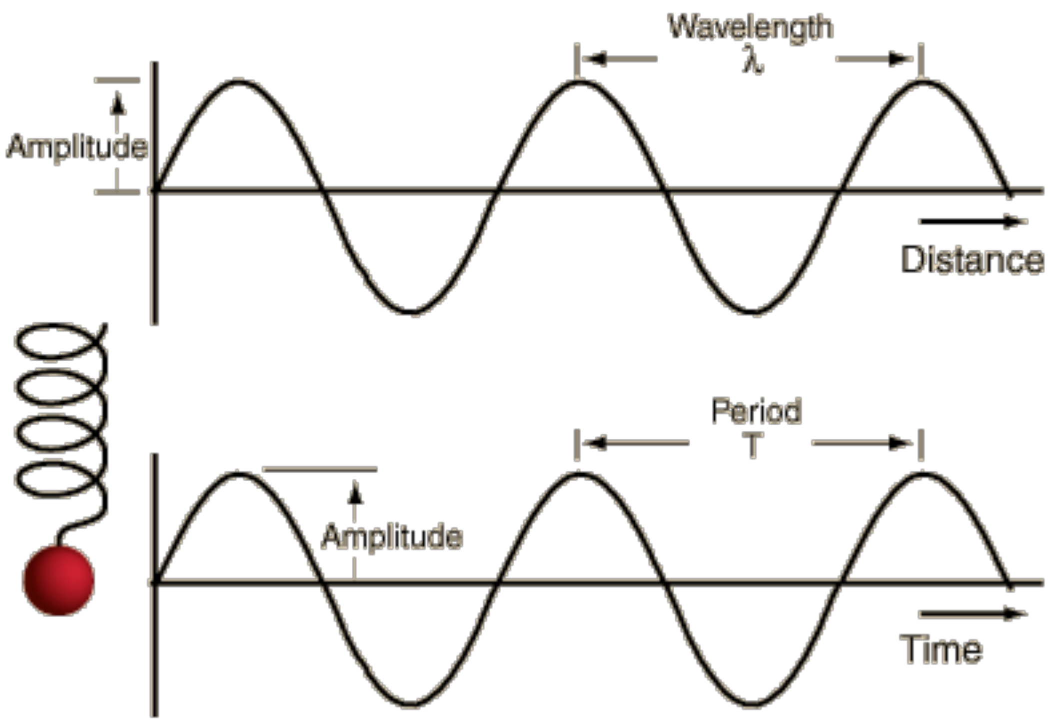
Chapter 6

Fourier Optics and High Resolution TEM

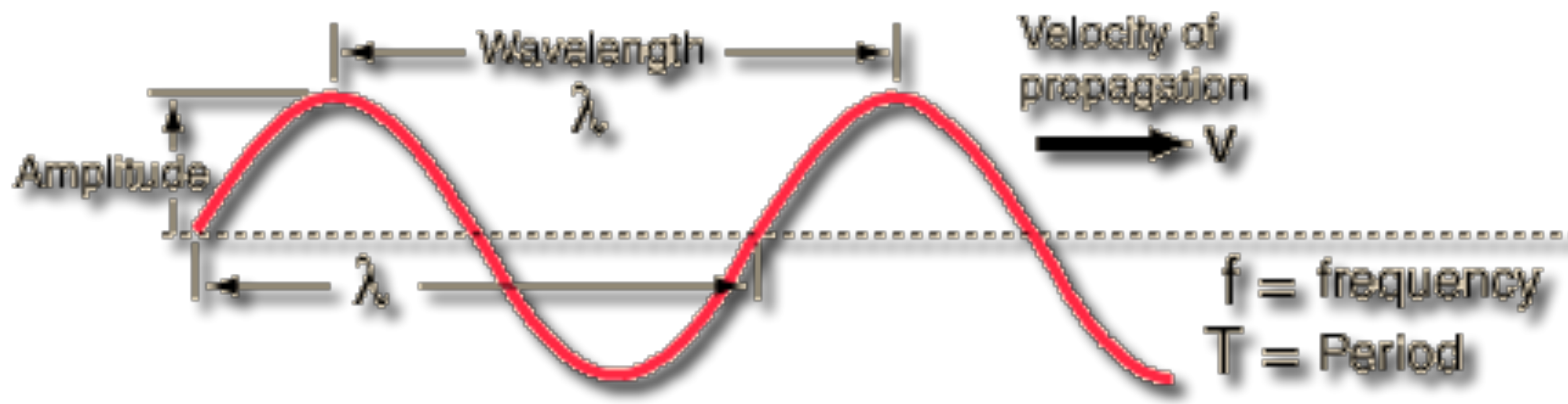
(Chapter 28)

