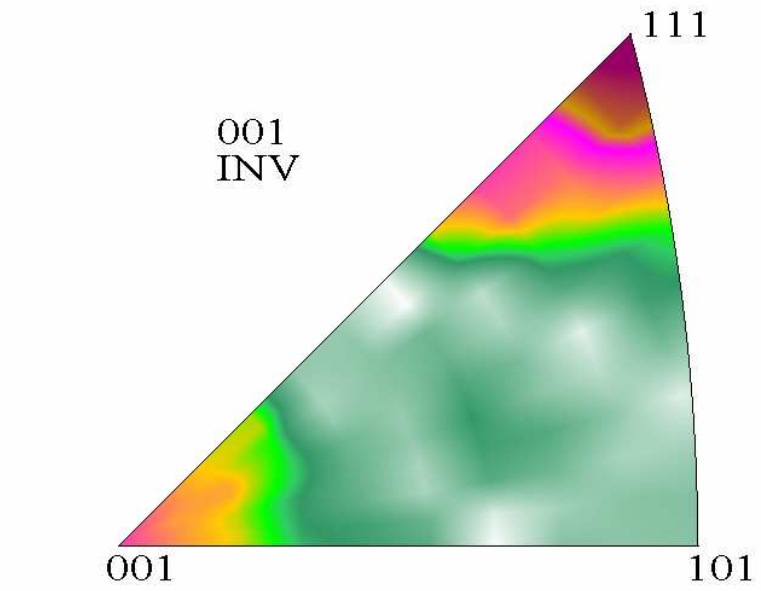
LABSOFT

LaboTex

Version 3.0

The Texture Analysis Software for Windows



Piotr Ozga

The Nomenclature of Inverse Pole Figures Use in LaboTex

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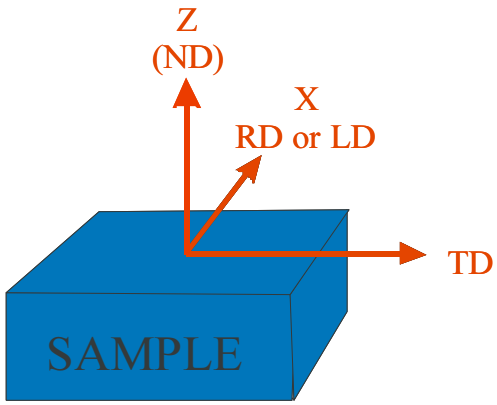
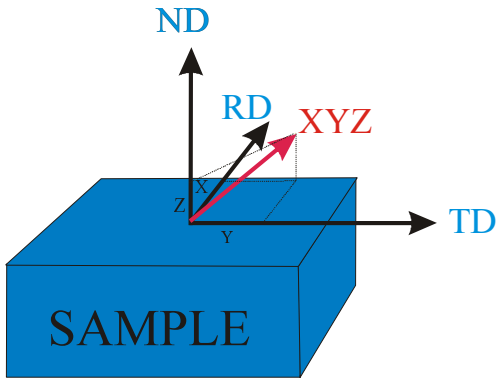
The Nomenclature of Inverse Pole Figures Use in LaboTex

The inverse pole figures answer for the question: "What crystallographic planes are preferentially perpendicular to the some sample direction". Intensity of inverse pole figure depend on numbers of crystal planes {hkl} perpendicular to chosen sample direction <XYZ>. This sample direction is input to LaboTex by user during inverse pole figure calculation. LaboTex can calculate inverse pole figures for many directions defined on the basis of sample axes frame. 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):

Denotation of inverse pole figure (sample direction)	Description
001	**Orientation distribution of a sample ND axis on a stereogram**
100	**Orientation distribution of a sample RD/LD axis on a stereogram**
010	**Orientation distribution of a sample TD axis on a stereogram**
XYZ	**Orientation distribution of a XYZ direction on a stereogram (for example 111 direction)**

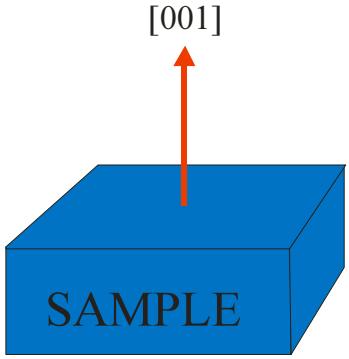


Sample Axes Definition

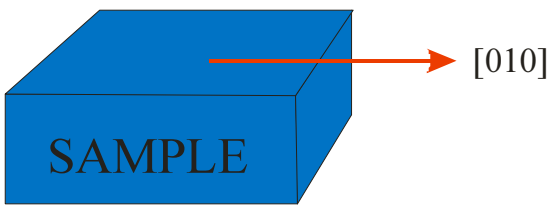


XYZ Direction

Examples:

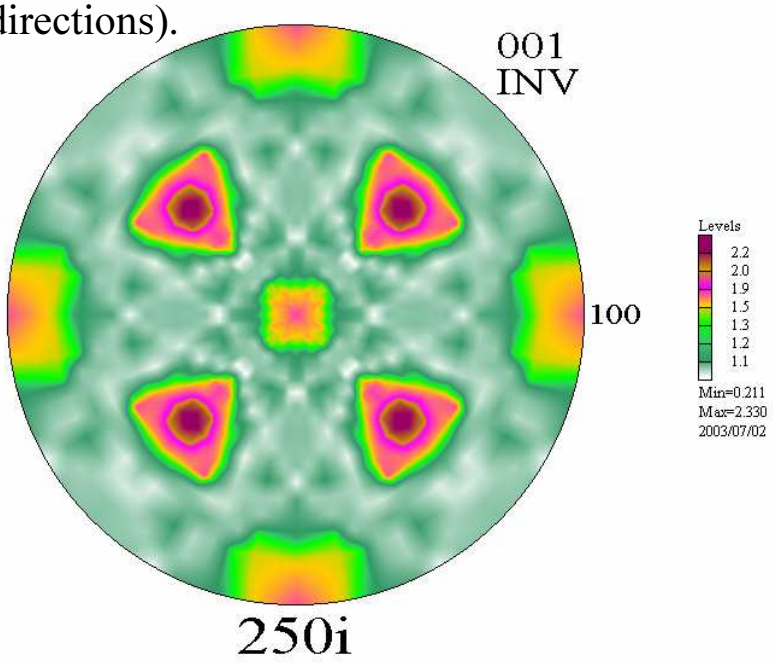


[001] Sample Direction



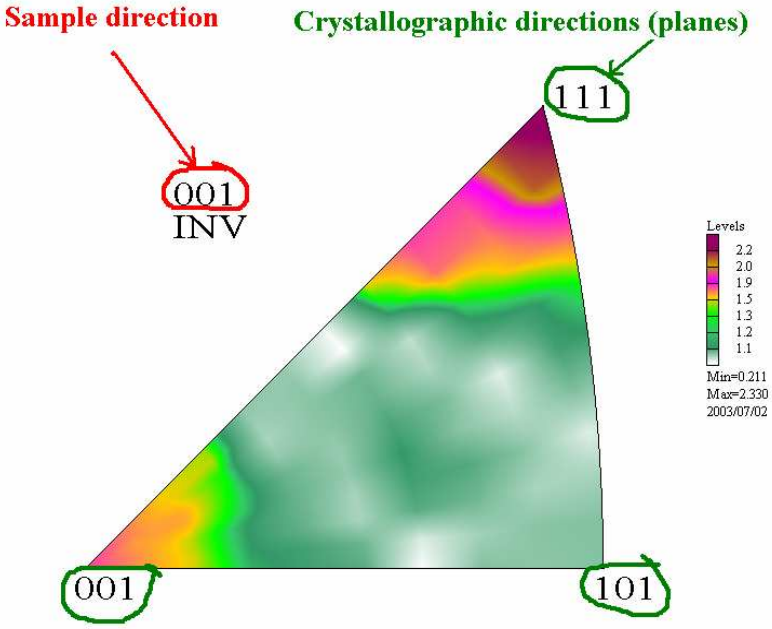
[010] Sample Direction

Complete Inverse Pole Figure - orientation distribution of a sample axis or XYZ direction on a stereogram plotted with respect to crystallographic orientation (axis or directions).



