

3 14, 13 13:55

ReflWidthStill.py

Page 1/8

```

import os,sys,math
from numpy import *
from Amat import *

class ReflWidthStill:

    def __init__(self,amatfile,divv,divh,mosaic,dispersion,wavelength=1.24):
        self.amatfile=amatfile
        self.mosaic=mosaic
        self.dispersion=dispersion          #UNIT: degree
        self.divv=divv                      # UNIT: degree
        self.divh=divh                      # UNIT: degree
        self.cuspflag=1
        self.width_max=3.0                  # UNIT: degree
        self.isPrepDELEPS=False
        self.isSetMisset=False
        self.wl=wavelength

        # Some flags
        self.isInit=False
        self.isSolved=False

    def init(self):
        #      S0 vector (anti-parallel to the x-ray)
        self.s0=array((-1,0,0))
        #      E3 vector (Z axis: rotation axis)
        self.e3=array((0,0,1))

        # A matrix file open and read 'A matrix'
        amatftmp=Amat(self.amatfile)
        self.amat=amatftmp.getAmat()

        self.isInit=True

    def setMosaic(self,mosaic):
        self.mosaic=mosaic

    def setMisset(self,rx,ry,rz):
        rotx=self.makeRotX(rx)
        roty=self.makeRotY(ry)
        rotz=self.makeRotZ(rz)

        rot_xy=dot(rotx,roty)
        self.misset=dot(rot_xy,rotx)
        self.isSetMisset=True
        #print self.misset

    # hkl: array of reflection index (type: integer)
    # phistart: phi start angle [degrees]

    # phistart: start PHI angle
    # phiend : end PHI angle
    # used in MOSFLM integration
    def setHKL(self,hkl,phistart,phiend):
        if self.isInit==False:
            self.init()
        self.isPrepDELEPS=False

        ## HKL -> XYZ in reciprocal space
        # convert int -> float
        tmp_hkl=[]
        tmp_hkl.append(float(hkl[0]))
        tmp_hkl.append(float(hkl[1]))
        tmp_hkl.append(float(hkl[2]))
        self.hkl=hkl

        self.phimid=(phistart+phiend)/2.0

        # Rotation matrix with phimid ((startphi+endphi)/2.0 in MOSFLM)
        phimid_matr=self.makeRotMat(self.phimid)

        # Amat x Rotation matrix (@end phi)
        self.amat_midphi=dot(phimid_matr,self.amat)
        if self.isSetMisset:

```

```

        self.amat_midphi=dot(self.misset,self.amat_midphi)

# Amat*HKL -> XYZ in reciprocal space
float_hkl=array(tmp_hkl)

# XYZ1: RLP at start phi
self.xyz1=dot(self.amat_midphi,float_hkl)

# E1/E2/E3 vectors are calculated from XYZ1(RLP@ start phi)
##      E2 vector (E3xRLP/E3xRLP)
self.e2=cross(self.e3,self.xyz1)/linalg.norm(cross(self.e3,self.xyz1))
#      E1 vector (E2 x E3)
self.e1=cross(self.e2,self.e3)

## d* value is calculated from XYZ1(RLP@start phi)
## Calculating d* value
self.dstar=linalg.norm(self.xyz1)
self.dstar2=self.dstar*self.dstar
self.dst4=self.dstar2*self.dstar2*0.25

## XRLP .vs. Ewald sphere
## Diffraction condition
# CEA.cos(phic)+CEB.sin(phic)=CEC
# 1) CEA=(XRLP.E1)*(E1.S0)
# 2) CEB=(XRLP.E1)*(E2.S0)
# 3) CEC=0.5*(XRLP.E1)^2+0.5*(XRLP.E3)^2-(XRLP.E3)*(E3.S0)
# 4) CEABSQ=CEA^2+CEB^2 (=0.0 -> XRLP on rotation axis)

## DEBUG
#print "E1=",self.e1
#print "E2=",self.e2
#print "E3=",self.e3

# Preparation
# xe1: XRLP.E1
xe1=dot(self.xyz1,self.e1)
# xe3: XRLP.E3
xe3=dot(self.xyz1,self.e3)
# XE1D
e1_dot_s0=dot(self.e1,self.s0)
e2_dot_s0=dot(self.e2,self.s0)
e3_dot_s0=dot(self.e3,self.s0)

## DEBUG
#print "XE1/3=",xe1,xe3
#print "E1.S0/E2.S0/E3.S0=",e1_dot_s0,e2_dot_s0,e3_dot_s0

####
# CEA,CEB,CEC
self.cea=xe1*e1_dot_s0
self.ceb=xe1*e2_dot_s0
self.cec=0.5*pow(xe1,2.0)+0.5*pow(xe3,2.0)-(xe3*e3_dot_s0)
#print "CEA=",self.cea
#print "CEB=",self.ceb
#print "CEC=",self.cec

self.ceabsq=pow(self.cea,2.0)+pow(self.ceb,2.0)
#print "CEABS %12.5f"%self.ceabsq

#####
# There are 2 solutions where RLP crosses Ewald Sphere
#####
if self.ceabsq!=0.0:
    self.arg1=self.cec/sqrt(self.ceabsq)
    #print "ARG=",self.arg1
    return True
else:
    return False

def getD(self):
    # d=(wavelength/self.dstar)
    # dstar_true=(self.dstar/wavelength)
    return (1.0/self.dstar*self.wl)

```

```

def solvePhi(self):
    dtor=4.0*arctan(1.0)/180.0

    #####
    # self.arg1 value is not in the reasonable range
    #####
    if self.arg1>1.0:
        self.arg1=1.0
    elif self.arg1<-1.0:
        self.arg1=-1.0

    # solutions in unit of radians
    t1=arccos(self.arg1)
    t2=arctan2(self.ceb,self.cea)

    # 1st solution in unit of degree
    phic=degrees(t1+t2)
    phia=self.phimid+phic
    # 2nd solutin in unit of degree
    self.phic=degrees(-t1+t2)
    phib=self.phimid+self.phic;

    # Choosing the solution
    diff1=fabs(phia-self.phimid)
    diff2=fabs(phib-self.phimid)

    # DEBUG
    #-print "T1/T2=",t1,t2
    #print "PHIA/PHIB=",phia,phib
    #-print "DIFF1/DIFF2=",diff1,diff2

    # self.phi UNIT:degrees
    if diff1<diff2:
        self.phi=phia
    else:
        self.phi=phib

    #print "solved PHI",self.phi
    self.isSolved=True

def makeRotMat(self,phideg):
    phirad=radians(phideg)
    #print "PHIRAD/COS(PHIRAD)/SIN(PHIRAD)=",phirad,cos(phirad),sin(phirad)
    tpl=matrix( (
        ( cos(phirad), -sin(phirad),0.),
        ( sin(phirad), cos(phirad),0),
        ( 0., 0., 1.)
    ) )
    mat=array(matrix((tpl)).reshape(3,3))
    return mat

def makeRotZ(self,phideg):
    phirad=radians(phideg)
    #print "PHIRAD/COS(PHIRAD)/SIN(PHIRAD)=",phirad,cos(phirad),sin(phirad)
    tpl=matrix( (
        ( cos(phirad), -sin(phirad),0.),
        ( sin(phirad), cos(phirad),0),
        ( 0., 0., 1.)
    ) )
    mat=array(matrix((tpl)).reshape(3,3))
    return mat

def makeRotX(self,phix):
    phirad=radians(phix)
    #print "PHIRAD/COS(PHIRAD)/SIN(PHIRAD)=",phirad,cos(phirad),sin(phirad)
    tpl=matrix( (
        ( 1., 0., 0.),
        ( 0.,cos(phirad), -sin(phirad)),
        ( 0.,sin(phirad), cos(phirad))
    ) )
    mat=array(matrix((tpl)).reshape(3,3))
    return mat

def makeRotY(self,phiy):

