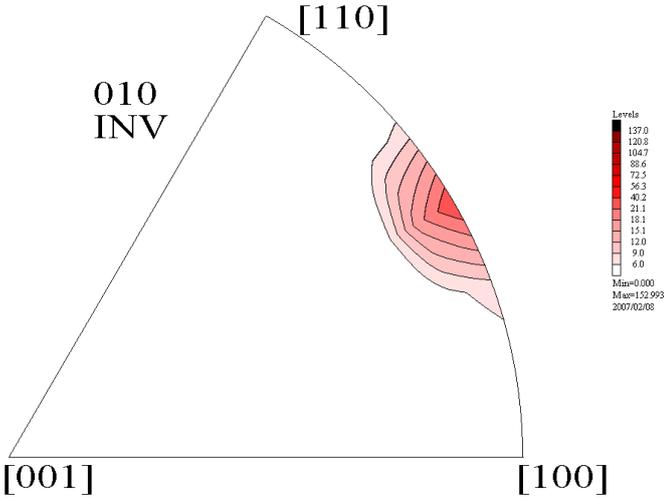
In case of orientation {0-10}<100> which is shown on the figure below
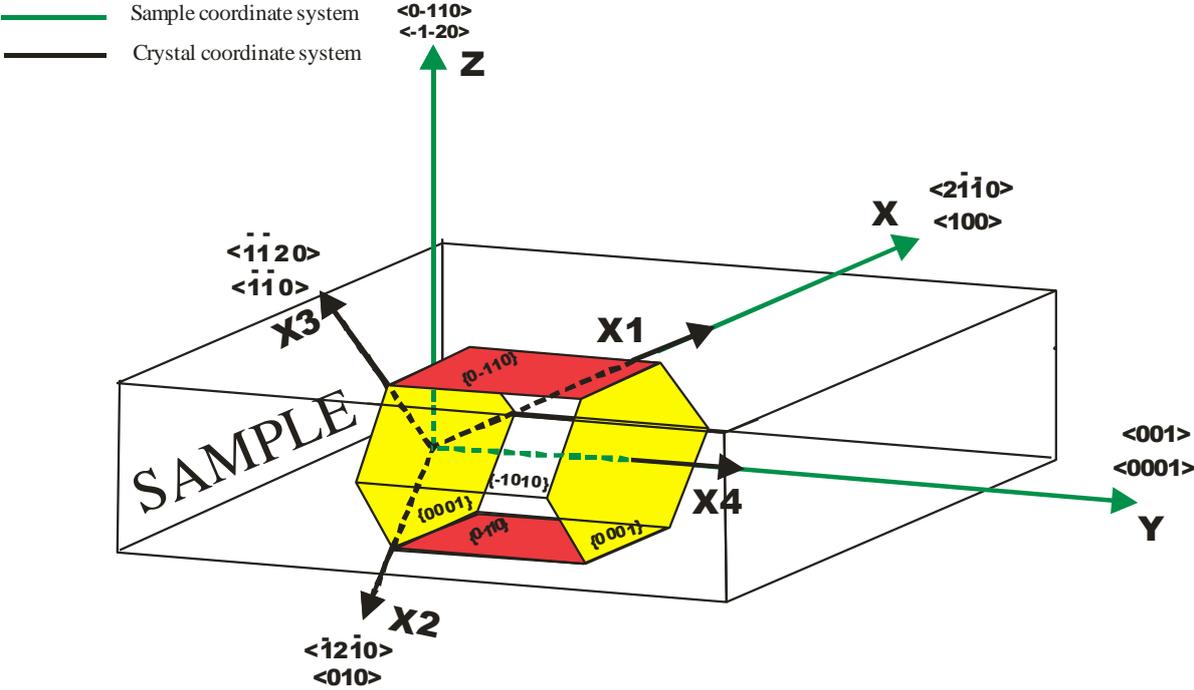
the basal planes are perpendicular to TD (Y) direction hence in this case the inverse pole figure calculated for this direction shows maximum for <001> direction:
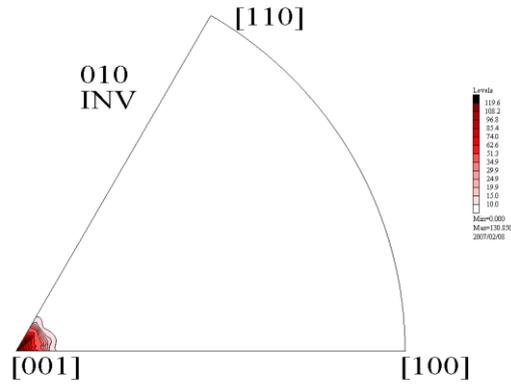
Inverse pole figure calculated for direction TD
(Model of component {0-10}<100>, FWHM 10 degrees)