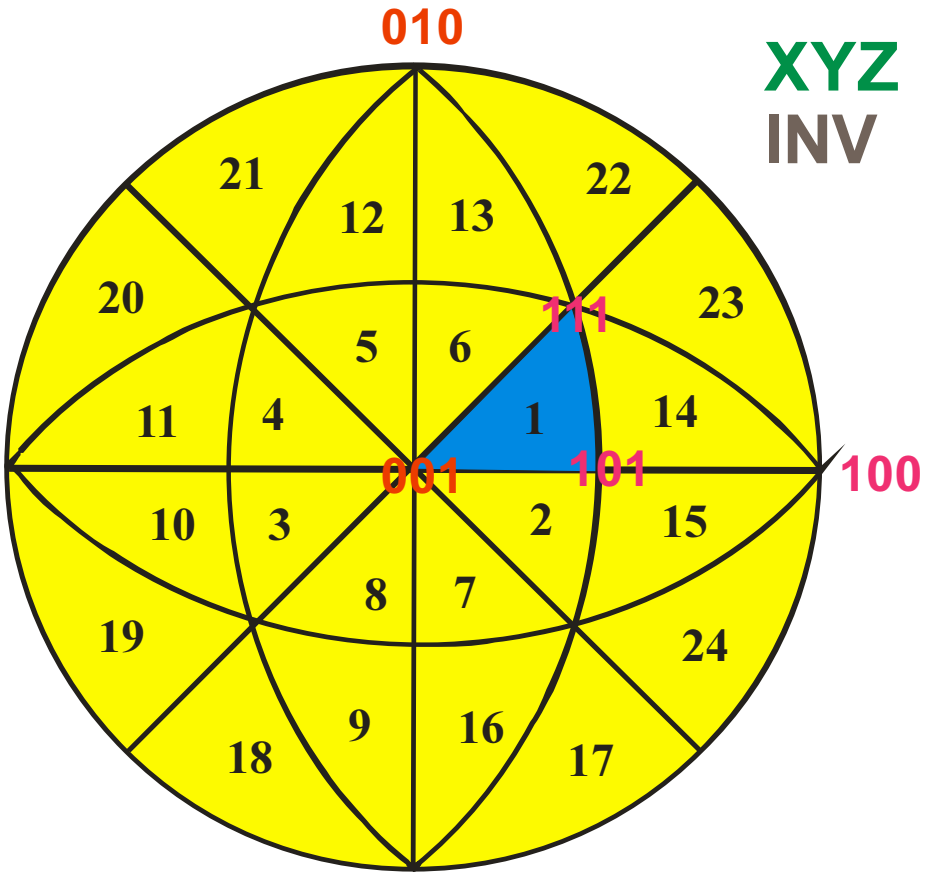
Example of the Complete Inverse Pole Figure (orientation distribution of 001 or ND sample axis. 010 and 100 - crystallographic axis. In center - 001 crystallographic axis)

Partial Inverse Pole Figure (Inverse Pole Figure in Basic Region) - orientation distribution of a sample axis or XYZ direction on a standard stereographic triangle (eliminate of redundant information of complete IPF). The icon  change IPF visualization from complete to partial.



Example of the Partial Inverse Pole Figure for Cubic System (distribution of 001/ND sample axis. 001, 101 and 111 - crystallographic direction)

24 Equivalent regions of complete inverse pole figure for cubic system



1..24 - equivalent regions of complete inverse pole figure for cubic system

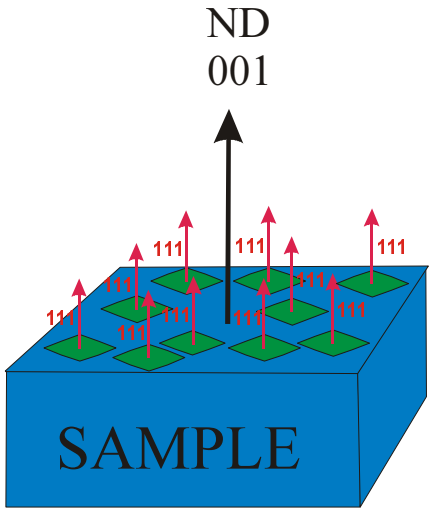
001, 010, 100, 111, 101 - crystallographic axes and directions

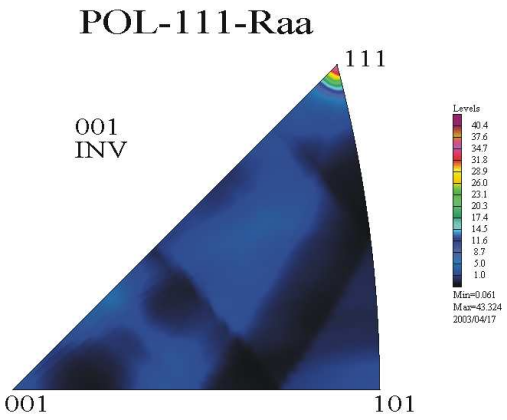
INV - type of pole figure (inverse pole figure)

XYZ - sample direction for which orientation distribution is plotted

1 - basic region (main area) of complete IPF (partial IPF, standard stereographic triangle)

Schematic interpretation of the IPF



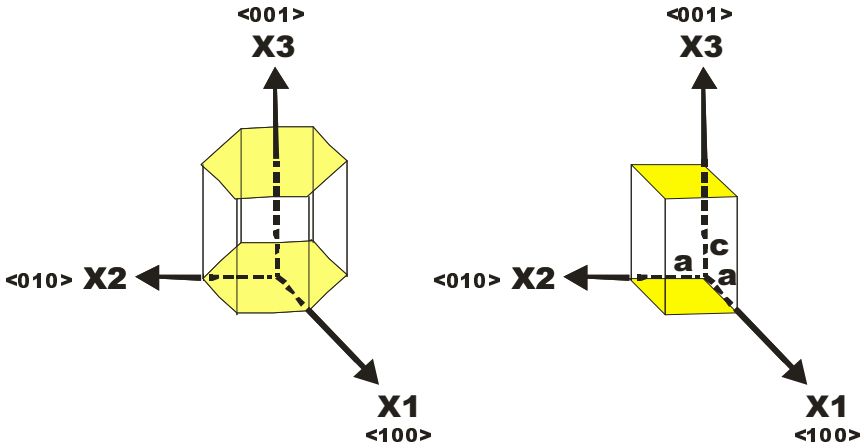


{111} crystal plane oriented in ND/<001> sample direction (normal direction)

Inverse pole figures in hexagonal system

In Hexagonal System are used two notations:

1) Miller Notation (3 Axis Notation)

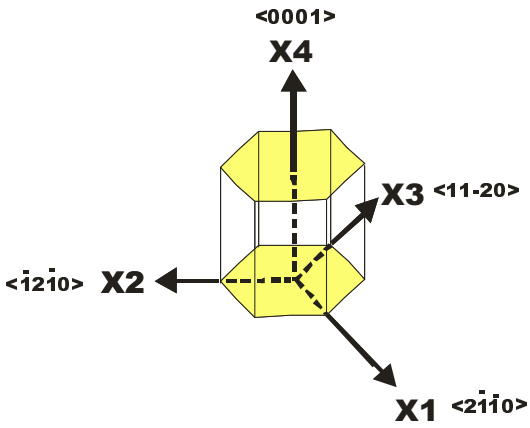


Plane in Miller Notation: {hkl}
Direction in Miller Notation <uvw>
If the direction <uvw> lies in the plane {hkl}, then:

hu + kv + lw = 0 (Weiss Zone Law – true in all crystal systems)

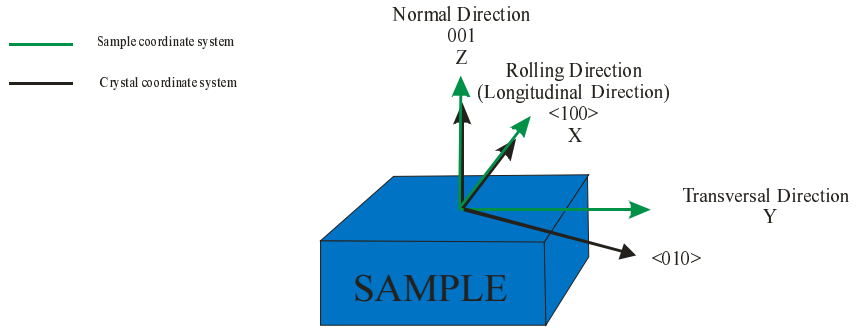
In hexagonal system <uvw> direction in Miller Notation is not perpendicular to {uvw}plane as in cubic system.
For example: the {100} plane is perpendicular to direction <210> (not <100> as in cubic system).

