A description of Pan v. 1.979

August 31, 2015

Pan is a simple program for manipulating parameters of crystal(lite) orientations and analyzing the so-called orientation relationships. It is mainly intended for solving very simple problems in analysis of crystallographic textures. The direct access to crystallographic indices of planes and directions allows for analysis of geometry of phase transformations, crystal slip systems, slip transfer across interfaces, twinning systems, crystal interfaces et cetera. Pan can also be used for relating Miller indices corresponding to
– different conventions for reference frames (e.g, hexagonal vs. rhombohedral, three- vs. four-index),
– different conventions for the 'zero' orientation (e.g., $\mathbf{a} \parallel \mathbf{e}_x$ vs. $\mathbf{b} \parallel \mathbf{e}_y$ in the hexagonal case).

To run the program, the screen resolution needs to be set to '96 DPI' or 'small text'.[1]

Pan is a tool for composition of *proper* rotations with the capability of representing results in the form of crystallographic indices.[2] The user interface of the program consists of two main windows: Pan – Orientation calculator and Pan – OR (Orientation Relationship). Below, they are briefly referred to as 'OC' and 'OR'. Data (orientations or misorientations) are passed between 'OC' and 'OR' using right click on `Apply` buttons.

Lattices
The first step of every analysis is to provide crystal point symmetries and parameters of crystal lattices. The two lattices of the crystals can be specified by clicking on the buttons `C1` and `C2/S` in 'OR'. The window 'Lattice parameters' is self-explanatory; one needs to provide Cartesian components of (direct lattice) basis vectors **a**, **b** and **c**.

Miller indices ('OR' window)
The 'OR' window (with Miller indices) is designed to determine crystallographic plane and direction in crystal no. 1 (upper frame) parallel to a given crystallographic plane and direction in crystal no. 2 (lower frame).
After modifying the indices in the lower frame, the user should click on `Apply` to get the corresponding data in the upper frame for the current (mis)orientation. BY default, the current (mis)orientation is the zero (mis)orientation. It can be changed using the other ('OC') window: right click on `Apply`in the 'OC' window transfers the rotation specified in 'OC' to 'OR'.
Right click on `Apply` in the 'OR' window shows (in the 'OC' window) the parameters of the (best) rotation relating the planes and directions displayed in 'OR'.
Only the indices in the lower frame of 'OR' can be changed by the user. If the upper frame needs to be modified, click on `Swap`, to swap the lattices.
The 'OR' window can also be used to get a crystallographic plane and direction in crystal no. 1 which are parallel to some plane and direction in the *sample* coordinate system. [Typically, the sample coordinate system will be Cartesian, no symmetry will be assumed (the *a* lattice type), the plane will be the 'rolling' plane (001), and the direction will be the 'rolling' direction [100]. Clearly, other options (like higher sample symmetry, or other planes and directions) are allowed.]

(Mis)orientation ('OC' window)
If certain indices are specified in both frames in 'OR', one can calculate the rotation transforming the vectors corresponding to the data of the lower frame to a position best matching the vectors corresponding to the data of the upper frame. As was mentioned above, that rotation is obtained by right click on `Apply` in 'OR'. This shows the rotation parameters in the 'OC' window.
The calculator works similarly to the old version Pan 1.1, except that the rotation axis in `AXIS + ANGLE` is opposite to that of Pan 1.1. The other important difference is that, after selecting certain parameters, if you want to see the corresponding representation in the form of Miller indices in the

[1] Windows XP, 2000: right-click the Windows desktop → Properties → Settings (tab) → Advanced (button) → General (tab) → 96 DPI in a list in the Display area; restart your computer to allow the changes to take effect. Windows 7-8: Screen Resolution → Make text and other items larger or smaller.

[2] In the case of enantiomorphic crystals and, generally, crystals without center of inversion, the user must keep track of improper rotations (e.g., using the property that the transformation by a mirror plane is a composition of inversion and a half-turn about the axis perpendicular to the plane) and the handedness of transformed coordinate systems. For crystals having inversion in their point groups, each improper rotation is equivalent to some proper rotation.

'OR' window, you need to use right-click on `Apply` in the 'OC' window. This fixes the (mis)orientation in 'OR', i.e., in all further steps in 'OR', this (mis)orientation will be used, until it is replaced by a different one by right-click on `Apply` in the 'OC' window.
The calculator does not assume symmetry, unless one or both check-boxes in 'OC' are checked.

Symbols and shortcuts

A. Focus on the 'OR' window
`Apply` right click – update rotation parameters in the 'OC' window
Ctrl + a = `Apply`.
Ctrl + d = `Apply` right click.
Ctrl + s = `Swap`.
Ctrl + i – save the current lattices in the file 'Pan.ini'. If this file exists, each time the program is executed, it will load the lattices from 'Pan.ini'.
The symbol $\vdash$ indicates that the direction `[uvw]` (`[uvtw]`) is in the plane `(hkl)` (`(hkil)`).
Shift + v = click on $\vdash$ in the upper frame = perpendicularity.
Ctrl + v = switch perpendicularity check-box.
Click on `(hkl)` (`(hkil)`) or `[uvw]` (`[uvtw]`) to get inter-planar spacing or magnitude of the (direct lattice) vector, respectively; they are shown in 'OC'.

