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Supporting information for article:

Calculating temperature-dependent X-ray structure factors of α -quartz with an extensible Python 3 package

John P. Sutter, James Pittard, Jacob Filik and Alfred Q. R. Baron

S1. Example script SF-vs-T_Dextro-z+_101.py used in Section 10.1

```
import numpy as np
import sys

from general_crystals import CrystalFactory
from general_crystals.alphaquartz_dextro_zp import AlphaQuartz_Dextro_zp
from general_crystals.alphaquartz_dextro_zp_isodwf import
AlphaQuartz_Dextro_zp_isodwf
from Structure_Factor_Calculator.structure_factor_calc import Structure_Factor

print("sys.path = ",sys.path)
descriptions = CrystalFactory.get_descriptions()

# User parameters

hk11 = [1,0,1]
hk12 = [1,0,-1]
tempmin_K = 20
tempmax_K = 838
energy_eV = 10000
OutFile1 = 'SF_Out_hk11=101.txt'
OutFile2 = 'SF_Out_hk12=10-1.txt'
OutFileIso1 = 'SFIso_Out_hk11_101.txt'
OutFileIso2 = 'SFIso_Out_hk12_10-1.txt'

# Crystal object initialization

AQzD1 = AlphaQuartz_Dextro_zp(tempmin_K,hk11,energy_eV)
AQzD2 = AlphaQuartz_Dextro_zp(tempmin_K,hk12,energy_eV)
AQzDIso1 = AlphaQuartz_Dextro_zp_isodwf(tempmin_K,hk11,energy_eV)
AQzDIso2 = AlphaQuartz_Dextro_zp_isodwf(tempmin_K,hk12,energy_eV)
```

```
# Calculation and output of structure factors versus temperature

for tempdK in range(tempmin_K,tempmax_K+1):

    AQzD1.set_temp_miller_energy(tempdK,hkl1,energy_eV)

    ThBragg_deg = AQzD1.environment.angle_deg

    SF = Structure_Factor.F_hkl(AQzD1,AQzD1.environment)

    SF_H = SF[0][0]
    SF_H_Mag = np.abs(SF_H)**2
    SF_H_Angrad = np.angle(SF_H)

    SF_Hbar = SF[1][0]
    SF_Hbar_Mag = np.abs(SF_Hbar)**2
    SF_Hbar_Angrad = np.angle(SF_Hbar)

    SF_0 = SF[2][0]
    SF_0_Mag = np.abs(SF_0)**2
    SF_0_Angrad = np.angle(SF_0)

    with open(OutFile1,'a') as out:
        out.write( '{0:d} {1:5f} {2:5f} {3:5f} {4:5f} {5:5f} {6:5f} {7:5f}'.format(
            tempdK, ThBragg_deg, SF_H_Mag, SF_H_Angrad, SF_Hbar_Mag, SF_Hbar_Angrad, SF_0_Mag,
            SF_0_Angrad ) + '\n' )

    AQzD2.set_temp_miller_energy(tempdK,hkl2,energy_eV)

    ThBragg_deg = AQzD2.environment.angle_deg

    SF = Structure_Factor.F_hkl(AQzD2,AQzD2.environment)

    SF_H = SF[0][0]
    SF_H_Mag = np.abs(SF_H)**2
    SF_H_Angrad = np.angle(SF_H)
```

```
SF_Hbar = SF[1][0]
SF_Hbar_Mag = np.abs(SF_Hbar)**2
SF_Hbar_Angrad = np.angle(SF_Hbar)

SF_0 = SF[2][0]
SF_0_Mag = np.abs(SF_0)**2
SF_0_Angrad = np.angle(SF_0)

with open(OutFile2,'a') as out:
    out.write( '{0:d} {1:5f} {2:5f} {3:5f} {4:5f} {5:5f} {6:5f} {7:5f}'.format(
tempdK, ThBragg_deg, SF_H_Mag, SF_H_Angrad, SF_Hbar_Mag, SF_Hbar_Angrad, SF_0_Mag,
SF_0_Angrad ) + '\n' )

AQzDIso1.set_temp_miller_energy(tempdK,hkl1,energy_eV)
ThBragg_deg = AQzDIso1.environment.angle_deg
SF = Structure_Factor.F_hkl(AQzDIso1,AQzDIso1.environment)

SF_H = SF[0][0]
SF_H_Mag = np.abs(SF_H)**2
SF_H_Angrad = np.angle(SF_H)

SF_Hbar = SF[1][0]
SF_Hbar_Mag = np.abs(SF_Hbar)**2
SF_Hbar_Angrad = np.angle(SF_Hbar)

SF_0 = SF[2][0]
SF_0_Mag = np.abs(SF_0)**2
SF_0_Angrad = np.angle(SF_0)

with open(OutFileIso1,'a') as out:
    out.write( '{0:d} {1:5f} {2:5f} {3:5f} {4:5f} {5:5f} {6:5f} {7:5f}'.format(
tempdK, ThBragg_deg, SF_H_Mag, SF_H_Angrad, SF_Hbar_Mag, SF_Hbar_Angrad, SF_0_Mag,
SF_0_Angrad ) + '\n' )
```

```
AQzDIso2.set_temp_miller_energy(tempdK,hkl2,energy_eV)

ThBragg_deg = AQzDIso2.environment.angle_deg

SF = Structure_Factor.F_hkl(AQzDIso2,AQzDIso2.environment)

SF_H = SF[0][0]
SF_H_Mag = np.abs(SF_H)**2
SF_H_Angrad = np.angle(SF_H)

SF_Hbar = SF[1][0]
SF_Hbar_Mag = np.abs(SF_Hbar)**2
SF_Hbar_Angrad = np.angle(SF_Hbar)

SF_0 = SF[2][0]
SF_0_Mag = np.abs(SF_0)**2
SF_0_Angrad = np.angle(SF_0)

with open(OutFileIso2,'a') as out:
    out.write( '{0:d} {1:5f} {2:5f} {3:5f} {4:5f} {5:5f} {6:5f} {7:5f}'.format(
tempdK, ThBragg_deg, SF_H_Mag, SF_H_Angrad, SF_Hbar_Mag, SF_Hbar_Angrad, SF_0_Mag,
SF_0_Angrad ) + '\n' )
```