2) Miller-Bravais Notation (4 Axis Notation)



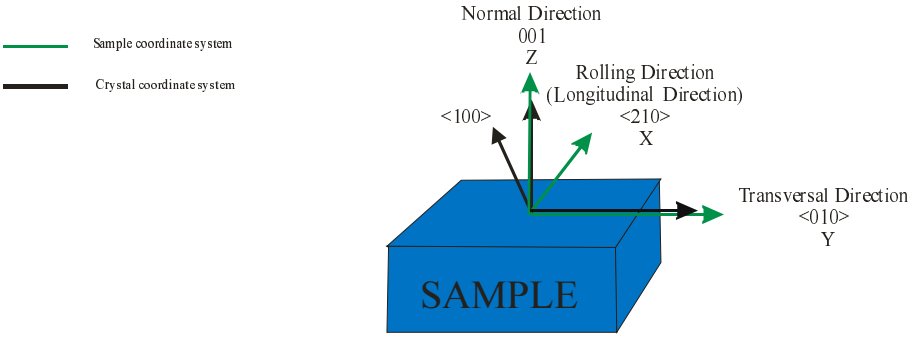
Plane in Miller-Bravais Notation: {HKTL}
Direction in Miller-Bravais Notation <UVTW>
T=-(H+K) (redundant information)
<UVTW> direction in Miller-Bravais Notation is perpendicular to {UVTW} plane (similar as in Miller Notation in cubic system).

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 Axis Definition
Euler Angles (0,0,0)

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:

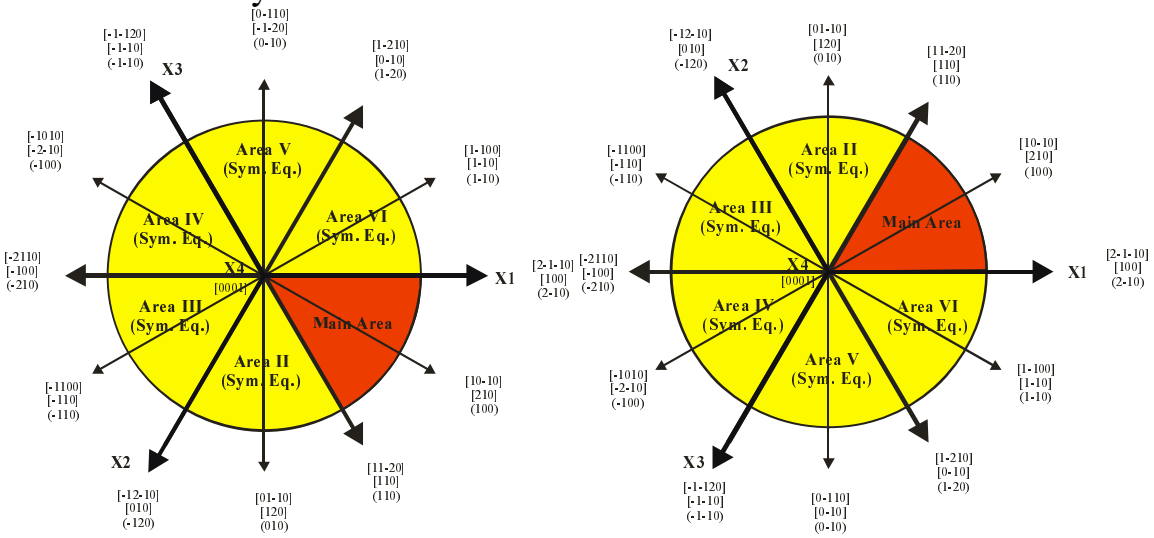


Sample Axis Definition
Euler Angles (0,0,0)

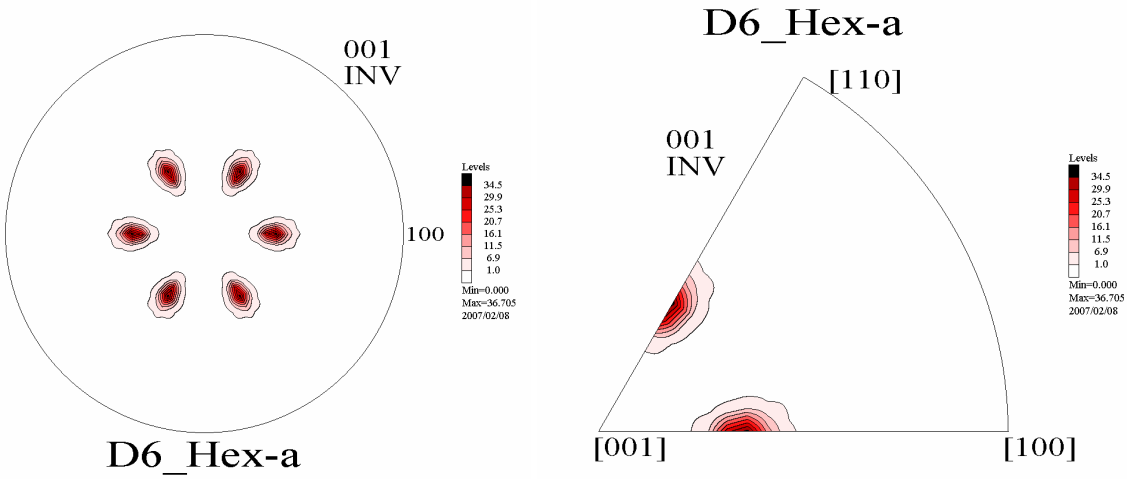
More information about both systems and about conversion of indices you can find in manual: "*Hexagonal Axes: Convention & Conversion*" (www.labotex.com).

The LaboTex displays complete and partial inverse pole figures in hexagonal system. 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:



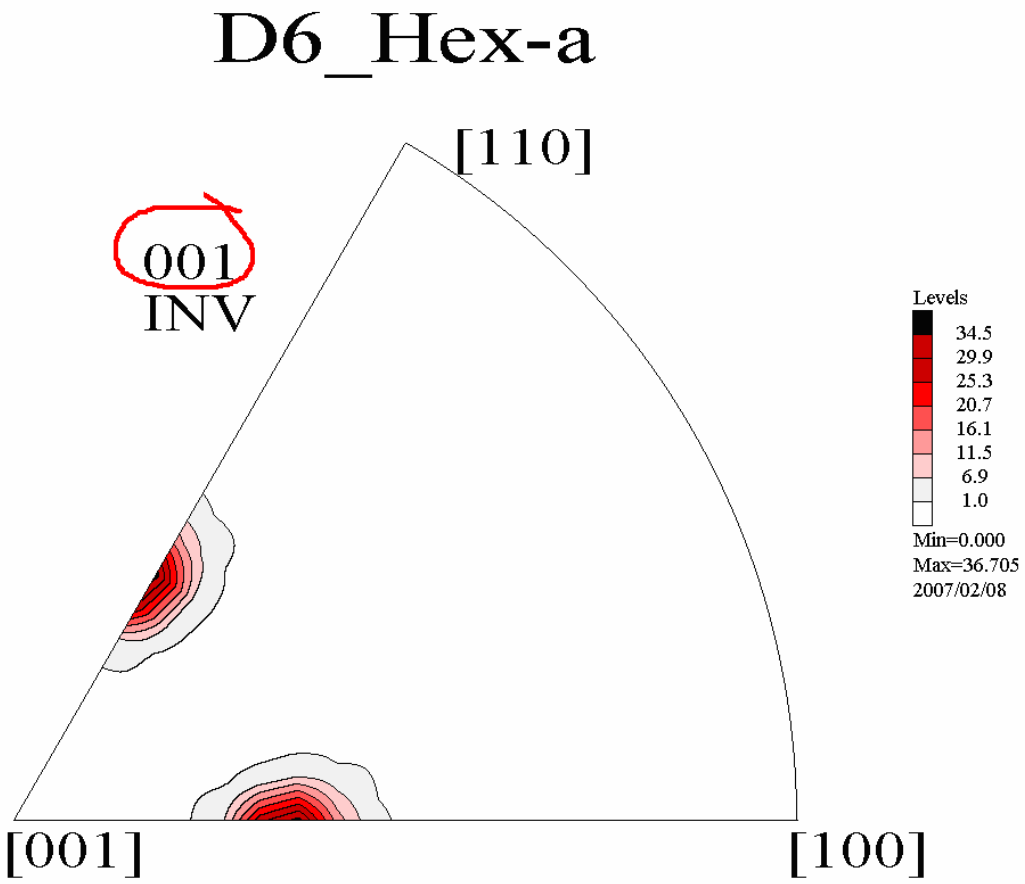
Below you can see examples of complete (full) and partial inverse pole figures for hexagonal crystal system (example calculated for strong component {-124}<210>, c/a=1.6 with FWHM 10 degrees):



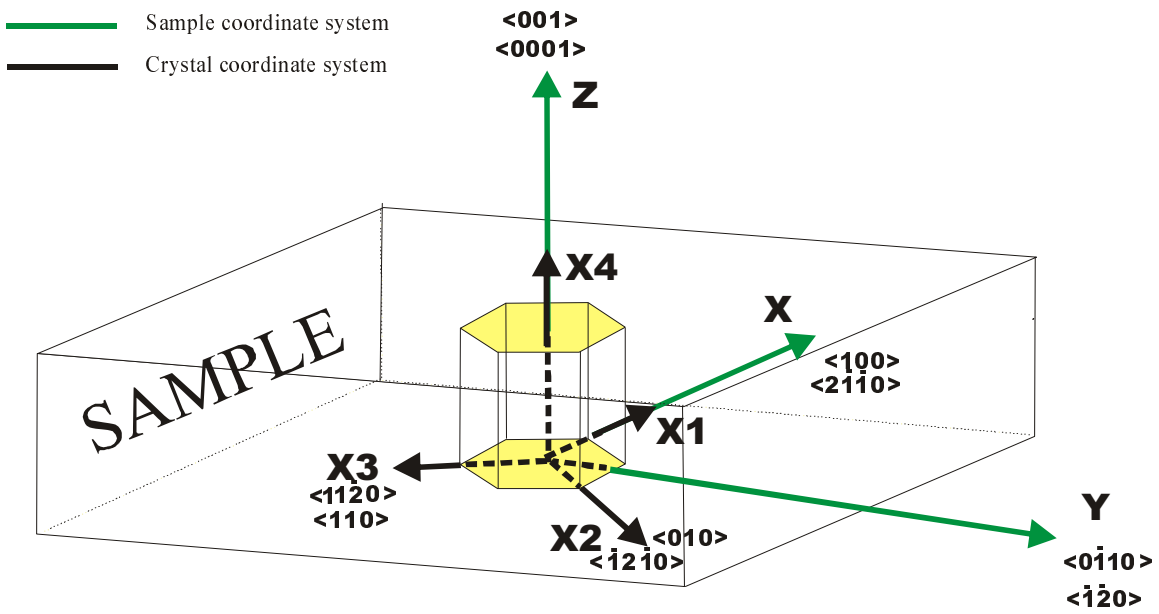
In some works the unit triangle is presented in smaller region than presented above i.e. only 30 degrees instead 60 degrees

LaboTex calculates main inverse pole figures (001),(100) and (010) for hexagonal system 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 on the partial inverse pole figure of hexagonal system in the left side of inverse pole figure (it is marked red line):

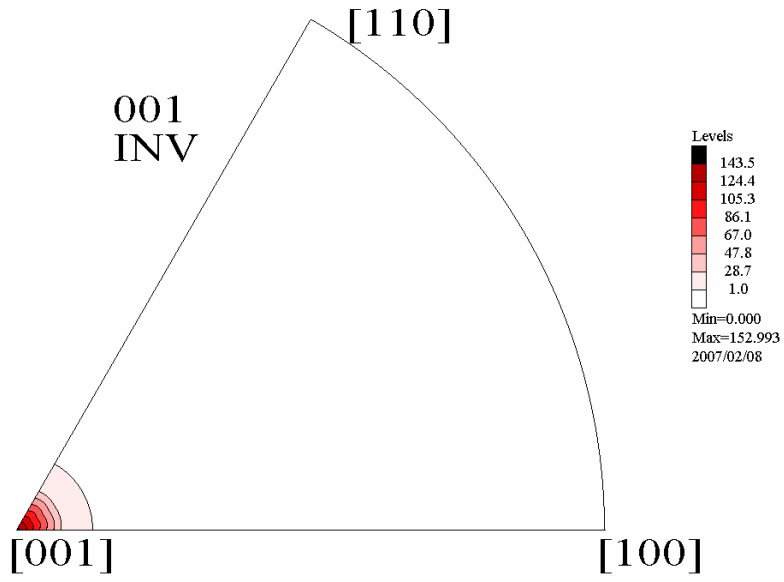


Intensity of inverse pole figure depend on numbers of crystal planes {hkl} perpendicular to chosen sample direction (<XYZ>). On the inverse pole figure the plane is represented by direction perpendicular for this plane (Warning: please remember during analysis that in hexagonal system the plane and the direction have the same indices in Miller-Bravais notation. In three indices notation - Miller notation - plane and direction perpendicular to this plane have usually different indices). 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) .