Below you can see the pole figures {100} and {001} calculated for model model of component *{0-10}<100>*
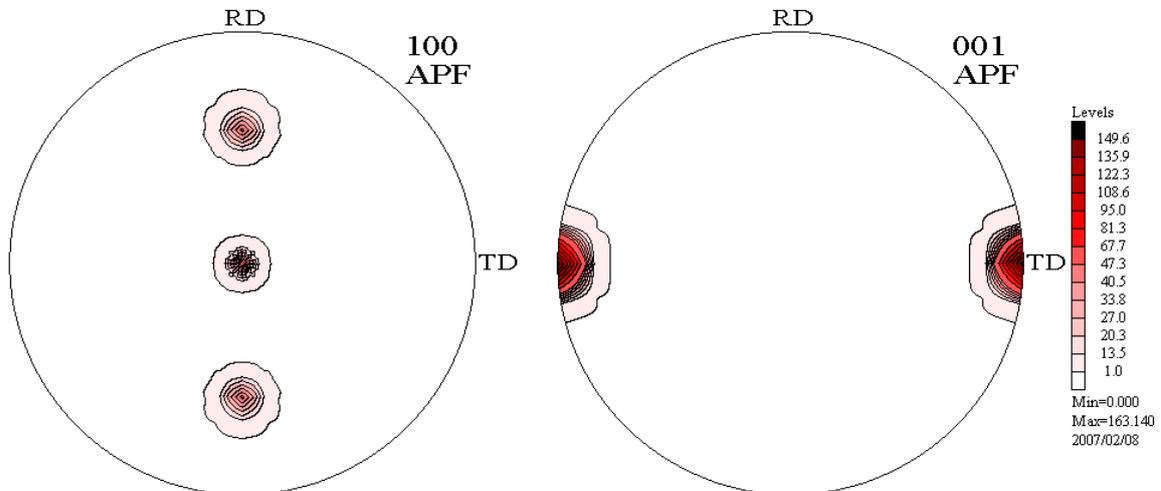
Please remember that orientation noted by Miller indices when is expressed by Euler angles has different notation for each hexagonal axes convention.
For example orientation {0-10}<100> is equivalent orientation {0,90,0} in the first convention and {0,90,30} in the second hexagonal axes convention. Pole figures and inverse pole figures are the same for orientation {0-10}<100> in both convention. Orientation {0,90,0) in the first convention is different from orientation {0,90,0) in the second convention hence orientation expressed by Miller indices, pole figures and inverse pole figures are different in the both conventions.

6. Anisotropy Factors & Kearns Factors

Anisotropy is very important parameter which described properties of hexagonal materials. LaboTex calculates two kinds of texture factors which are used to characterize the hexagonal materials. The anisotropy factors and Kearns factors have found use for correlations and materials characterization of hexagonal materials (thermal expansion, irradiation growth, elastic properties in zirconium and titanium alloys, etc.). LaboTex calculates anisotropy texture factors also for Orthorhombic and Tetragonal Crystal Systems.

Analysis of texture based on partial (incomplete) pole figures or on the Theta-2Theta scans may lead to errors in estimation of anisotropy factors hence LaboTex calculates anisotropy texture factors from ODF (orientation Distribution Function). The ODF contains complete information about texture of sample. Very important is that LaboTex can calculate ODF using incomplete data (partial pole figures) from only one technique:

- X-Ray reflection (partial pole figures)
- X-Ray transmission (partial pole figures)
- Neutron diffraction (partial pole figures)
- EBSD

The first kind of anisotropy factors inform us about **fractions** of basal pole [0002] in each from three principal directions :

- X (Rolling Direction or Axial Direction),
- Y (Transverse Direction or Circumferential Direction)
- Z (Normal Direction or Radial Direction).