```

3 14, 13 13:55

ReflWidthStill.py

Page 4/8

```

    phirad=radians(phiy)
    #print "PHIRAD/COS(PHIRAD)/SIN(PHIRAD)=",phirad,cos(phirad),sin(phirad)
    tpl=matrix( (
        ( cos(phirad), 0., sin(phirad)),
        ( 0., 1., 0.)),
        ( -sin(phirad), 0., cos(phirad)),
    ) )
    mat=array(matrix((tpl)).reshape(3,3))
    return mat

def distEwaldToRLP(self) :
    if self.isSolved==False :
        self.solvePhi()
        # Ewald sphere (x+1)^2 + y^2 + z^2 = 1.0
    #####
    ## XRLP at start phi
    #####
    x1=self.xyz1[0]
    y1=self.xyz1[1]
    z1=self.xyz1[2]

    # Some short cut variants
    # for XYZ1@start phi
    x1_2=(x1+1.0)*(x1+1.0)
    y1_2=y1*y1
    z1_2=z1*z1
    #print "XYZ1 %12.5f %12.5f %12.5f"%(x1,y1,z1)
    #print "XYZ2 %12.5f %12.5f %12.5f"%(x2,y2,z2)
    #####
    # Distance from XYZ to Ewald sphere
    #####
    self.dell=sqrt(x1_2+y1_2+z1_2)-1.0
    self.adell=fabs(self.dell)

    return True

def getPHI(self):
    return self.phi

def getLorentz(self):
    return self.lorentz_factor

def calcLorentz(self):
    # Matrix required for Lorentz factor estimation
    tmp1=cross(self.e3,self.s0)
    # RLP coordinates at the 'solved phi' angle
    # self.phic [degrees]
    #print "LOR: ",self.phic
    phicrotmat=self.makeRotMat(self.phic)
    xrlpe=dot(phicrotmat,self.xyz1)

    # Holton factor
    htmp=dot(self.e3,xrlpe)
    if htmp==0.0:
        self.holton_factor=0.0
    else:
        self.holton_factor=1.0/fabs(dot(self.e3,xrlpe))
    # Lorentz factor is estimated at the beginning rotation angle
    t3=dot(tmp1,xrlpe)
    if t3==0.0:
        self.lorentz_factor=0.0
        return 0.0
    else:
        self.lorentz_factor=fabs(1.0/t3);
        #print self.holton_factor,self.lorentz_factor

def calcRspot(self):
    # Divergence
    #---- Conventional source geometry
    # Radius of reciprocal lattice point along radius of Ewald sphere
    # RSPOT = 0.5*(DIVERGENCE+dispersion*tan(theta) )*DSTAR*COS(THETA)
    # and as DSTAR*COS(THETA) = SQRT(DSTAR**2-0.25*DSTAR**4)
    # Note that the divergence parameters DIVH,DIVV and the mosaic spread

