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```
% CORRECTION_SAMPLE_MISALIGNMENT Correcting for sample misalignments in Horace
%
% Corrections of the sample mis-alignments and lattice parameter
% refinement. (from the script on the Horace website )
% To be done after the creation of the .sqw file
%
% 1) Check which Bragg peak to deal with (in 3 directions)
% 2) Once the notional Braggs are defined, refine the Braggs
% 3) Compute the corrections
% 4) Apply corrections to the .sqw file
%
clear, close all
```

## Parameters to enter

```
sqw_file = 'spe/Alcur_155K.sqw'; % .sqw file to correct
% projection axes
proj.u = [1,1,0];
proj.v = [0,0,1];
proj.type = 'rrr';
proj.uoffset = [0,0,0,0];
% Lattice parameters
alatt = [8.22,8.22, 11.02];
angdeg = [90,90,120];
```

## Look for Braggs

```
%Make a series slices in order to work out what Bragg positions we have.
dQ = 0.025;
H = 0; dH = dQ;
K = 0; dK = dQ;
L = 0; dL = dQ;
E = 0; dE = 0.125;
alignment_slice1=cut_sqw(sqw_file,proj, dH, dK,[L-dL, L+dL],[E-dE, E+dE],'-nopix');
alignment_slice2=cut_sqw(sqw_file,proj, [H-dH, H+dH], dK,dL,[E-dE, E+dE],'-nopix');
alignment_slice3=cut_sqw(sqw_file,proj, dH, [K-dK, K+dK],dL,[E-dE, E+dE],'-nopix');

plot(compact(alignment_slice1)); keep_figure; lc 0 1
plot(compact(alignment_slice2)); keep_figure; lc 0 1
plot(compact(alignment_slice3)); keep_figure; lc 0 1
```

## Define notional Bragg peaks

Notional Bragg peaks = rlu

```
bp=[1,1,0; 2,2,0; 0,0,6; 1,1,2; 1,1,-2];
```

## Refine the Bragg peak positions

```

%Get true Bragg peak positions

% longitudinal extend, bin width, thickness
% transversal extend, bin width, thickness
% dE
%
% longitudinal cuts:
% w1 = cut_sqw(sqw_file, proj, [-longit. extend/2, longit. bin, lomngit. extend/2], ...
%                               [-transverse thick, transverse bin, +transverse thick], ...
%                               [-transverse thick, transverse bin, +transverse thick], [-dE,
+dE], '-nopix');
%
% transverse cuts:
% wt1= cut_sqw(sqw_file, proj, [-longit. thick/2,+longit. thick/2], ...
%                               [-trans. extend/2, trans. bin,+trans. extend/2], ...
%                               [-trans. thick/2,+trans. thick/2], [-dE, +dE], '-nopix');
%
% wt2= cut_sqw(sqw_file, proj, [-longit. thick/2,+longit. thick/2], ...
%                               [-trans. thick/2,+trans. thick/2], [-dE, +dE], ...
%                               [-trans. extend/2, trans. bin,+trans. extend/2], '-nopix');
%
%
[rlu0,~,wcut,wpeak]=bragg_positions(sqw_file, bp, ...
    -0.5, 0.0125, 0.25,...
    0.5, 0.0125, 0.25, 0.1, 'gauss','bin_ab');

%Check how well the function did:
bragg_positions_view(wcut,wpeak)

```

```

-----
Peak 1:  [1  1  0]    scan: 1 (radial scan)
-----
Peak 1:  [1  1  0]    scan: 2 (transverse scan)
-----
Peak 1:  [1  1  0]    scan: 3 (transverse scan)
-----
Peak 2:  [2  2  0]    scan: 1 (radial scan)
-----
Peak 2:  [2  2  0]    scan: 2 (transverse scan)
-----
Peak 2:  [2  2  0]    scan: 3 (transverse scan)
-----
Peak 3:  [0  0  6]    scan: 1 (radial scan)
-----
Peak 3:  [0  0  6]    scan: 2 (transverse scan)
-----
Peak 3:  [0  0  6]    scan: 3 (transverse scan)
-----
Peak 4:  [1  1  2]    scan: 1 (radial scan)
-----
Peak 4:  [1  1  2]    scan: 2 (transverse scan)
-----
Peak 4:  [1  1  2]    scan: 3 (transverse scan)
-----
Peak 5:  [1  1 -2]    scan: 1 (radial scan)
-----
Peak 5:  [1  1 -2]    scan: 2 (transverse scan)
-----
Peak 5:  [1  1 -2]    scan: 3 (transverse scan)
-----

```

## Compute the corrections

```

%Determine corrections to lattice and orientation:
[rlu_corr,alatt,angdeg] = refine_crystal(rlu0, alatt, angdeg,
bp,'fix_angdeg','fix_alatt_ratio');

```

## Apply changes to sqw file

```

choice = questdlg('Apply changes to sqw file?', 'Confirm dialog', 'Ok', 'Cancel','Cancel');
if strcmp(choice,'Ok')
    change_crystal_horace(sqw_file, rlu_corr);

```

end

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