Perfect alignment of the basal poles in one direction gives an 'f' value of '1' in that direction and '0' in second and third directions. The sum of anisotropy factors in the three direction is equal 1.0:

$$f_1^{RD} + f_2^{TD} + f_3^{ND} = 1.0$$

For sample with none crystallographic texture (texture "free" sample) all factors are equal 1/3.

There are also the anisotropy factors, 'f' factors, defined by Kearns (Kearns factors (JJ Kearns, "Thermal expansion and preferred orientation in Zircaloy", Bettis Atomic Power Laboratory, Report WAPD-TM-473,1965 and JJ Kearns, CR Woods, J. Bucl. Mater. 20 (1966) 241). If we make assumption that for single hexagonal crystal contribution to the bulk property (P) depends on the angle between reference direction and the [0001] crystal direction (Kearns on the basis of „Anisotropy of Metals", W.Boas and J.K.Mackenzie, 1950) as following:

$$P_{ref.} = P_{[0001]} \cos^2 \varphi + P_{\perp[0001]} (1 - \cos^2 \varphi)$$

where $P_{ref.}$ is the property in the reference direction, $P_{[0001]}$ and $P_{\perp[0001]}$ are the single crystal values parallel and perpendicular to [0001], and φ is the angle between the reference direction and [0001], then for polycrystalline hexagonal materials :

$$f = \int_0^{\frac{\pi}{2}} I(\varphi)\sin(\varphi)\cos^2\varphi \cdot d\varphi$$

$$P_{ref.} = P_{[000\bar{1}]}f + P_{\perp[000\bar{1}]}(1-f)$$

where f is orientation parameter – Kearns factor.

The Kearns factors can be defined for principal directions:

$f_L = f_1^{RD} = FL = f_{ra}$ (*Axial or Rolling or Longitudinal Direction*)

$f_T = f_2^{TD} = FT = f_{rc}$ (*Circumferential or Transverse Direction*)

$f_N = f_3^{ND} = FN = f_r$ (*Radial or Normal Direction*)

The sum of Kearns factors in the three direction is also equal 1.0:

$$f_L + f_T + f_N = 1.0$$

as also the "f" factors for texture "free" sample are equal 1/3, similar as earlier defined anisotropy factors. The Kearns factors can be determined from Theta-2Theta scan (Kearns method) which should be made for each principal plate direction or for longitudinal and transverse directions in case of rod and similar materials. We can calculate these factors with greater accuracy using ODF which can be determined on the basis of the pole figures measured with only one principal direction. The Kearns method use several interpolations hence it is difficult to indicate whether the results of calculation are good or poor (see for example to the paper *„Generalized Kearns texture factors and orientation texture measurement"* by Gruber et. all in the *Journal of Nuclear Materials, Volume: 408, (2011), pp. 176-182)*. Please see on the figure below (comparison of ODF and Kearns methods), where dependence $I(\varphi)$ (red line) is interpolated from experimental points determined on the basis of peaks from 18 (hkil) planes (black points and black lines).
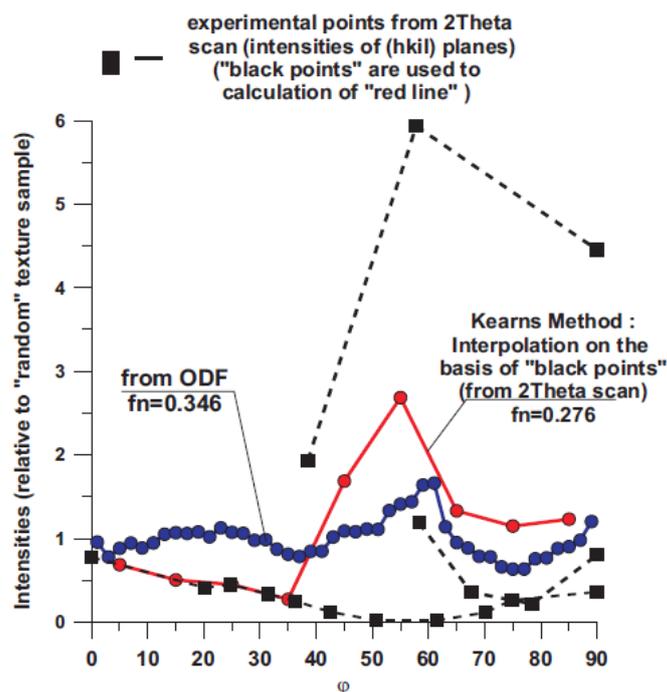
The radial Kearn's texture parameter (f_r) is usually greater than 0.5 for Zircaloy nuclear fuel clad tubing. (See also: Van Swam, L. F. P. et al; "*Relationship Between Contractible Strain Ratio R and Texture in Zirconium Alloy Tubing*"; Metallurgical Transactions A, Volume 10A, pages 483-487. (1979)).