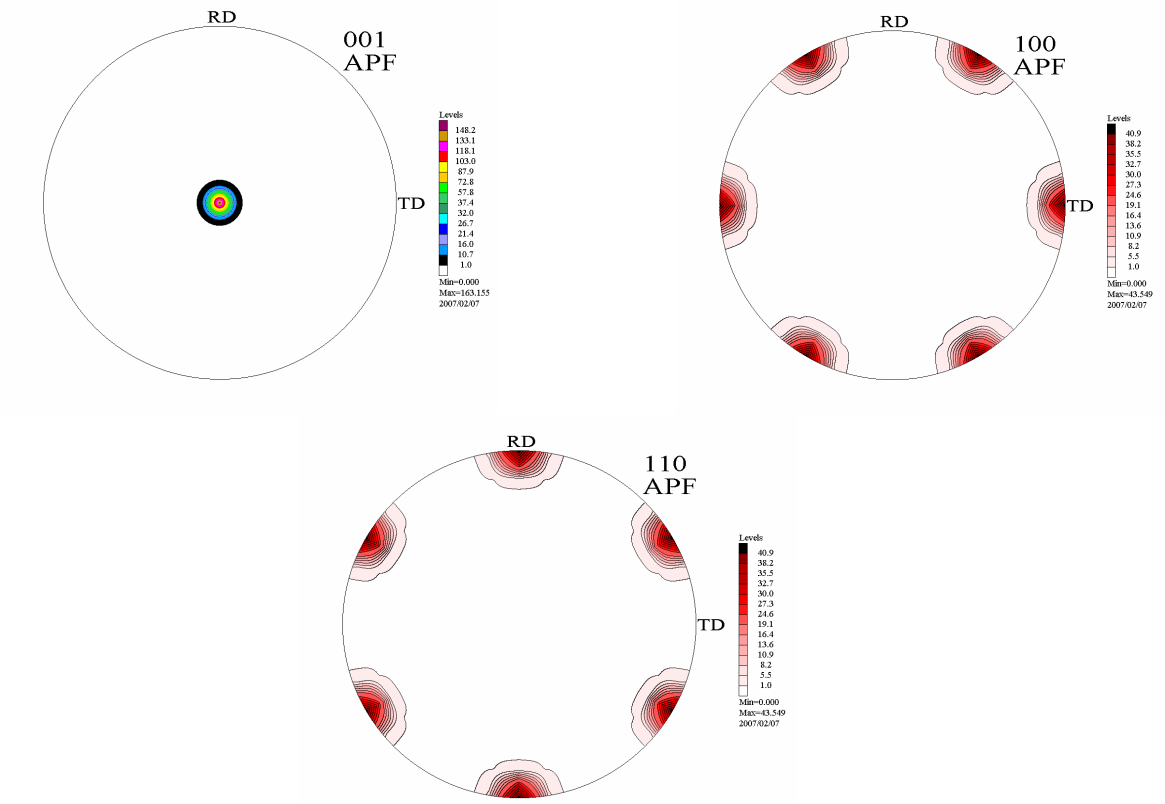


Orientation {001}<100>

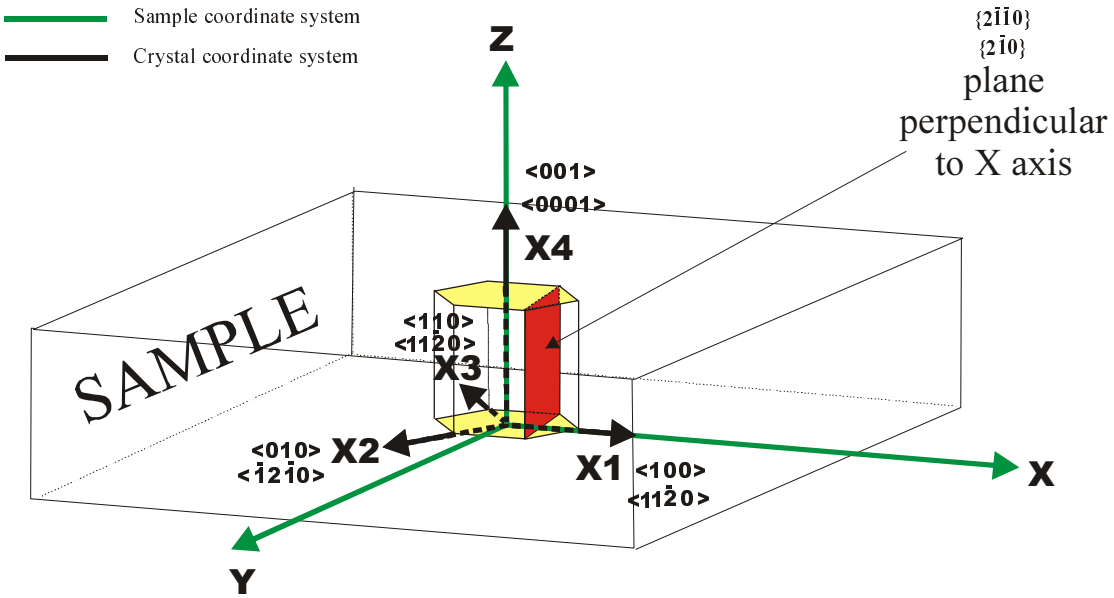
Below, you can see this maximum on the inverse pole figure which were calculated for model which have 100% volume fraction of {001}<100> component and FWHM equal 10 degrees:



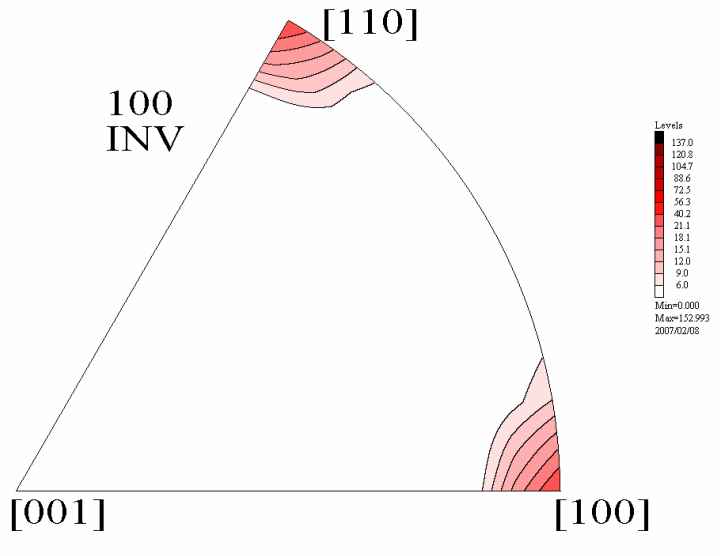
Pole figures (001), (100) and (110) for orientation {001}<100> show position of basal planes {0001}, first order prism planes {10-10} and second order prism planes {2-1-10}:



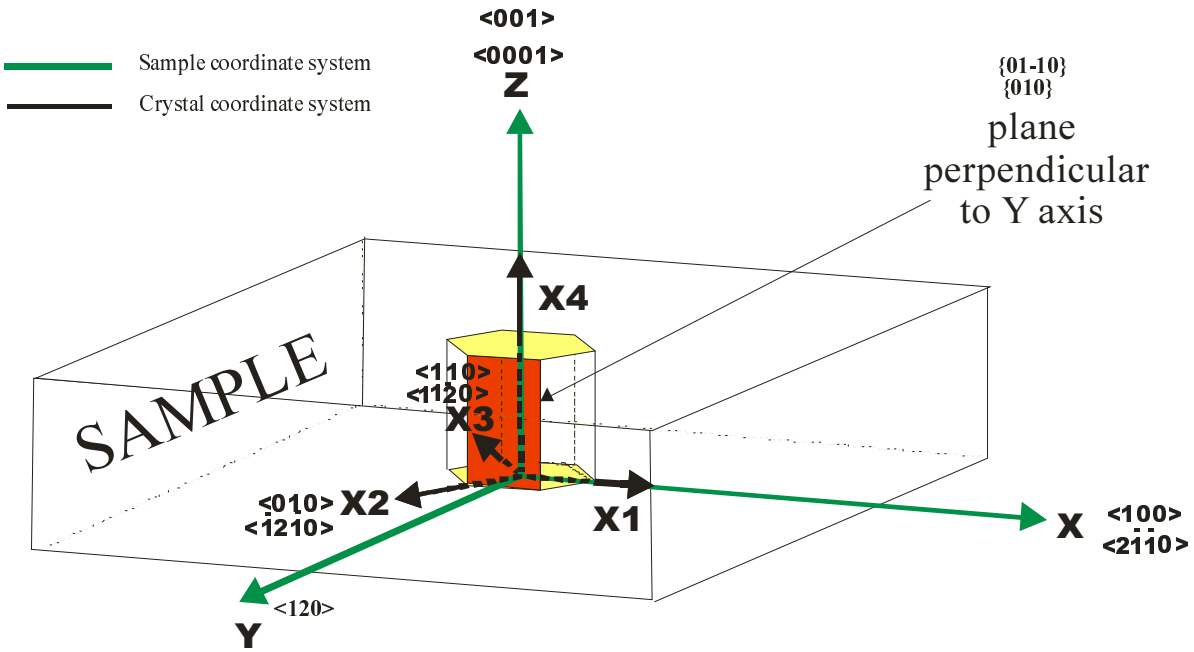
In case of inverse pole figures for RD and TD directions (XYZ=<100> and XYZ=<010>) we can observe the different positions of maximum for orientation {001}<100>. The plane perpendicular to X axis is {2-1-10}:



