Supplementary Material

Thin film disorientation measurement using the single crystal Nonius Kappa CCD diffractometer

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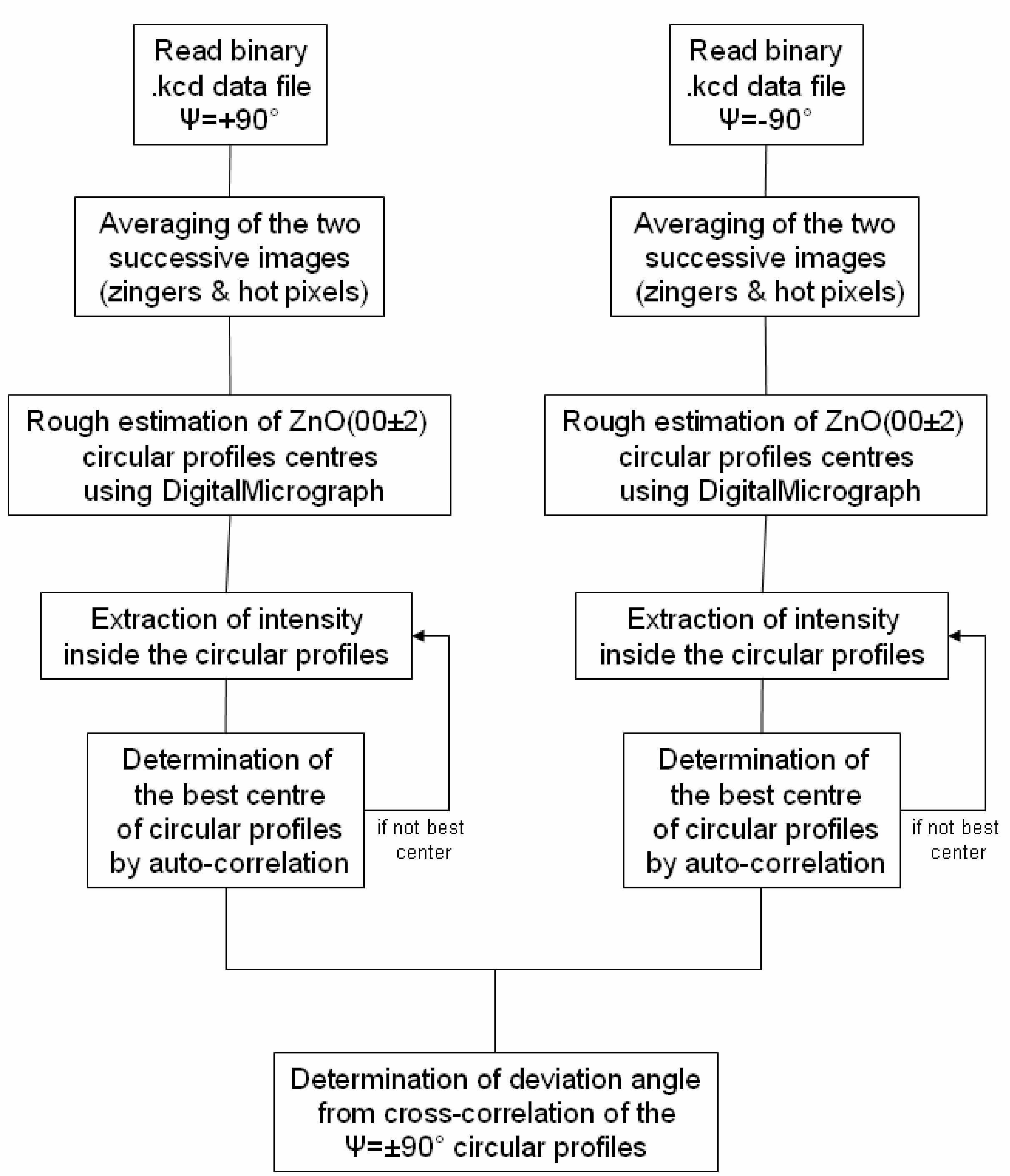
Annexes

Flow chart of the Fortran routines used


Read binary .kcd data file Ψ=+90°
Read binary .kcd data file Ψ=-90°
Averaging of the two successive images (zingers & hot pixels)
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Rough estimation of ZnO(00±2) circular profiles centres using DigitalMicrograph
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Extraction of intensity inside the circular profiles
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Determination of the best centre of circular profiles by auto-correlation
if not best center
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if not best center
Determination of deviation angle from cross-correlation of the Ψ=±90° circular profiles

Fortran77 Routines used (code dealing with binary file handling is platform dependent)