Calculation of Anisotropy Factors

You can start dialog '**Calculation of Anisotropy Factors**' from menu '**Calculation**'.

When you click on the button 'Calculate' LaboTex shows results of calculation for the current Sample and Job. The calculation are made on the basis of ODF.

LaboTex displays:
- Anisotropy factors – f_1, f_2, f_3 – fractions of Basal Planes (001) in Sample Directions (on the basis of angles between normal to Basal Plane (resultant) and Sample Directions;
- Angles between normal to Basal Plane (resultant) and Sample Directions;
- Kearns Factors (fL,fT, fN) – fraction in physical property
- normalized texture index ("0" – random, "1" monocrystal)

Example 1:

We can build the model texture which contains 100% of texture component (Phi1=0,Phi=22.5,Phi2=0) (i.e. the angle between [0002] direction and ND direction is equal 22.5 degrees),
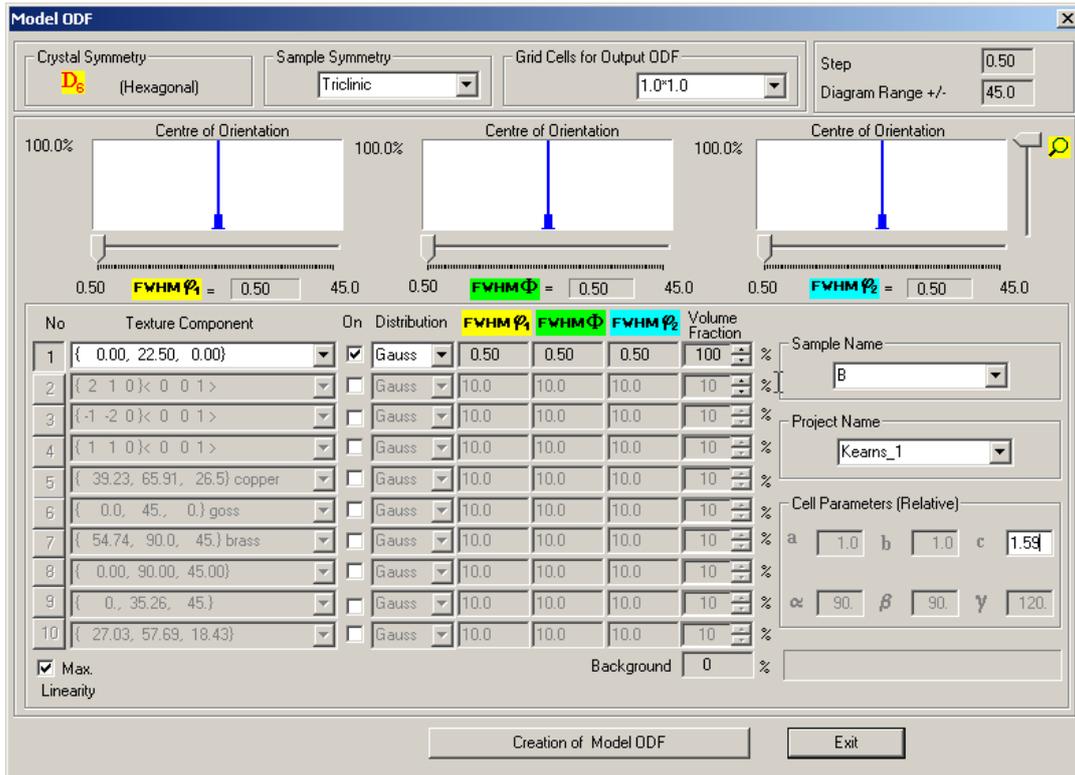
Because model of ODF was created for triclinic sample symmetry hence complete pole figure (0002) shows only one maximum:
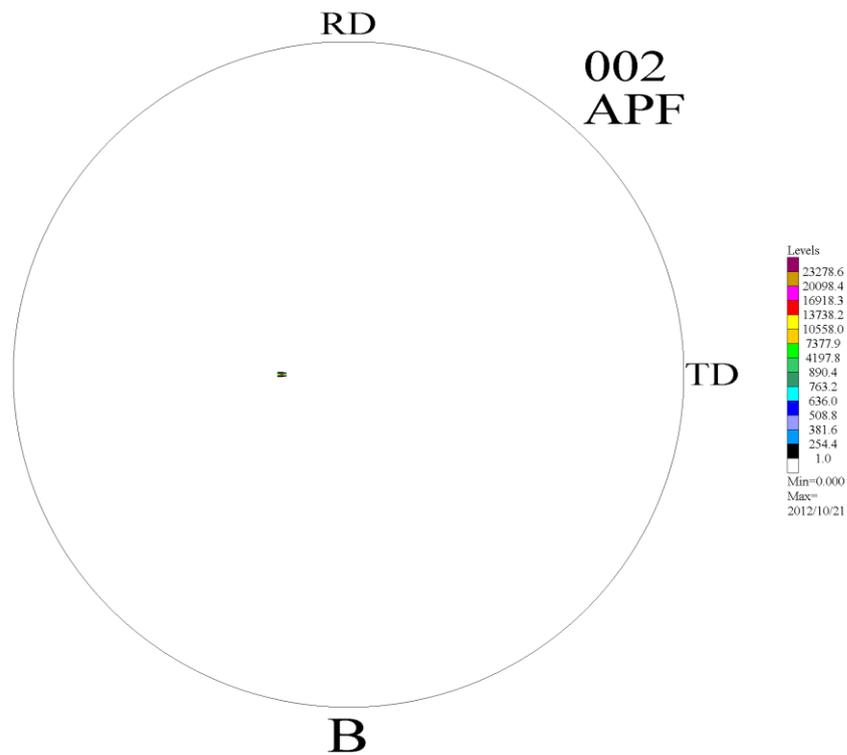
The results of Kearns factors calculation are the following:

The texture index equal 1.0 indicates that our texture correspond to pure monocrystal. The angles between direction [0002] of this monocrystal ("resultant" monocrystal) and direction ND is equal 22.5 degrees when for TD direction is equal 67.5 degrees. Hence anisotropy factors f_1, f_2, f_3 are close to 0.0, 0.25 and 0.75:

- for ND direction: ((90.0-22.5)/[(90-22.5)+(90-67.5)+(90.0-90.0)]=0.75
- for TD direction: (90.0-67.5)/ [(90-22.5)+(90-67.5)+(90.0-90.0)]=0.25
- for LD direction: (90.0-90.0)/ [(90-22.5)+(90-67.5)+(90.0-90.0)]=0.0

In case of Kearns factors, the fractions in physical property are the following:

- for ND direction: the angle ND/[0002] is equal 75 degrees hence $f_N = \cos^2(22.5°)=0.853$
- for TD direction: the angle TD/[0002] is equal 67.5 degrees hence $f_T= \cos^2(67.5°)=0.147$
- for LD direction: the angle LD/[0002] is equal 90.0 degrees hence $f_L= \cos^2(90.0°)=0.0$

Example 2:
We can build the model of ODF which contains:
- 20% planes with [0002] in ND direction,
- 30% planes with [0002] in TD direction and
- 50% planes with [0002] in RD/LD direction