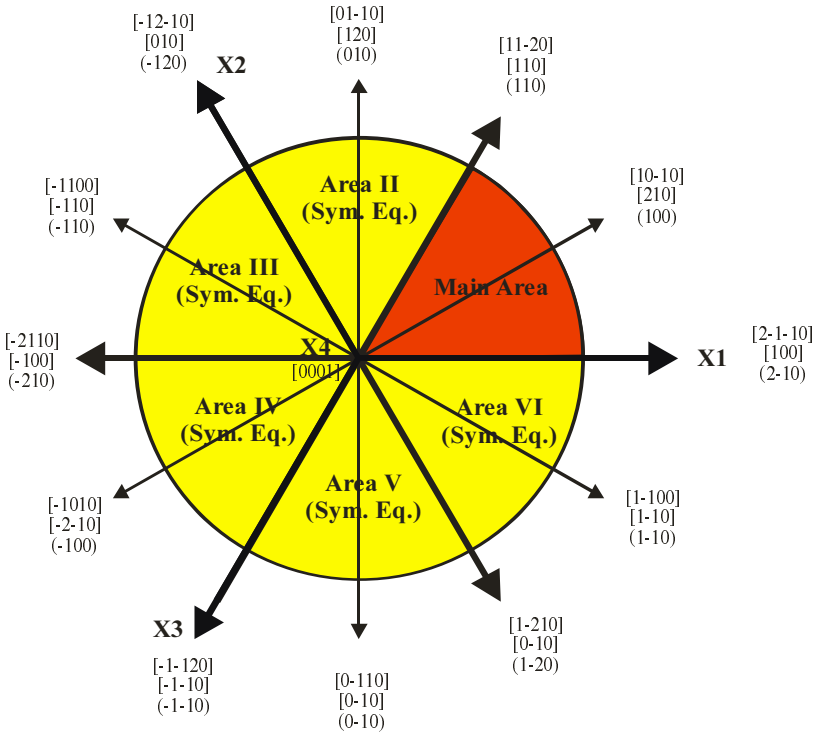
hence the maximum intensity is observed for direction equal [100] as also on symmetrically equivalent direction [110]:



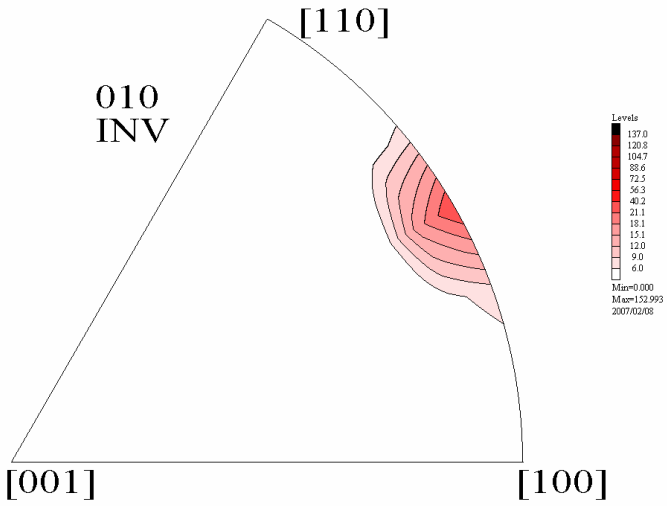
Below you can see that when you choose Y (i.e. (010) or TD) direction for inverse pole figure then the planes type {010}(the plane (010) is marked on the red in the figure) is perpendicular to this direction for orientation {001}<100>.



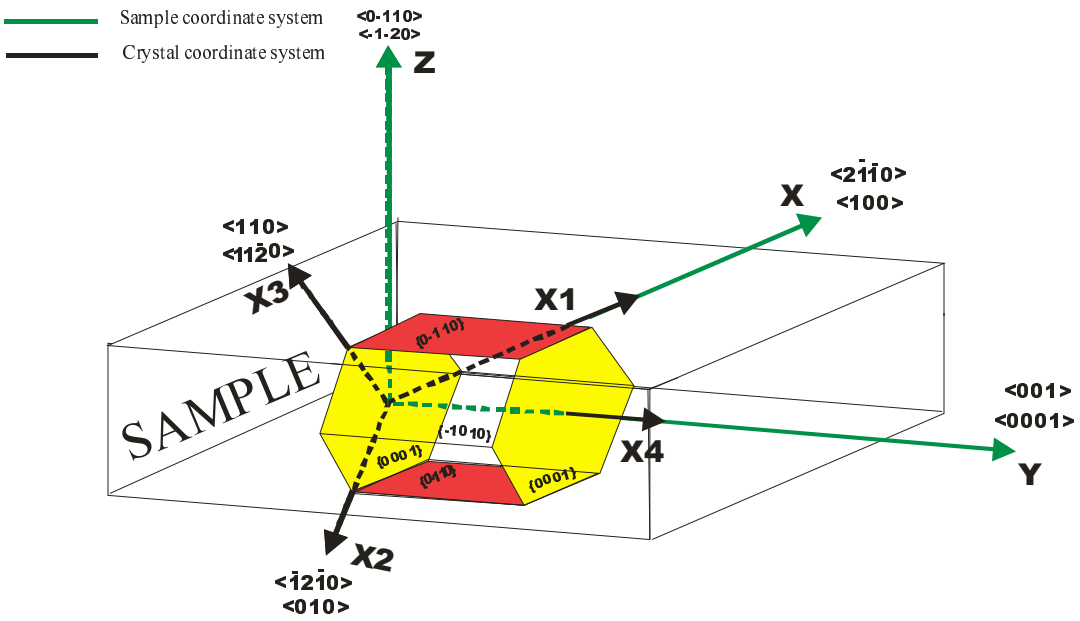
The perpendicular direction <120> will represent this plane on the inverse pole figure. Because direction <120> doesn't belong to the unit triangle (main, fundamental area) the equivalent direction <210> from unit triangle is chosen:



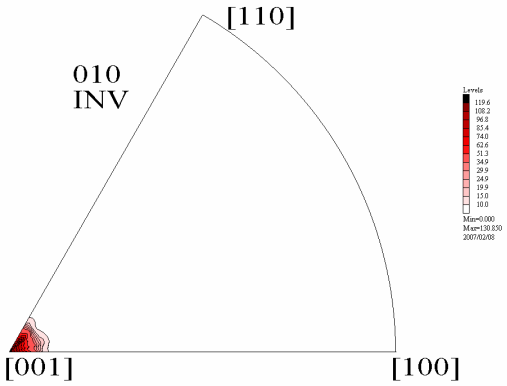
Below you can see the inverse pole figure for TD direction with maximum for direction <210> (<10-10>) determined the planes: {100} or {10-10}.



In case of orientation {0-10}<100> which is shown on the figure below

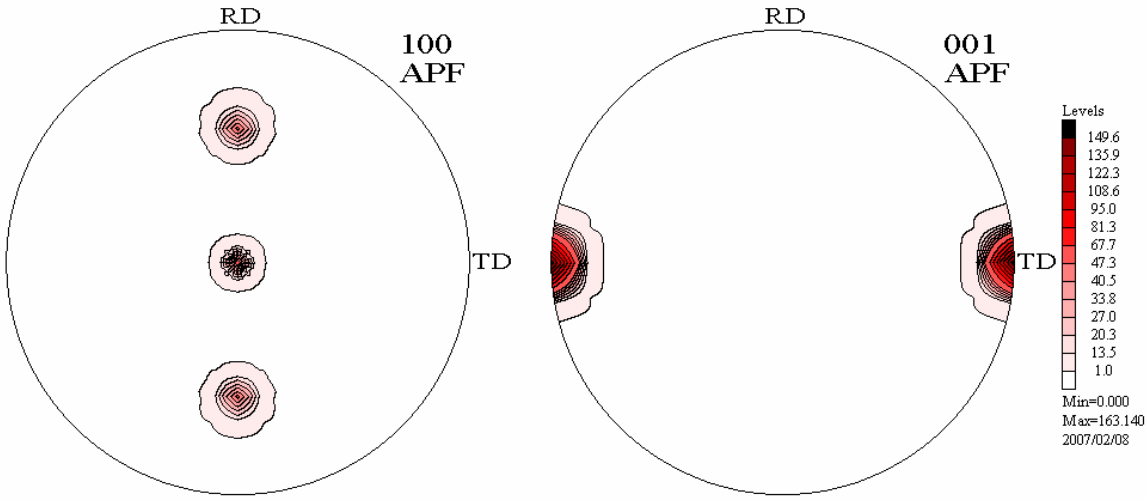


the basal planes are perpendicular to TD (Y) direction hence in this case the inverse pole figure calculated for this direction shows maximum for <001> direction:



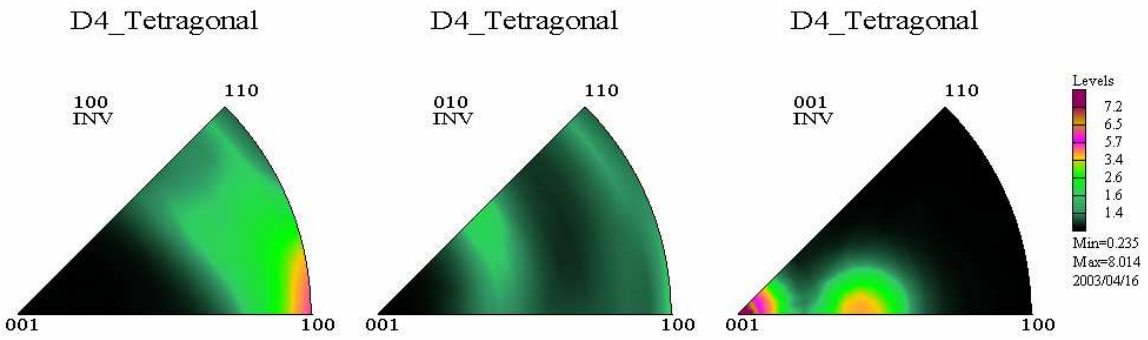
Inverse pole figure calculated for direction TD
(Model of component {0-10}<100>, FWHM 10 degrees)

Below you can see the pole figures {100} and {001} calculated for model model of component *{0-10}<100>*

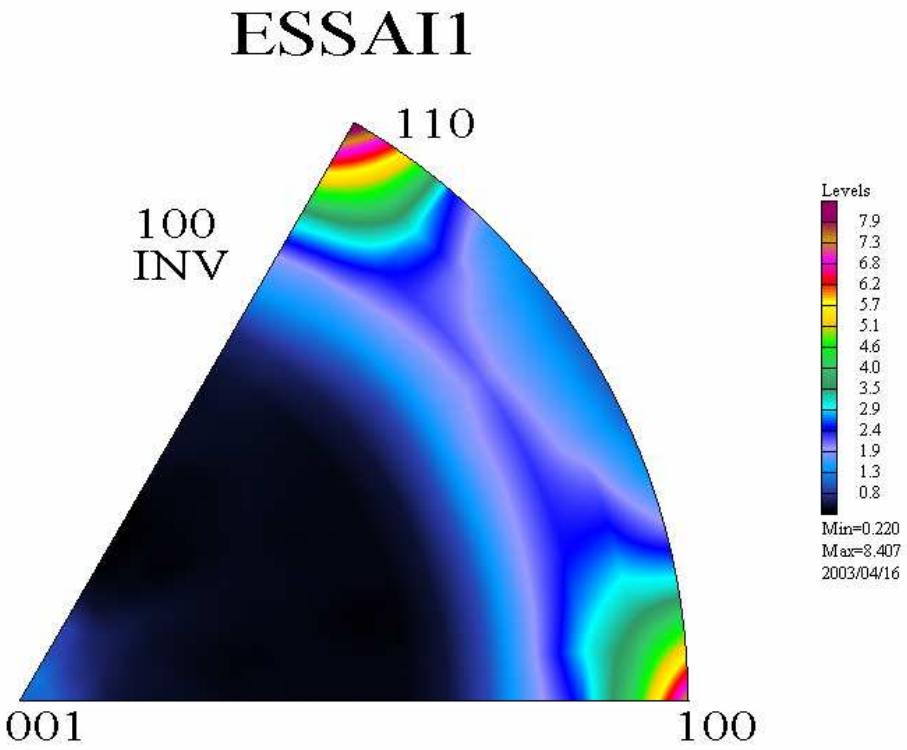


Please remember that orientation noted by Miller indices when is expressed by Euler angles has different notation for each hexagonal axes convention.
For example orientation {0-10}<100> is equivalent orientation {0,90,0} in the first convention and {0,90,30} in the second hexagonal axes convention. Pole 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.

Examples for other Systems

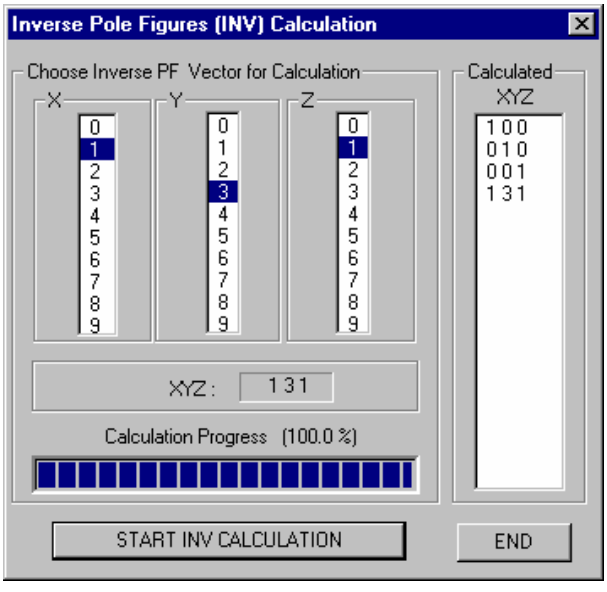


Example of the Partial Inverse Pole Figures for Tetragonal System (distribution of 100/RD, 010/TD and 001/ND sample axis).



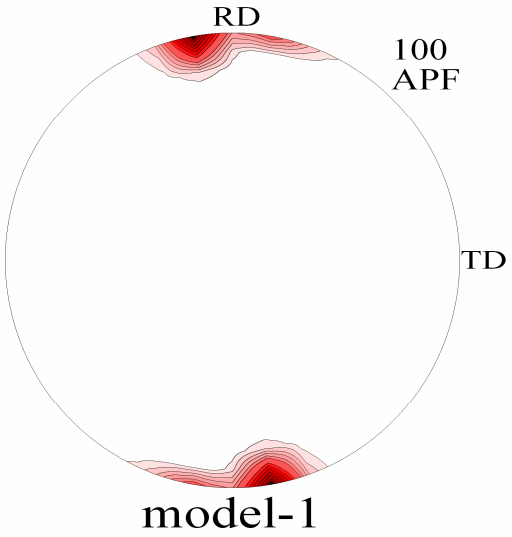
Example of the Partial Inverse Pole Figures for Trigonal System (distribution of 100/RD axis).

LaboTex calculates Inverse Pole Figure 100, 010 and 001 during ODF calculation. User can calculate IPF for other direction (XYZ) using dialog window (click mouse on the icon)



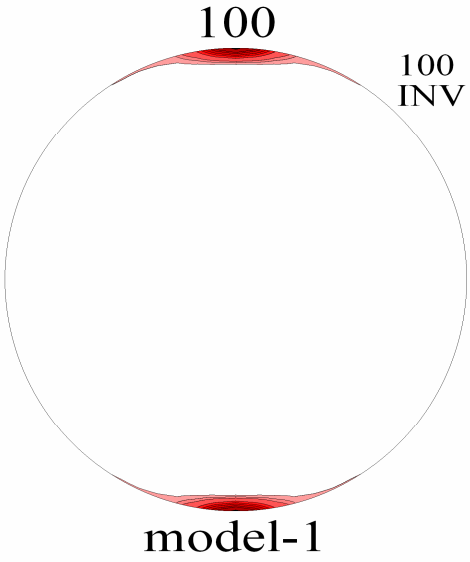
Warning: LaboTex calculate XYZ IPF for integer X,Y, Z in the range 0 to 9.