6.1 Periodicity and Frequency

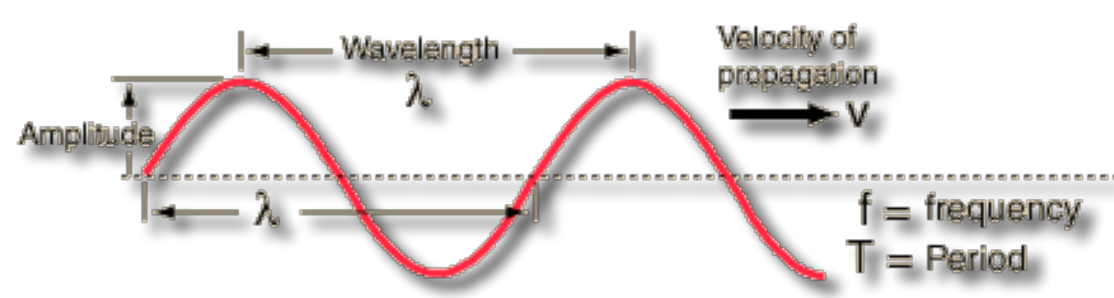
NTHU



Long λ, Larger period, Low frequency
slow fluctuation in signal



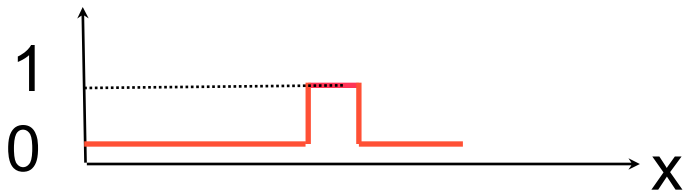
Short λ, smaller period, High frequency
rapid fluctuation in signal



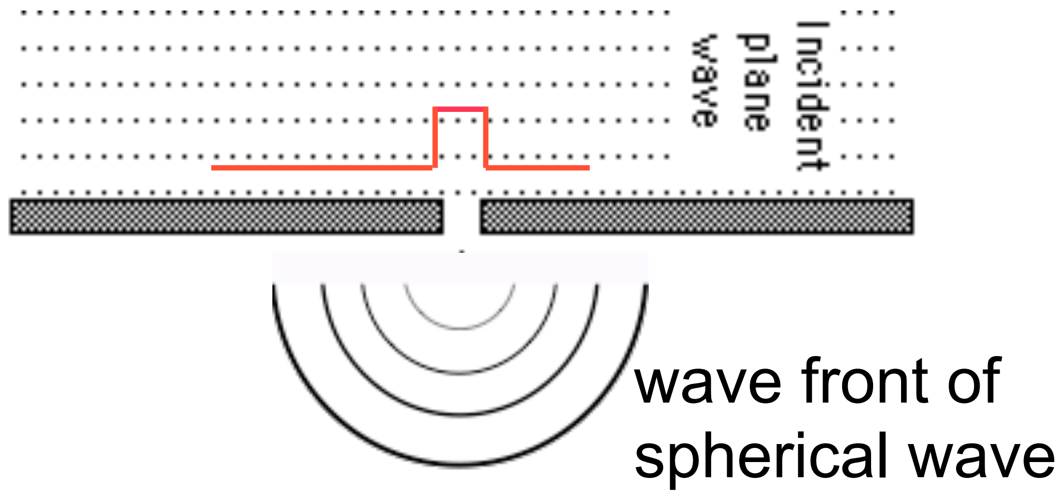
$\lambda = v \times T$
$= v/f$

$T = 1/f$

6.2.1 Fresnel and Fraunhofer Diffraction of Single Slit

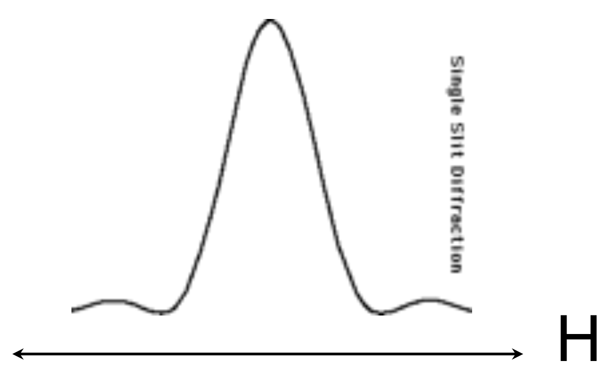


Fresnel Diffraction
(near field)