Extraction of pixel intensity information from .kcd file and removal of zingers and hot pixels

```
      integer*2 II
      integer*4 image1(1:576,1:625), image2(1:576,1:625)
      integer*4 zingers(1:576,1:625), hotpixels(1:576,1:625),
     &  imagef(1:576,1:625)
      integer i,j,m,n,ip,jp,imoy,igood,I12
      real xs1,xs2,xs,xz,xh

      open(unit=1,file='kcd.kcd',form='unformatted',
     & status='old',access='direct',recl=2)
      open(unit=2,file='kcd.ave',form='unformatted',
     & status='unknown',access='direct',recl=2)
      open(unit=3,file='zingers',form='unformatted',
     & status='unknown',access='direct',recl=2)
      open(unit=4,file='hotpixels',form='unformatted',
     & status='unknown',access='direct',recl=2)

   50 print*,'Criteria for zingers (3)'
      read(5,*) xz
      print*,'Criteria for hot pixels (1.5)'
      read(5,*) xh
      print*,xz,' ',xh

C     Table Initialization
      do i=1,576
         do j=1,625
            image1(i,j)=0
            image2(i,j)=0
            zingers(i,j)=1
            hotpixels(i,j)=1
            imagef(i,j)=0
         enddo
      enddo
C     Loading of the two sub-images in memory
  100 do i=1,576
         do j=1,625
            m=2050+((i-1)*625+j)
            read(1,rec=m) II
           if (II.lt.-0.1) then
                         image1(i,j)=II+65536
                           else
                         image1(i,j)=II
                           endif

            n=(i-1)*625+j+576*625+2050
            read(1,rec=n) II
            if (II.lt.-0.1) then
                         image2(i,j)=II+65536
                           else
                         image2(i,j)=II
                           endif
         enddo
      enddo
```

```
C     Definition of zingers
      do i=1,576
         do j=1,625
            if (i.eq.1.or.i.eq.576.or.j.eq.1.or.j.eq.625) then
                xs1=sqrt(image1(i,j)*1.0)
                xs2=sqrt(image2(i,j)*1.0)
                xs=(xs1+xs2)/2
                                                          else
                xs=0.0
                do ip=-1,1
                    do jp=-1,1
                         xs1=sqrt(image1(i+ip,j+jp)*1.0)
                         xs2=sqrt(image2(i+ip,j+jp)*1.0)
                         xs=xs+(xs1+xs2)/2
                    enddo
                enddo
                xs=xs/9.0
                                                          endif
            if (abs(image1(i,j)-image2(i,j)).gt.(xz*xs))
     &          then
                       zingers(i,j)=0
                endif
             II=zingers(i,j)
             write(3,rec=(i-1)*625+j) II
         enddo
      enddo

C     Definition of hot pixels
      do i=1,576
         do j=1,625
             imoy=0
             igood=0
             do ip=-1,1
                do jp=-1,1
                  if (ip.ne.0.and.jp.ne.0) then
                   imoy=imoy+(image1(i+ip,j+jp)+image2(i+ip,j+jp))/2
     &              *zingers(i+ip,j+jp)
                   igood=igood+zingers(i+ip,j+jp)
                                           endif
                enddo
             enddo
             if (igood.eq.0) then
                   imoy=65535
                             else
                   imoy=imoy/igood
                             endif
            I12=(image1(i,j)+image2(i,j))/2
            if (I12.gt.xh*imoy) hotpixels(i,j)=0
            II=hotpixels(i,j)
            write(4,rec=(i-1)*625+j) II
         enddo
      enddo

C     Intensity correction from zingers and hot pixels
      do i=1,576
         do j=1,625

            if (i.eq.1.or.i.eq.576.or.j.eq.1.or.j.eq.625) then
               imagef(i,j)=0
                                                          else
             imoy=0
             igood=0
             do ip=-1,1
                do jp=-1,1
                  if (ip.ne.0.and.jp.ne.0) then
                   imoy=imoy+(image1(i+ip,j+jp)+image2(i+ip,j+jp))/2
     &              *zingers(i+ip,j+jp)*hotpixels(i+ip,j+jp)
                   igood=igood+zingers(i+ip,j+jp)*hotpixels(i+ip,j+jp)
                                           endif
                enddo
             enddo
             if (igood.eq.0) then
                   imoy=65535
                             else
                   imoy=imoy/igood
                             endif

            I12=(image1(i,j)+image2(i,j))/2
            if ((zingers(i,j)*hotpixels(i,j)).eq.0)  then
                                        imagef(i,j)=imoy
                                                     else
                                        imagef(i,j)=I12
                                                     endif
                                                          endif
            n=(i-1)*625+j
            II=imagef(i,j)
            write(2,rec=n) II
         enddo
      enddo

  900 stop
      end
```