In case of crystal symmetry lower than cubic is important proper denotation of axis in the inverse pole figure plot. You also should input parameters of cell in proper manner (details you can find in manual: “Pole Figues: Registration and Plot Conventions”). You can check correctness of axis denotation. Please prepare model for symmetry in which you want work (LaboTex-->Menu-->Modelling--->Model ODF). Let in this model pole figure {100} has maximum in RD/L direction (build pole figure from ODF using LaboTex-->Menu-->Calculation--->ODF to APF). Next build from model ODF inverse pole figure for XYZ = 100 (inverse pole figure for RD/L direction) (LaboTex-->Menu-->Calculation--->ODF to INV).

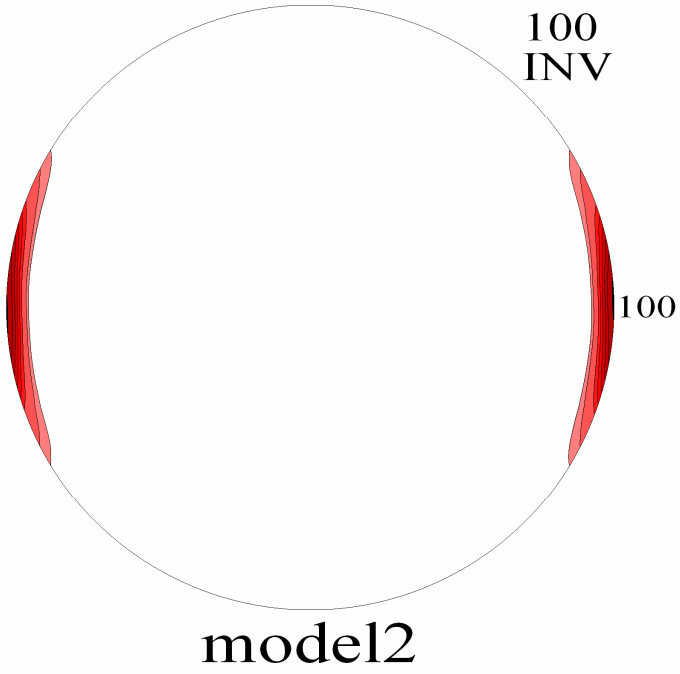


Pole figure {100} with maximum around {RD/L} direction.

In the case when maximum in the inverse pole figure {100} is in top of pole figure you should write (Menu Edit-->LaboTex options) denotation of crystallographic axis ‘100’ to editbox ‘Y’ :



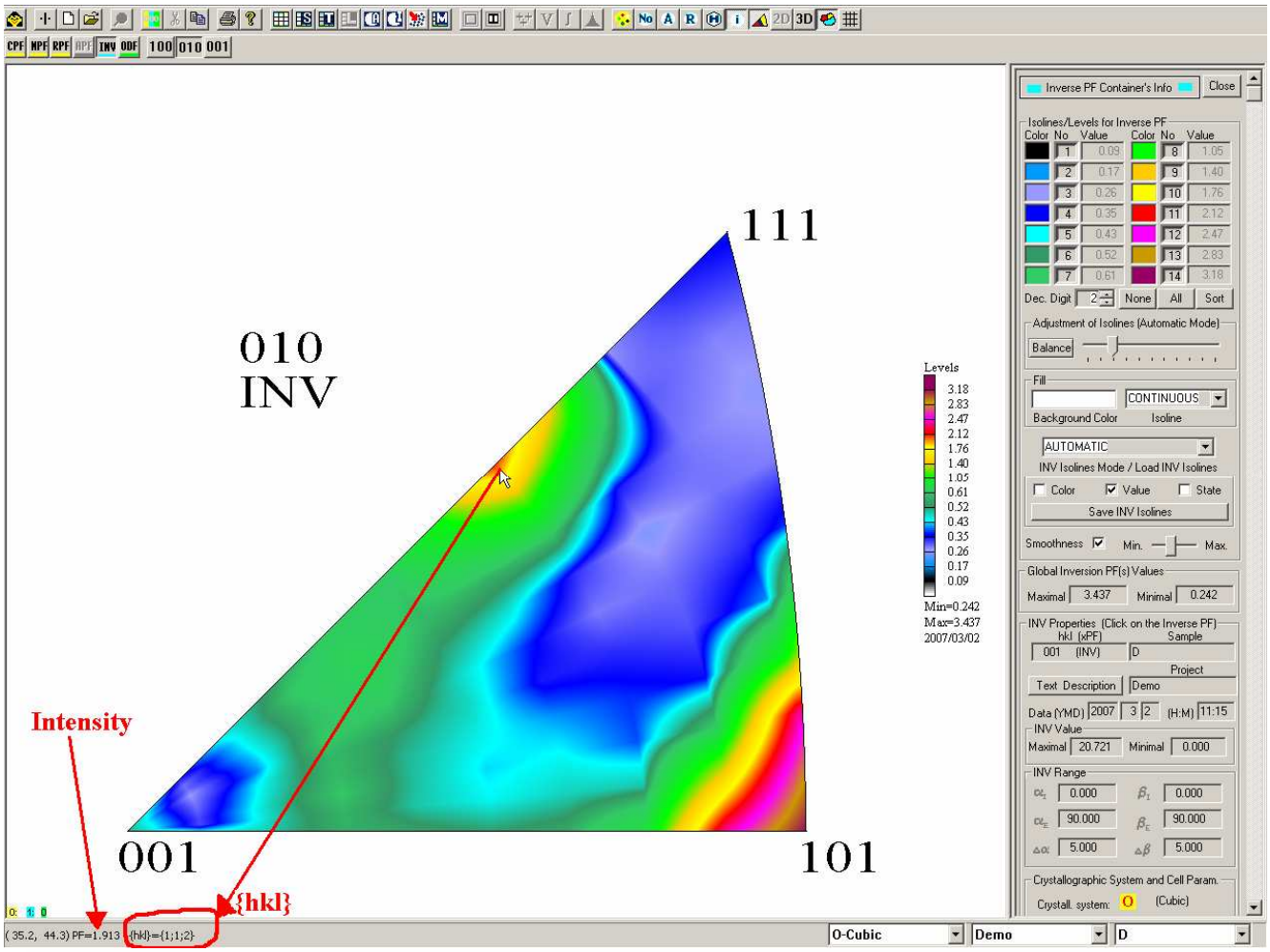
When maximum is from left side of pole figure then you should write denotation ‘100’ to editbox ‘X’ :



Analysis of inverse pole figures in LaboTex

You can analyze inverse pole figures using cursor. LaboTex displays on the left side of ‘Status Bar’ intensity of inverse pole figure in position of cursor. It also displays {hkl} of plane in cursor position and values of angles. In case of hexagonal and trigonal crystal systems LaboTex use Miller-Bravais indices: {hkil}. LaboTex shows proper {hkl} indices if you introduce cell parameters and indices of pole figures to ODF calculation in convention described in manual: “Pole figures: registration and plot conventions”. Position of plane on the inverse pole figure is depend on cell parameters for crystal symmetry lower than Cubic. LaboTex shows {hkl} or {hkil} for indices up to maximal value equal 15. You can decrease this value using dialog ‘Max. Value of Miller Indice’ from menu ‘Analysis’.

Below you can see example of partial inverse pole figure for Cubic C.S. and 'Status Bar' with information about intensity of inverse pole figure in position of cursor (close to local maximum) and information about hkl of planes which lies in position indicates by cursor (i.e. {112} in this example).



Below you can see change of the position of planes {21-34} on the inverse pole figures for samples with different cell parameters (Hexagonal Crystal System).