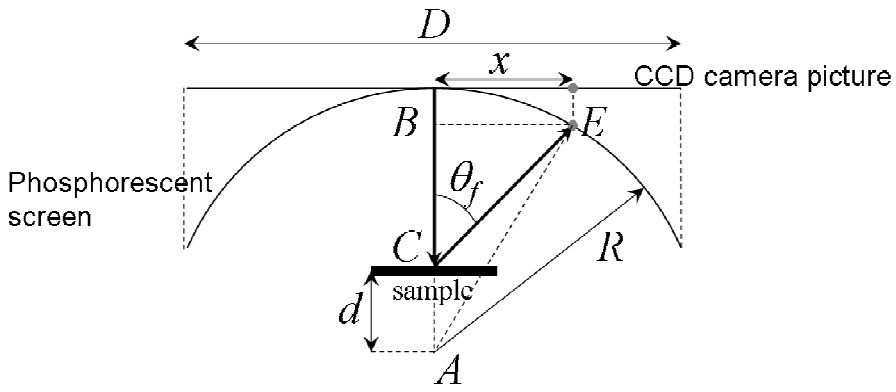
Annexes

Annex 1. Determination of θ_f for LEED



$$BE = CB.\tan\theta_f \rightarrow x = CB.\tan\theta_f$$

$$\left.\begin{array}{l} CB = AB - CA \rightarrow CB = AB - d \\ AB = \sqrt{AE^2 - BE^2} \rightarrow AB = \sqrt{R^2 - x^2} \end{array}\right\} \rightarrow CB = \sqrt{R^2 - x^2} - d$$

$$\Rightarrow \theta_f = \text{arctg}\left(\frac{x}{\sqrt{R^2 - x^2} - d}\right)$$

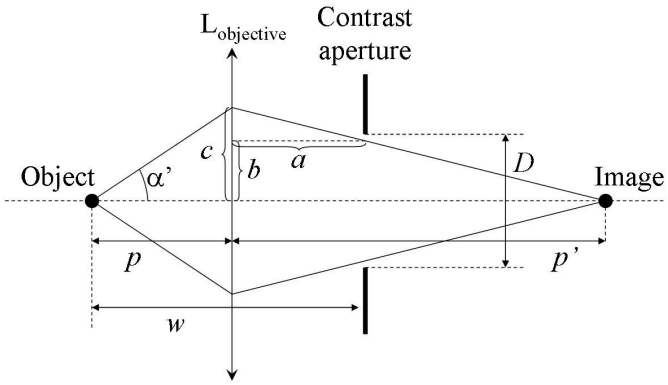
Annex 2. Determination of α' for PEEM aberrations

From optical geometry theory:

$$\frac{1}{f} = \frac{1}{p} + \frac{1}{p'} \tag{1}$$

$$G = \frac{i}{o} = -\frac{p'}{p} \tag{2}$$

p and p' are defined hereafter :



The focal distance can be calculated by using experimental results: if the projective lenses are set to column potential (i.e. the magnification power of these lenses is 0), an object (*o*) with a diameter of 80µm gives an image (*i*) of 1.2cm on the fluorescent screen through the electrostatic system of the PEEM. According to equation (2), the magnification *G* equals 150. Hence,

$$p' = 150\,p \tag{3}$$

Because of the geometry of the PEEM:

$$\begin{aligned} p + p' &= 650 \text{ mm} \\ w &= 17.4 \text{ mm} \end{aligned} \tag{4}$$

Substituting (3) in (4) leads to

$$\begin{aligned} p &= 4.3 \text{ mm} \\ p' &= 645.7 \text{ mm} \end{aligned} \tag{5}$$

Results (5) inserted in equation (1) give the focal distance of the objective lenses:

$$f = 4.3 \text{ mm} \tag{6}$$

From the figure presented above, it is easy to see that:

$$\frac{p'}{c} = \frac{p + p' - w}{b} \qquad (7)$$

Because b is the radius of the contrast aperture (i.e. $D/2$) and using results (4), (5) and (7), the distance c can be calculated:

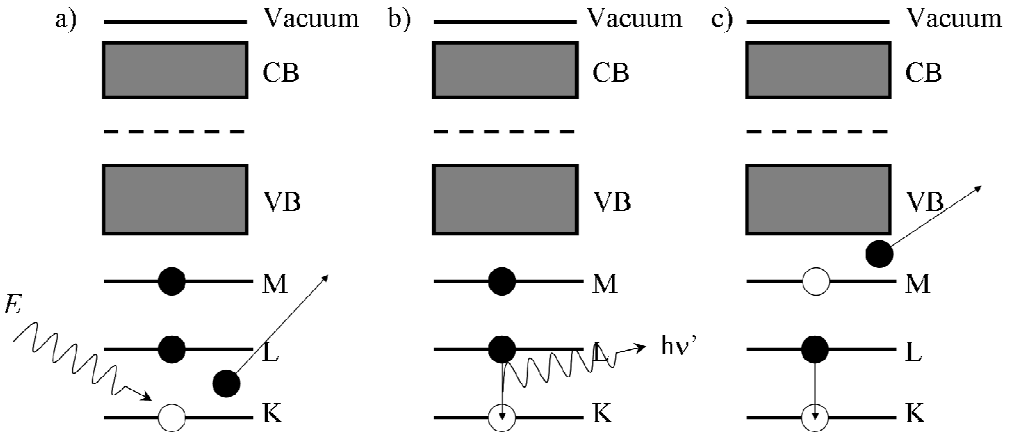
$$c = \frac{p'.b}{p + p' - w} = \frac{645.7D}{2(650 - 17.4)} = 0.51D \qquad (8)$$

Hence, the value of α' is:

$$\tan\alpha' \cong \alpha'(rad) = \frac{c(m)}{4.3\ 10^{-3}} = 119.D(m) \qquad (9)$$

Annex 3. Auger effect

When an incident beam of particles with an energy *E* hits a surface, the quantum can be absorbed, leading to the emission of a core level electron if the incident energy is higher than the binding energy of the electron. The ionized atom with a core level hole is in an excited state. The fundamental state is recovered when an electron from a higher energy level relaxes in order to fill the hole created by the emitted electron (see figure hereafter).



a) Emission of a core level electron; b) Stabilization by fluorescence; c) Stabilization by KLM Auger electron emission.

The energy difference *E'* between the level of the stabilizing electron and that of core level hole can be restituted to the surrounding environment by two different mechanisms:

- Fluorescence: the emission of a photon with an energy hν' = *E'* (Figure b);
- Auger effect: the emission of an electron from a higher level or from the same level as the stabilizing electron (Figure c).The kinetic energy (E_k) of the Auger electron is equal to $E_k = E' - E_b$ with E_b being the binding energy of this electron. The kinetic energy is different for each element of the periodic table and depends on the energy levels of the hole, the stabilizing electron and the Auger electron. When the Auger electrons are collected, peaks appear in the spectra, according to these three levels. The peaks are labeled with 3 letters, the first indicating the level of the hole, the second the level of the stabilizing electron and the third the level of the Auger electron (ex: C_{KLL} for an Auger electron emitted from the L level of a carbon atom and created from the relaxation of the excited atom by an electron from the L level to fill a hole in the K level).