```

3 14, 13 13:55

ReflWidthStill.py

Page 5/8

```

# are stored in the generate file as the FULL WIDTHS in degrees.
# These are converted to HALF WIDTHS in radians prior to the prediction
# calculations.
# Add the contribution due to finite block size.

#print "DEG: divv,divh=",self.divv,self.divh
#print "DEG: mosaic=",self.mosaic
#print "RAD: divv,divh=",radians(self.divv),radians(self.divh)
#print "RAD: mosaic=",radians(self.mosaic)

# Mosaic/Divergence conversion which can match to MOSFLM
# For strategy option ON ???
divv=radians(self.divv)/2.0
divh=radians(self.divh)/2.0
mosaic=radians(self.mosaic)/2.0

# Energy dispersion?
delcor=0.0001
# z1 of XRLP
z1=self.xyz1[2]
# ymid : in the MOSFLM (Y@phistart+Y@phiend)/2.0
ymid=self.xyz1[1]
yms=ymid*ymid

# Preparation of parameters required for divergence calculation
esyn_h=delcor*self.dstar2+z1*divh
esyn_v=divv*ymid
# Divergence calculation
divergence=sqrt((pow(esyn_h,2.0)+pow(esyn_v,2.0))/(yms+z1*z1))
# Reflection spot radius
self.rspot=(divergence+mosaic)*sqrt(self.dstar2-self.dst4) \
+0.25*self.dispersion*self.dstar2
#print "DIVERG/ETA/DSTAR2/RSPOT=",divergence,mosaic,self.dstar2,self.rspot
#print "RSPOT=",self.rspot
return self.rspot

def cuspcheck(self):
    csmin=0.5*self.dstar2+self.rspot
    csmin2=self.dst4+self.dstar2*self.rspot
    x,y=self.xyz1[0],self.xyz1[1]
    xys=x*x+y*y
    #=====
    # What should csimin test be ? The spot can still appear on image
    # even if the centre of the rlp never cuts the sphere (ie lies in
    # the cusp region) providing any part of the rlp touches the sphere.
    # In this case, the test on line below is the right one, but this
    # seems to overpredict in practice, so limit it to case where the
    # centre of the rlp must intersect the sphere.
    #=====
    if xys<=csmin2:
        ## A part of spot is in cusp region
        self.cuspflag=-3
    elif(xys<self.dst4):
        ## Whole spot is included in cusp region
        self.cuspflag=-4
        self.inCusp=true

## Reflection width and start/end phi of diffraction
def diffWidth(self) :
    ## Full width of reflection condition (UNIT:radians)
    dtor=4.0*arctan(1.0)/180.0

    # self.phiw = spot angular radius in unit:degrees
    self.phiw=2.0*self.rspot*self.lorentz_factor/dtor
    self.phis=self.phi-0.5*self.phiw
    self.phie=self.phis+self.phiw

def numframes(self) :
    ## Estimating max frames of this reflections
    maxframes=(int)(self.width_max/oscstep)
    #- print maxframes

    ## Find start BATCH in which this reflection is observed
    for i in range(1,maxframes+1):

```

3 14, 13 13:55

ReflWidthStill.py

Page 6/8

```

        if phistart-(i-1)*oscstep<=self.phis:
            self.istart=i
            break

    for i in range(1,maxframes+1):
        if phiend+(i-1)*oscstep>=phie:
            self.iend=i;
            break;
    self.iwidth=self.istart-1+self.iend-1+1;
    #- print self.iwidth,self.istart,self.iend
## Estimation of deleps1,deleps2. this is the objective of this CLASS

def prepDELEPS(self):
    self.solvePhi()
    self.distEwaldToRLP()
    self.calcLorentz()
    self.calcRspot()
    self.diffWidth()
    self.cuspcheck()
    self.isPrepDELEPS=True

def getPhiw(self):
    if self.isPrepDELEPS==False:
        self.prepDELEPS()
    return self.phiw

def calcDELEPS(self):
    # Preparation
    if self.isPrepDELEPS==False:
        self.prepDELEPS()

## Calculate distance of edge of spot from sphere at end of rotation
    dist1=self.adell-self.rspot;

    #print self.adell,self.adel2
    #print "DIST1/DIST2=%12.5f %12.5f"%(dist1,dist2)

## Test if spot is cut at beginning of rotation
## Set DELEPS to a negative value
## NOTE: sign change depending on whether Y is +ve/-ve

    x1,y1,z1=self.xyz1[0],self.xyz1[1],self.xyz1[2]

    self.deleps1=0.0

    # Flag for partial/full reflection
    self.isFull=True

    #print "DIST",dist1,dist2

    # ADEL1 -> Cross section between E.S and RLP (UNIT:radians)
    # Firstly, check CUSP flag
    if self.cuspflag<0:
        self.isFull=False

    elif dist1<0.0:
        self.isFull=False
        if y1<0.0:
            sign=-1
        else :
            sign=1

        # DELEPS1 calculation
        self.deleps1=-(sign*self.dell/self.rspot+1.0)*0.5

    return self.deleps1

def DEBUG_calcPartiality(self):
    print "===== PART CALC ====="
    dist1=self.adell-self.rspot
    dist2=self.adel2-self.rspot

    if dist1<0.0:
        print "Start point is on ES %12.6f %12.6f"%(self.deleps1,self.deleps2)