Extraction of circular profiles

```
C     6789012345678901234567890123456789012345678901234567890123456789012345678901
      integer*2 II
      integer*4 III,image(1:576,1:625)
      integer*4 i,j,m,Rayon,Epaiss,som,N,xc,yc
      real*8 x,bet

      open(unit=1,file='kcd.ave',form='unformatted',
     & status='old',access='direct',recl=2)
      open(unit=2,file='profil.txt',form='formatted',
     & status='unknown')

  100 x=0.0
  101 format(I6)
      do i=1,576
         do j=1,625
            m=((i-1)*625+j)
            read(1,rec=m) II
            if (II.lt.-0.1) then
                               III=II+65536
                            else
                               III=II
                            endif
            image(i,j)=III
            x=x+image(i,j)
         enddo
      enddo
      Rayon=150
      Epaiss=20
      xc=296
      yc=325
      print*,'centre xc'
      read 101,xc
      print*,'centre yc'
      read 101,yc

      print*,'Average radius '
      read 101,Rayon
      print*,'Radius = ', Rayon
      print*,'delta R '
      read 101,Epaiss
      print*,'Delat R =',Epaiss

      N=360
      print*,'Nomber of radius = '
      read 101,N
      print*,'N= ', N

  200 do nn=1,N
           bet=nn*(360.0/N)
           call Iradial(x,Rayon,Epaiss,bet,image,xc,yc)
           write(2,250) bet,x
       enddo

  250 format(D15.9,' ',D15.9)

  900 stop
      end

C     Radial Integration
      SUBROUTINE Iradial(xirad,R,dR,xbeta,imaget,xcc,ycc)
      integer*4 imaget(1:576,1:625)
      integer*4 mm,M,ii,jj,R,dR,xcc,ycc
      real*8 xirad,xr,x,y,xbeta
  100 M=40
  101 format(I6)
      xirad=0.0
C     print*,'Radius is pixels'
C     read 101, M
C     print*,'M= ',M
  200 do mm=1,M
           xr= (R-dR)+(2.0*dR/(M-1))*(mm-1)
           x=xcc*1.0-xr*cos(xbeta*3.14159265359/180.0)
           y=ycc*1.0-xr*sin(xbeta*3.14159265359/180.0)
           ii=int(x)
           jj=int(y)
           if (ii.gt.1.and.ii.lt.576.and.jj.gt.1.and.jj.lt.625) then
                xirad=xirad+imaget(ii,jj)
                                                                endif
       enddo
       xirad=xirad/(M-1)
       return
       END
```

Auto-correlation of circular profile for best centre determination:

```
C     678901234567890123456789012345678901234567890123456789012345678901

      real*8 xbeta(1:7200),xsi1(1:7200),xmod(1:5000),
     & x1,xx1

      open(unit=1,file='profil.zno',form='formatted',
     & status='old')
      open(unit=2,file='zno-zno.txt',form='formatted',
     & status='unknown')
      open(unit=3,file='test.txt',form='formatted',
     & status='unknown')

  100 format(D15.9,' ',D15.9)
  110 format(D15.9,' ',D15.9)
  200 do i=1,7200
         read(1,100,end=900) xbeta(i),xsi1(i)
      enddo
      do i=1,5000
         xmod(i)=xsi1(i+1000)
      enddo

C     Profiles are 360° with 0.05° steps.
      do j=0,4999
         x1=0.0
         do i=1,5000
           if ((i+j).lt.5000) then
                  xx1=xmod(i)*xmod(i+j)
                              else
                  xx1=xmod(i)*xmod(i+j-5000)
                              endif
           x1=x1+xx1
          enddo
          write(2,110) j*0.05 ,x1
          if ((j.gt.3000).and.(j.lt.4200)) write(3,110) j*0.05 ,x1
      enddo

  900 stop
      end
```

Correlation of two profiles: determination of the deviation angle

```
C     678901234567890123456789012345678901234567890123456789012345678901
      real*8 xbeta(1:7200),xsi1(1:7200),xsi2(1:7200),
     & x1,xx1,x2,xx2

      open(unit=1,file='profile.zno1',form='formatted',
     & status='old')
      open(unit=2,file='profile.zno2',form='formatted',
     & status='old')
      open(unit=3,file='beta.txt',form='formatted',
     & status='unknown')

  100 format(D12.6,' ',D12.6)
  110 format(D12.6,' ',D12.6)
  200 do i=1,7200
         read(1,100,end=900) xbeta(i),xsi1(i)
         if ((i.lt.1380).or.
     & (i.gt.1800.and.i.lt.4900).or.
     & (i.gt.5400)) then
                          xsi1(i)=0.0
                    endif
```

```
       read(2,100,end=900) xbeta(i),xsi2(i)
       if ((i.lt.1800).or.
   & (i.gt.2240.and.i.lt.5300).or.
   & (i.gt.6000)) then
                       xsi2(i)=0.0
                  endif
    enddo
    do j=0,7199
       x1=0.0
       x2=0.0
       do i=1,7200
         if ((i+j).lt.7200) then
                xx1=xsi1(i)*xsi2(i+j)
                            else
                xx1=xsi1(i)*xsi2(i+j-7200)
                            endif
         x1=x1+xx1
        enddo
        write(3,110) j*0.05 ,x1
    enddo

900 stop
    end
```