Annex 4. FORTRAN program for LEED simulation

```
program LEED
implicit none
integer(4)::i,j,k,l
integer(4)::height,X,Y,kminpix,kmaxpix,kpix
real(8)::latt,a,Z,Zstep,sigma,pi,Xstep,Ystep,tampon1,mu,ktemp,klength,radius,&
& comp,norme,energy
real(8),allocatable::amplitude(:,:,:),planXY(:,:),gauss(:)
!Parameters (3x3 hexagons in the XY plane)
pi=3.141592654
X=648 !125 pts between 2 nodes in a (111) plane along the [11-2] direction
Y=500 !100 pts between 2 nodes in a (111) plane along the [1-10] direction
write(*,*) "Give the lattice parameter of the zinc blende structure in Angstroem"
read (*,*)latt
write(*,*) "Give the LEED electron beam energy in eV"
read(*,*) energy
a=8*pi/(latt)    !Length of the unit cell in the reciprocal space
Z=2.0*pi*sqrt(3.0)/latt !Distance between two (111) planes
write(*,'(a,f5.3,a)') "Hexagonal length = ",a," Angstroem -1"
write(*,'(a,f5.3,a)') "Interplanar spacing in Z direction = ",Z," Angstroem -1"
height=int(1.024*sqrt(energy))
if (height<12) height=12
write(*,'(a,i2)')"Number of nodes in the Z direction = ",height
allocate (amplitude(X,Y,50*height+1)) !100 points for each Gaussian profile
allocate (planXY(X,Y))
allocate (gauss(50*height+1))
Xstep=a/125.0 !Value of 1 pixel in the [11-2] direction
Ystep=a/100.0 !Value of 1 pixel in the [1-10] direction
Zstep=Z/50.0 !Value of 1 pixel in the [111] direction
! Hexagonal XY plane: 3x3 hexagons
```

```
planXY(1,1)=1.
do i=100,500,100
planXY(1,i)=1.
end do
do i=72,648,72
planXY(i,1)=1.
end do
do i=1,9
do j=1,5
planXY(72*i,100*j)=1.
end do
end do
do i=0,8
do j=0,4
planXY(36+i*72,50+j*100)=1.
end do
end do
open(20,file='planXY.txt')
do i=1,648
do j=1,500
if (planXY(i,j)==1.) then
write(20,*) i,j
end if
end do
end do
close (20)
! Génération du profil gaussien
sigma=14.0
do j=1,51
mu=1.
gauss(j)=1/(sigma*sqrt(2*pi))*exp(-(((j)-mu)**2/(2*sigma**2)))
end do
do i=5,height,4 !Gaussian profile of blue nodes
do j=1,101
```

```
mu=real(50*(i-1)+1,8)
gauss(j+50*(i-2))=gauss(j+50*(i-2))+1/(sigma*sqrt(2*pi))* &
& exp(-(((j+50*(i-2))-mu)**2/(2*sigma**2)))
end do
end do
do i=2,height,4          !Gaussian profile of red nodes
do j=1,101
mu=real(50*(i-1)+1,8)
gauss(j+50*(i-2))=gauss(j+50*(i-2))+0.59*(1/(sigma*sqrt(2*pi))* &
& exp(-(((j+50*(i-2))-mu)**2/(2*sigma**2))))
mu=real(50*(i-1)+101,8)
gauss(j+50*(i-2)+100)=gauss(j+50*(i-2)+100)+0.59*(1/(sigma*sqrt(2*pi))* &
& exp(-(((j+50*(i-2)+100)-mu)**2/(2*sigma**2))))
end do
end do
do i=3,height,4          !Gaussian profile of yellow nodes
do j=1,101
mu=real(50*(i-1)+1,8)
gauss(j+50*(i-2))=gauss(j+50*(i-2))+0.17*(1/(sigma*sqrt(2*pi))* &
& exp(-(((j+50*(i-2))-mu)**2/(2*sigma**2))))
end do
end do
norme=maxval(gauss)          !Normalization of Gauss matrix
do i=1,50*height+1
gauss(i)=gauss(i)/norme
end do
open (30,file='gaussienne.txt')
do i=1,50*height+1
write(30,*) (i-1)*Zstep,gauss(i)
end do
close (30)
! Creation of the 3D reciprical space
open (40,file='reseau 3D.txt')