Fraunhofer Diffraction
(far field)

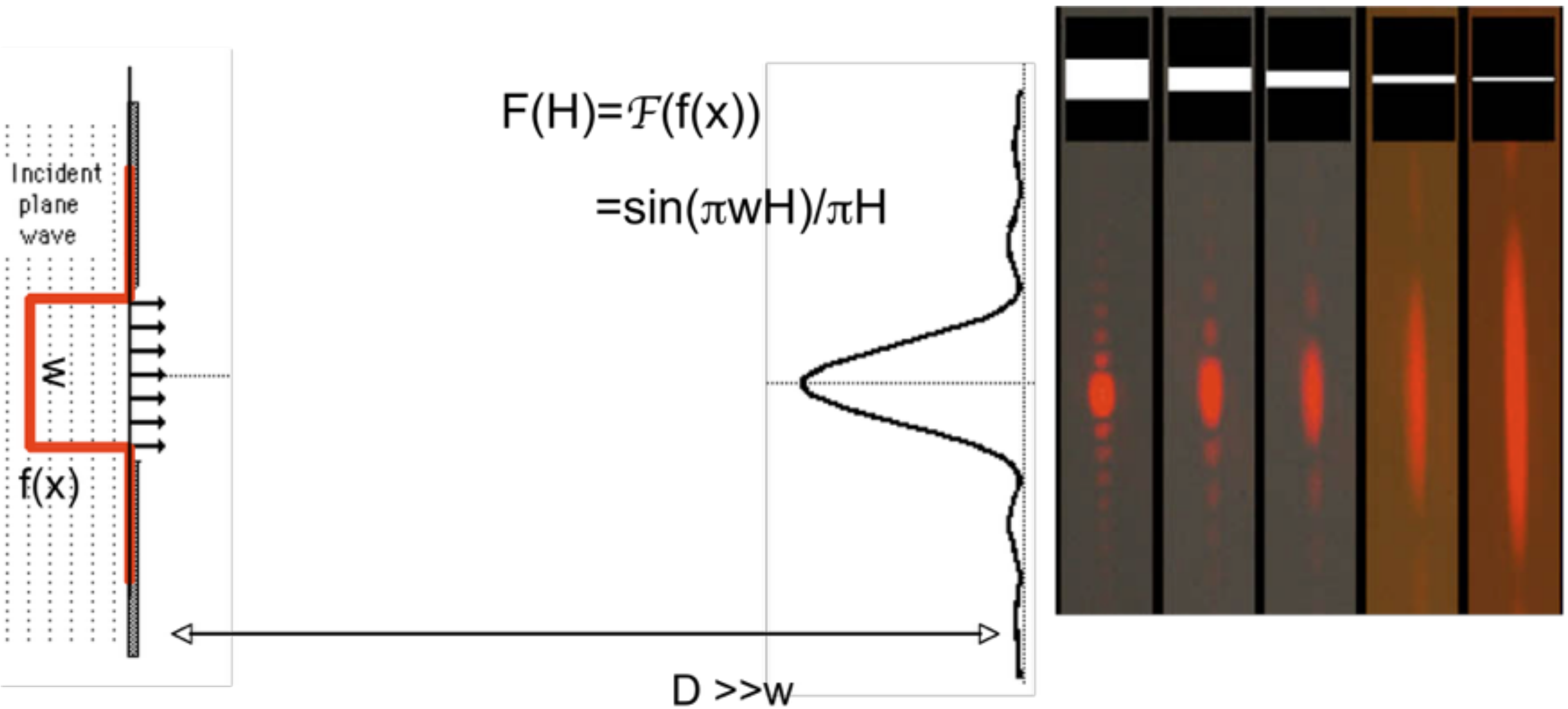
Fourier Transform of 1
flat hat functions