```

```

        if dist2<0.0:
            print "Both is on ES %12.6f %12.6f"%(self.deleps1,self.deleps2)
        elif dist2<0.0:
            print "After oscillation on ES %12.6f %12.6f"%(self.deleps1,self.deleps2)

        else:
            print "Hashinimo bounimo %12.6f %12.6f"%(self.deleps1,self.deleps2)

        return 1.0

def getDel(self):
    return self.adel1,self.adel2

def calcPartiality(self):
    dist1=self.adel1-self.rspot
    dist2=self.adel2-self.rspot

    ## Case1
    if self.isFull:
        p1=self.adel1/self.rspot
        p2=self.adel2/self.rspot
        self.pcalc=array([p1,p2]).min()
        #print self.pcalc
        return self.pcalc

    elif fabs(self.deleps2)<0.00001 :
        self.pcalc=0.5*(1.0-cos(self.deleps1*pi))
        return self.pcalc

    elif fabs(self.deleps1)<0.00001 :
        self.pcalc=0.5*(1.0-cos(self.deleps2*pi))
        return self.pcalc

    else:
        tmp=0.5*(1.0-cos(self.deleps1*pi))
        self.pcalc=tmp-(1.0-0.5*(1.0-cos(self.deleps2*pi)))
        return self.pcalc

def calcP_Rossmann(self):

    mr_model=lambda a:3.0*a*a-2.0*a*a*a

    if self.isFull:
        p1=self.adel1/self.rspot
        p2=self.adel2/self.rspot
        self.pcalc=array([p1,p2]).min()
        #print self.pcalc
        return self.pcalc

    elif fabs(self.deleps2)<0.00001 :
        self.pcalc=mr_model(self.deleps1)
        return self.pcalc

    elif fabs(self.deleps1)<0.00001 :
        self.pcalc=mr_model(self.deleps2)
        return self.pcalc

    else:
        tmp=mr_model(self.deleps1)
        self.pcalc=tmp-(1.0-mr_model(self.deleps2))
        return self.pcalc

def calcP_tsuki(self):

    model=lambda q:(q-(sin(2.0*pi*q))/2.0/pi)

    if self.isFull:
        p1=self.adel1/self.rspot
        p2=self.adel2/self.rspot
        self.pcalc=array([p1,p2]).min()
        #print self.pcalc
        return self.pcalc

    elif fabs(self.deleps2)<0.00001 :

```

3 14, 13 13:55

ReflWidthStill.py

Page 8/8

```

        self.pcalc=model(self.deleps1)
        return self.pcalc

    elif fabs(self.deleps1)<0.00001 :
        self.pcalc=model(self.deleps2)
        return self.pcalc

    else:
        tmp=model(self.deleps1)
        self.pcalc=tmp-(1.0-model(self.deleps2))
        return self.pcalc

if __name__=="__main__":
    tmp=ReflWidthBothEdge(sys.argv[1],0.02,0.02,0.5,0.0002,0.1)
    h,k,l=int(sys.argv[2]),int(sys.argv[3]),int(sys.argv[4])
    hklist=[array((h,k,l))]

    oscstart=0.0

    tmp.setMissetting(0.0,0.0,0.0)

    for hkl in hklist:
        #print "HKL type is ",type(hkl)
        if tmp.setHKL(hkl,oscstart)==True:
            tmp.calcDELEPS()
            print tmp.calcPartiality()

```