using dialog "Model ODF":
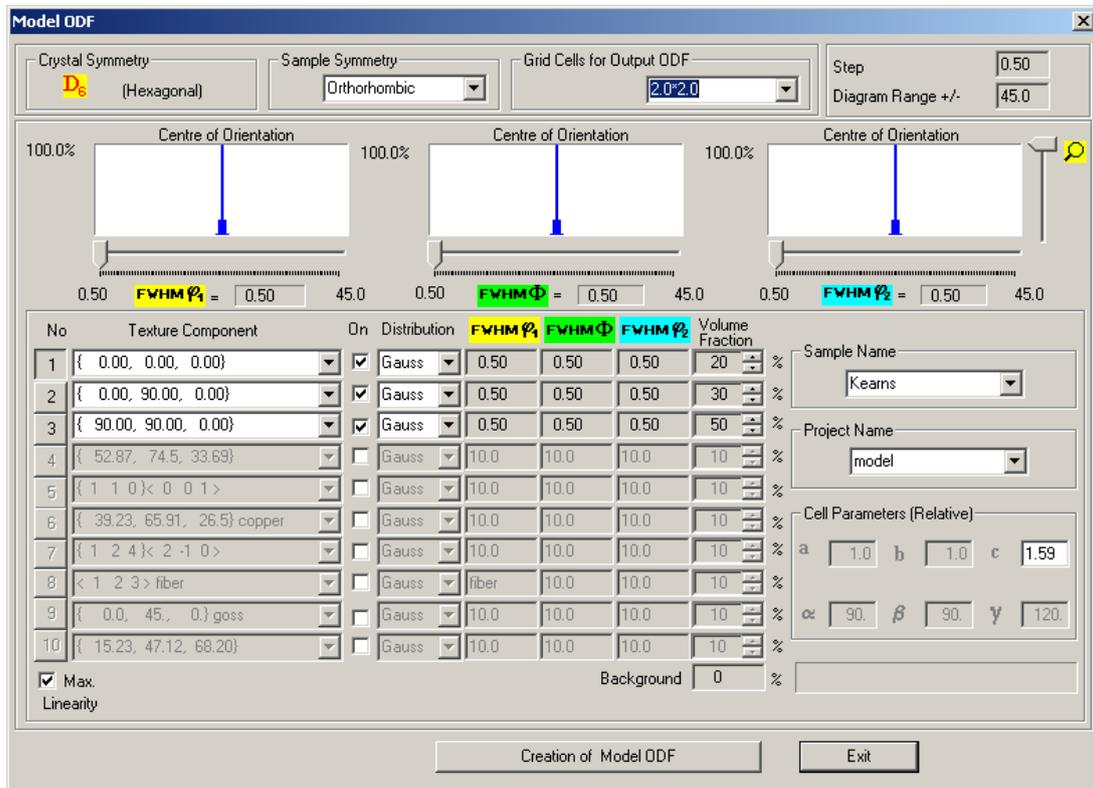
The pole figure for (0002) /basal plane/ calculated on the basis of the model ODF is following:
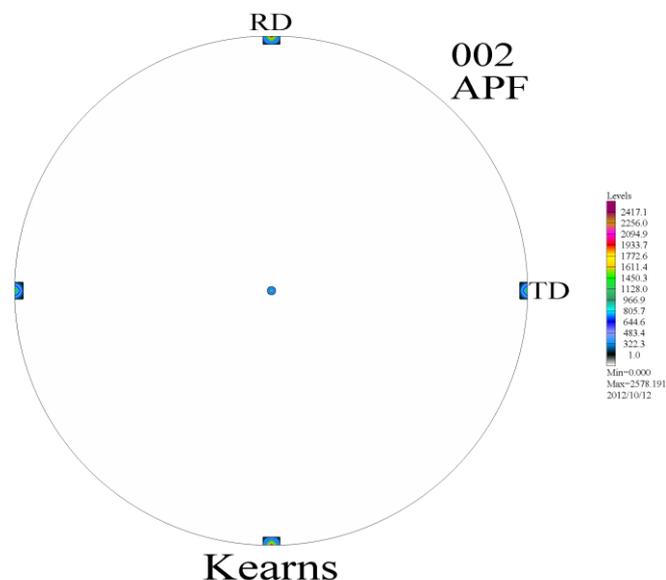
The results of Kearns factors calculation are compatible with assumptions of model:

Warning:
The Kearns factors (fL, fT, fN) are preferred for calculation of physical properties of sample in their principal directions on the base of data for monocrystal.

Example 3:

We have a hexagonal material which has

$P_{[0001]} = 3$ a.u.

$P_{\perp[0001]} = 1$ a.u.

where a.u. - arbitrary units and P - arbitrary property.