write(40,'(5X,a1,11X,a1,11X,a1,7X,a9)')"X","Y","Z","Intensity"
```

```
write(40,'(/)')
do i=1,648
do j=1,500
if (planXY(i,j)==1.0) then
if ((mod(j,100)==0.0).or.(j==1)) then          !Line 1 or multiple of 100
if ((mod(i,216)==0.0).or.(i==1)) then          !Point position
do k=1,50*height+1
amplitude(i,j,k)=gauss(k)
write(40,'(e11.5,X,e11.5,X,e11.5,X,e11.5)') Xstep*(i-1),Ystep* &
& (j-1),Zstep*(k-1),amplitude(i,j,k)
end do
else
if (mod((i-144),216)==0.0) then       !Cross position
do k=134,50*height+1
amplitude(i,j,k-133)=gauss(k)
write(40,'(e11.5,X,e11.5,X,e11.5,X,e11.5)') Xstep*(i-1),Ystep* &
& (j-1),Zstep*(k-134),amplitude(i,j,k-133)
end do
else     !Triangle position
do k=68,50*height+1
amplitude(i,j,k-67)=gauss(k)
write(40,'(e11.5,X,e11.5,X,e11.5,X,e11.5)') Xstep*(i-1),Ystep* &
& (j-1),Zstep*(k-68),amplitude(i,j,k-67)
end do
end if
end if
else     !The line pixel is a multiple of 50
if (mod((i-108),216)==0.0) then !Point position
do k=1,50*height+1
amplitude(i,j,k)=gauss(k)
write(40,'(e11.5,X,e11.5,X,e11.5,X,e11.5)') Xstep*(i-1),Ystep* &
& (j-1),Zstep*(k-1),amplitude(i,j,k)
end do
else
```

```
if (mod((i-36),216)==0.0) then          !Cross position
do k=134,50*height+1
amplitude(i,j,k-133)=gauss(k)
write(40,'(e11.5,X,e11.5,X,e11.5,X,e11.5)') Xstep*(i-1),Ystep* &
& (j-1),Zstep*(k-134),amplitude(i,j,k-133)
end do
else
if (mod((i-180),216)==0.0) then         !Triangle position
do k=68,50*height+1
amplitude(i,j,k-67)=gauss(k)
write(40,'(e11.5,X,e11.5,X,e11.5,X,e11.5)') Xstep*(i-1),Ystep* &
& (j-1),Zstep*(k-68),amplitude(i,j,k-67)
end do
end if
end if
end if
end if
end if
end if
end do
end do
close (40)
! Ewald sphere intersection with incident beam arricing in position (324,250,0) in pixels
open(50,file='Ewald coord.txt')
open (60,file='Ewald pixel.txt')
ktemp=0.512*sqrt(energy)
kpix=int(ktemp/Zstep)+1
klength=ktemp
write(50,'(a,3X,f5.1)') "Energy (eV) = ",(klength/0.512)**2
write(60,'(a,3X,f5.1)') "Energy (eV) = ",(klength/0.512)**2
do i=0,kpix !Analyse des cercles selon Z, d'une hauteur kpix à 2*kpix
radius=sqrt(abs(klength**2-(real(i,8)*Zstep)**2))
do j=1,648
do k=1,500
comp=sqrt((real(324-j,8)*Xstep)**2+(real(250-k)*Ystep)**2)
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```
if (comp<=1.15*radius.and.comp>=0.85*radius) then
if (planXY(j,k)==1.0) then
write(50,'(f7.4,5X,f7.4,5X,e13.4,5X,i3)') Xstep*j,Ystep*k,amplitude(j,k,kpix+i),kpix+i
write(60,'(i3,5X,i3,5X,e13.4,5X,i3,5X,f5.1)') j,k,amplitude(j,k,kpix+i),kpix+i, &
& (atan(radius/(real(i,8)*Zstep)))*180.0/pi
end if
end if
end do
end do
end do
close(50)
close(60)
open(70,file='point.txt')
open(80,file='cross.txt')
open(90,file='triangle.txt')
do i=1,50*height+1
write(70,'(e11.5,X,e11.5)') (i-1)*Zstep,amplitude(324,250,i)
write(80,'(e11.5,X,e11.5)') (i-1)*Zstep,amplitude(252,150,i)
write(90,'(e11.5,X,e11.5)') (i-1)*Zstep,amplitude(288,100,i)
end do
close(70)
close(80)
close(90)
end program LEED
```