B. Focus on the 'OC' window
Memory frame:
`MS` – Save in Memory as the next item.
`MR` – Recall selected item from Memory.
`MC` – Clear selected item from Memory.
`AC` – Clear All memory.
`S` – save memory in the file 'Pan.dat'.
`S` right click – save only Euler angles
`L` left click = `AC` + load memory file 'Pan.dat'.
`L` right click – append memory by data from the file 'Pan.dat',
Click on item in the list to mark an item. Double click on item in the list = `MR`.

`Clear` left click – clear parameter text boxes of 'OC' window.
`Clear` right click – clear everything in 'OC' window.
`R` left click – a random orientation.
`R` right click – a random orientation + `Smallest angle`.
`Apply` right click – updates Miller indices in the 'OR' window.
Right click on symmetry check-boxes – show the window with lattice parameters.

`< >` – ascribe the symmetry of a crystal to the other crystal (indicated by `===>` or `<===`).
`Smallest angle` – calculate parameters of a symmetrically equivalent rotation with the smallest rotation angle, and then with the largest n_1, and then with the largest n_2, and then with the largest n_3, where n_i are the Cartesian components of the rotation axis (in `AXIS + ANGLE`).
`All equivalent` – save (append to memory) parameters of all rotations symmetrically equivalent to the displayed rotation.
Double-click in the parameter frame (e.g., somewhere between the last Euler angle (φ_2) and `R`) to create/use lists of handy rotations. As the data are saved in the format of 'OC', the user is responsible for keeping the conventions of the reference frames right. Pre-defined lists can be restored by double-click on `1*`, `2*` or `3*`.

Ctrl + a = `Apply`
Ctrl + d = `Apply` right click
Ctrl + m = `Matrix/Parameters`
Ctrl + i = `Inverse`
Ctrl + s = `MS`
Ctrl + x = `AC`
Ctrl + r = `MR`
Ctrl + q = `Exit`
Shift + i = change the convention for the sign of the rotation axis in `Axis + angle`.

Shift + h = show history.
Shift + v = recording of programs (to be saved in 'Pan.rec').
Shift + s = saves history (in 'Pan.hst') or program (in 'Pan.rec').
Shift + x = clears the history or recording frame.
Shift + w – (un)link screen position of 'OR' (from) to that of 'OC', or change the distance between windows.

C. Focus on Lattice Parameters
Ctrl + i – shows corresponding point groups with inversion.

Graphic visualization
In order to get the window with graphic visualization of the orientation relationship, click on the graphic button in the 'OR' window. The figures show projections of some characteristic directions and planes for the crystallite `C1` (upper figure) and the reference system `C2/S` (lower figure). It must be stressed that these are *not* pole figures; a point represents a crystal direction not a crystal plane.
Shift + s changes the size of the window.
Shift + p switches between stereographic and equal-area projections.
Ctrl + s saves the picture as 'Pan.bmp'.
Ctrl + l loads 'Pan.bmp' as a background.
When initially called, the current (mis)orientation of 'OR' and planes and directions specified in 'OR' are displayed. Subsequent calls from 'OR', when the window with projections is visible, do not modify the (mis)orientation but update the Miller indices.
The orientations can be passed from (to) 'OC' by left (right) click on `< >` command buttons.
Click on the circle in the upper left corner to switch between the complete sphere and the upper hemisphere.
Move the mouse over the projection to see Miller indices of indicated directions; this applies to the upper hemisphere and shows indices in the rotated frame. In order to see the indices on the lower hemisphere, move the mouse with the right button pressed. In order to see the indices in the reference frame, move the mouse with the 'Ctrl' key pressed.
Click on the squares in the lower right corner to rotate the reference frames. Click on the bar below the squares to change the rotation step size; the possible steps are 10, 5, 2, 1, 0.5 and 0.1°. Press the 'Shift' key and left (right) click on one of the projections to indicate a rotation axis in the upper (lower) hemisphere. To remove the axis press the 'Shift' key and click outside the projection. The rotations in upper and lower figures are coupled when the box in the right-lower corner is checked.
Check-boxes on the right side allow for showing/hiding particular elements of the figure (the default colors are given in parentheses):
1. the external circle and the central disk (black),
2. the grid (light gray),
3. the directions of the basis vectors $\mathbf{e}_x$, $\mathbf{e}_y$ and $\mathbf{e}_z$ of the Cartesian frame plus fragments of the planes between these vectors (dark gray),
4. the directions of the lattice basis vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ (and $-(\mathbf{a}+\mathbf{b})$ in the hexagonal case) plus fragments of the planes between these vectors (green),
5. the plane and direction indicated in the text-boxes of the 'OR' window (red),
6. directions toward the corners of the unit cell plus fragments of the planes between some of these vectors (blue),
7. directions symmetrically equivalent to that indicated in the text-boxes of the 'OR' window (brown),
8. planes symmetrically equivalent to that indicated in the text-boxes of the 'OR' window (brown).

Creating Pan programs
Pan programs use data saved in the memory box. In these programs, `MC` must always be in a separate loop containing nothing else. The use of buttons of the 'OR' window is limited to right click on `Apply`. The lists of predefined rotations cannot be used.

Reporting bugs
Bugs, ideas, questions, comments: nmmorawi@cyf-kr.edu.pl.