

Generating SQW file

Generate the data file in the reciprocal space of the crystal (.sqw) from the datasets in the instrument frame (.spe) using the Horace distribution in Matlab.

The .spe files being generated before using, e.g., Lamp (see create .SPE files).

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```
% -----  
%  
%   create_17K_2p0A  
%  
% -----  
horace_on()  
  
clear, close all
```

```
!=====!  
!                               !  
!           HORACE              !  
!-----!  
! Visualisation of multi-dimensional neutron spectroscopy data !  
!-----!  
! T.G.Perring, J van Duijn, R.A.Ewings      November 2008    !  
!-----!  
! Matlab code: $Revision:: 558 $ ($Date:: 2011-07-19 11:06:05 $) !  
! Mex code:   Disabled or not supported on this platform      !  
!-----!
```

Define working directories

```
% -----  
% Define working directories  
% -----  
  
% Windows  
% dirroot = '\\serdon-nv\illdata\133\in5\exp_4-01-1230\';  
% dirfinal = [dirroot,'processed\spe'];  
% dirraw = [dirroot,'rawdata'];  
  
% linux  
dirroot = '/usr/illdata/133/in5/exp_4-01-1230/';  
dirfinal = [dirroot,'processed/spe/'];  
dirraw = [dirroot,'rawdata/'];  
  
indir = dirfinal; % directory of spe files  
par_file = [dirfinal,'in5psd_318_384_240.par']; % detector parameter file  
sqw_file = [dirfinal,'tmo_2p0A_17K.sqw']; % output sqw file
```

Initial parameters

```
Lambda = 2.0; % Wavelength [A]  
efix = 81.805/Lambda^2 ; % Ei [meV]  
emode = 1; % Direct geometry (2: inverse)  
alatt = [5.297, 5.831, 7.403]; % Crystal parameters (from literature)  
angdeg = [90.0,90.0,90.0];  
u = [0,1,0]; % 1st reference axis: u=// to incident beam  
v = [0,0,1]; % 2nd reference axis: v=perp to incident beam  
omega=0;dpsi=0; % Unuseful (?)  
gl=2.37; % Estimated from the Braggs at level  
gs=1.003; % ---  
% Or left to zero and orientation corrected on .SQW files later  
% (see horace_rotation_corrections).
```

Sample rotation offset

$\Omega = \Omega_0$ when K_i is parallel to the first reference axis (u)

```
% -----  
% Sample rotation offset (determined from Braggs positions)  
% -----  
Offset = 250.32 - 180.0;
```

Proceed

Give all sample rotation angles (as measured) and corresponding .spe files (generated in Lamp at present). Sort them (not compulsory), check Ω with the angle recorded in the raw datafiles and proceed to the projection in crystal reciprocal space (generate .sqw file).

```
% Sample rotation angles as given from the measurements  
Omega = [240:-2:234,232:-2:120,121:2:139,141:2:233]';  
% Run numbers corresponding to the sample rotation  
irun = [110017:110020,110023:110079,110080:110089,110091:110137]';  
[Omega, ind] = sort(Omega);  
  
% Sample rotation without offset  
psi = Offset - Omega;  
  
irun = irun(ind);  
nfiles = numel(irun);  
spe_file = cell(1,nfiles);  
  
% Cell matrix of spe files to use  
for k=1:nfiles  
    spe_file{k}=[indir,'sqw_',num2str(irun(k,1)),'_',num2str(irun(k,1)),'_318_384_240.spe'];  
end  
  
% Check consistency (compare the sample rotation angle with the value in each file)  
for k = 1:nfiles  
    rawFile = [dirraw,num2str(irun(k,1)),'.nxs'];  
    SROT=0;  
    SROT = hdf5read(rawFile, '/entry0/instrument/SROT/value');  
    fprintf('%d)\tPsi = %5.2f ( Om = %5.2f / SROT = %5.2f) -> %s \n',k, psi(k),Omega(k),SROT,spe_file{k});  
end
```

```
1) Psi = -49.68 ( Om = 120.00 / SROT = 120.01) -> /usr/illdata/133/in5/exp_4-01-1230/processed/spe/sqw_110079_110079_318_384_240.spe  
2) Psi = -50.68 ( Om = 121.00 / SROT = 120.99) -> /usr/illdata/133/in5/exp_4-01-1230/processed/spe/sqw_110080_110080_318_384_240.spe  
3) Psi = -51.68 ( Om = 122.00 / SROT = 122.01) -> /usr/illdata/133/in5/exp_4-01-1230/processed/spe/sqw_110078_110078_318_384_240.spe  
4) Psi = -52.68 ( Om = 123.00 / SROT = 122.99) -> /usr/illdata/133/in5/exp_4-01-1230/processed/spe/sqw_110081_110081_318_384_240.spe  
  
...  
  
116) Psi = -165.68 ( Om = 236.00 / SROT = 236.01) -> /usr/illdata/133/in5/exp_4-01-1230/processed/spe/sqw_110019_110019_318_384_240.spe  
117) Psi = -167.68 ( Om = 238.00 / SROT = 238.01) -> /usr/illdata/133/in5/exp_4-01-1230/processed/spe/sqw_110018_110018_318_384_240.spe  
118) Psi = -169.68 ( Om = 240.00 / SROT = 239.99) -> /usr/illdata/133/in5/exp_4-01-1230/processed/spe/sqw_110017_110017_318_384_240.spe
```

```
% Generate the .SQW file  
gen_sqw (spe_file, par_file, sqw_file, efix, emode, alatt, angdeg, u, v, ...  
        psi, omega, dpsi, gl, gs);
```

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