We calculated ODF on the basis of pole figures for ND direction of sample and we have calculated anisotropy factors. We received for example following data:

$$P_{ref.} = P_{[0001]}f + P_{\perp[0001]}(1-f)$$
$$P_{ND} = P_{[0001]}0.5 + P_{\perp[0001]}(1-0.5)$$
$$P_{ND} = 3.0 \cdot 0.5 + 1.0 \cdot (1-0.5) = 2.0 a.u.$$
$$P_{TD/LD} = P_{[0001]}0.25 + P_{\perp[0001]}(1-0.25)$$
$$P_{TD/LD} = 3.0 \cdot 0.25 + 1.0 \cdot (1-0.25) = 1.5 a.u.$$

The property *P* in direction ND is equal 2.0a.u. when in direction TD and LD is equal 1.5a.u.

User can find the maximal value of the property for calculation of Kearns factors for transformed ODF for other positions of sample frames (by changes of Phi1 and Phi angles). The calculation on the base of the resultant monocrystal (as in example 1) give good results only in some cases.

Example 4:

Pole figure (0002) (intensity of basal plane) for initial position of sample frame.


Titanium_x
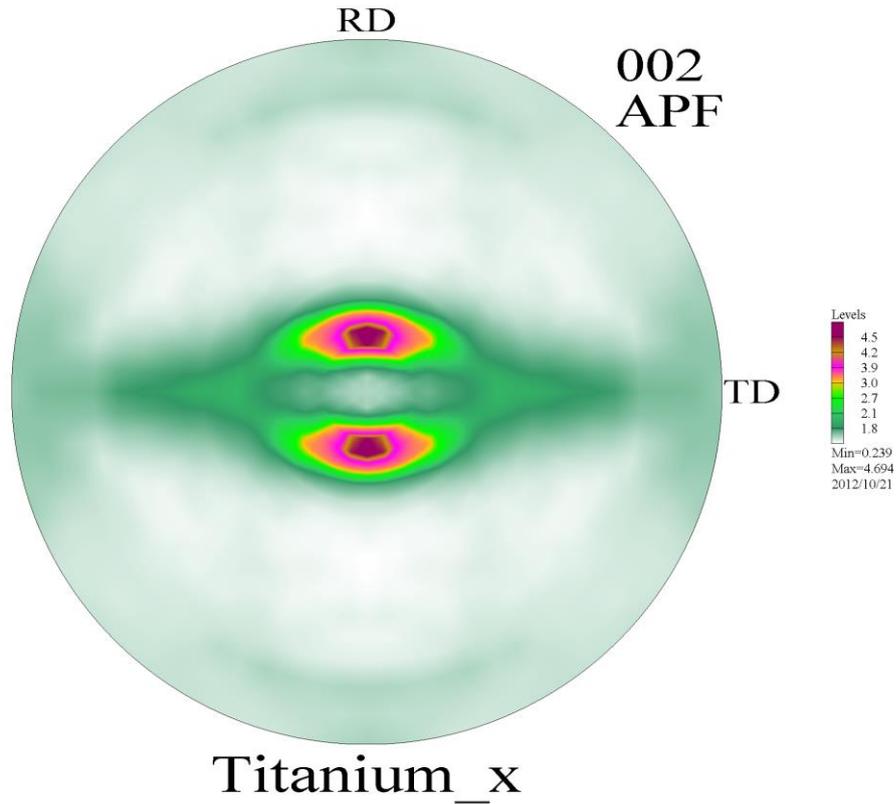
The calculation of anisotropy factors for initial sample frame are the following:

The calculation of ODF for new sample frame position, rotation about (Phi1=0; Phi=90;Phi2=0 i.e. rotation about 90 degrees around RD axis:
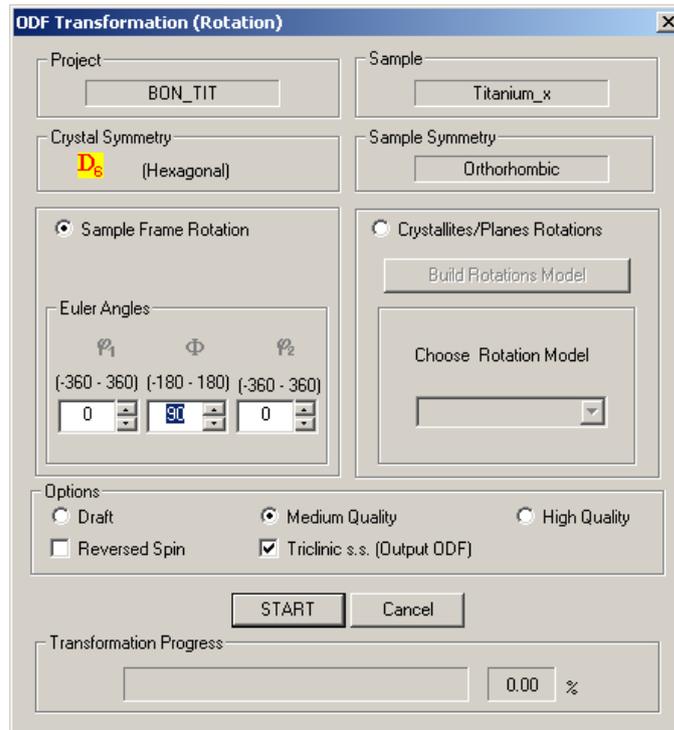
The pole figure (002) after sample frame change (ND<->TD):
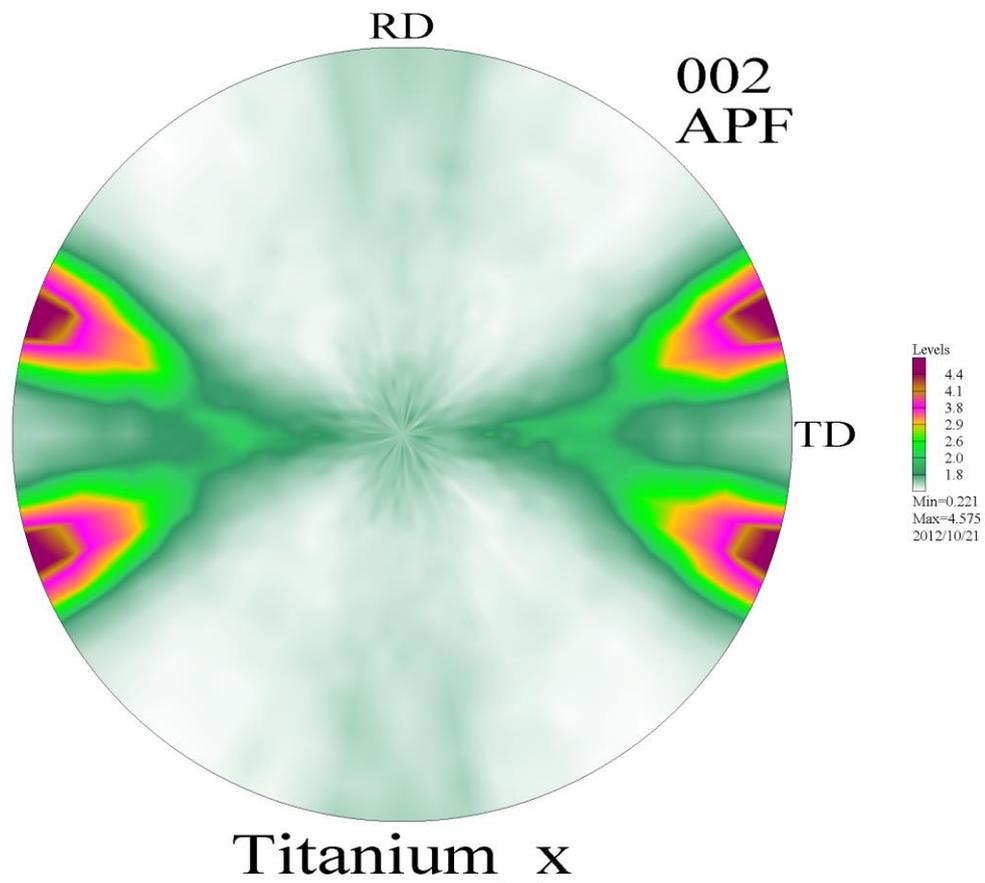
The Kearns factor for LD (f_L) is the same in both case (the rotation was around this axis). The factor for TD (f_T) is now equal factor for factor f_N in the initial frame and factor for ND (f_N) is now equal f_T in the initial frame.

Warning:
We can calculate Kearns factors for any position of sample frame by change of the initial sample frame in dialog "ODF Tranformation". If you have the experimental results (pole figures) for only one sample frame position you can calculate anisotropy factors for any other positions of sample frame. The above is true if texture in your sample is homogeneous (none or small changes with depth).