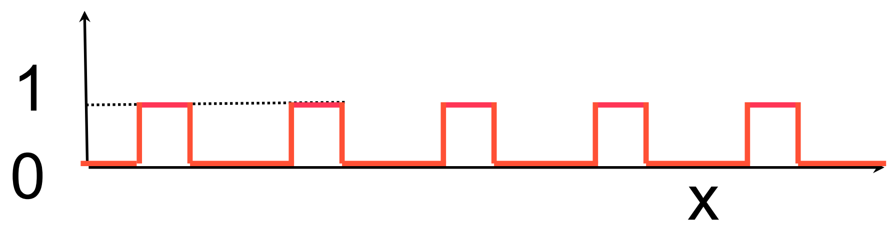
Fourier Transform of Top-Hat Function

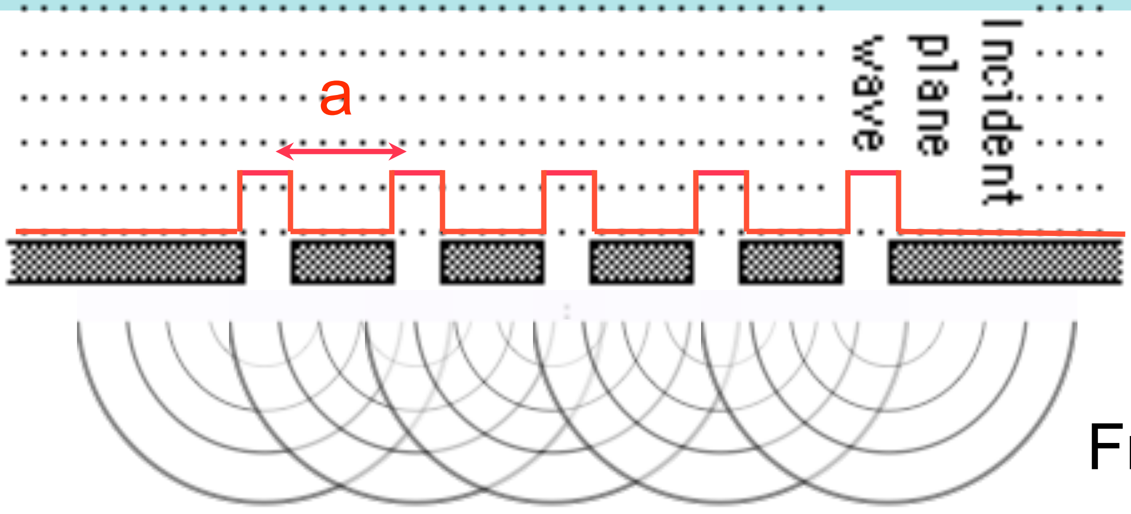
Fraunhofer Diffraction

NTHU



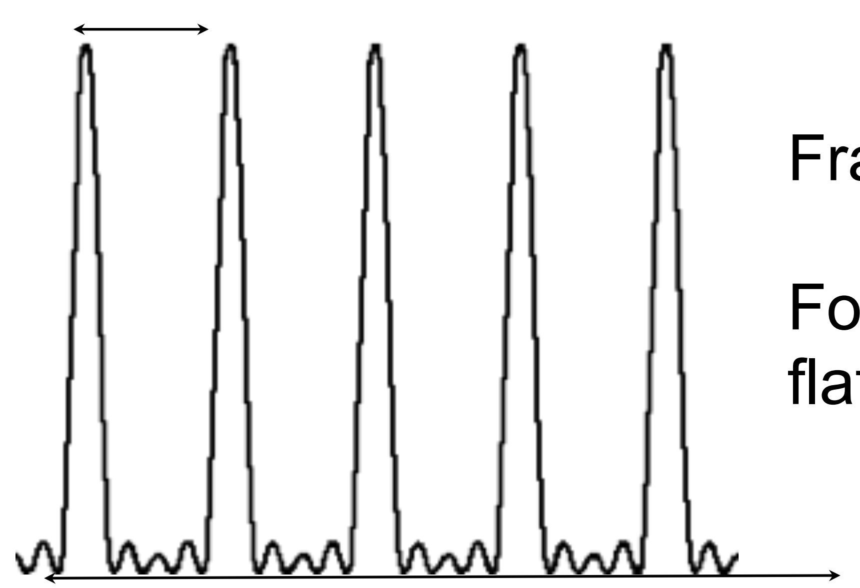
6.2.2 Fresnel and Fraunhofer Diffraction of Multi-grating





Fresnel Diffraction

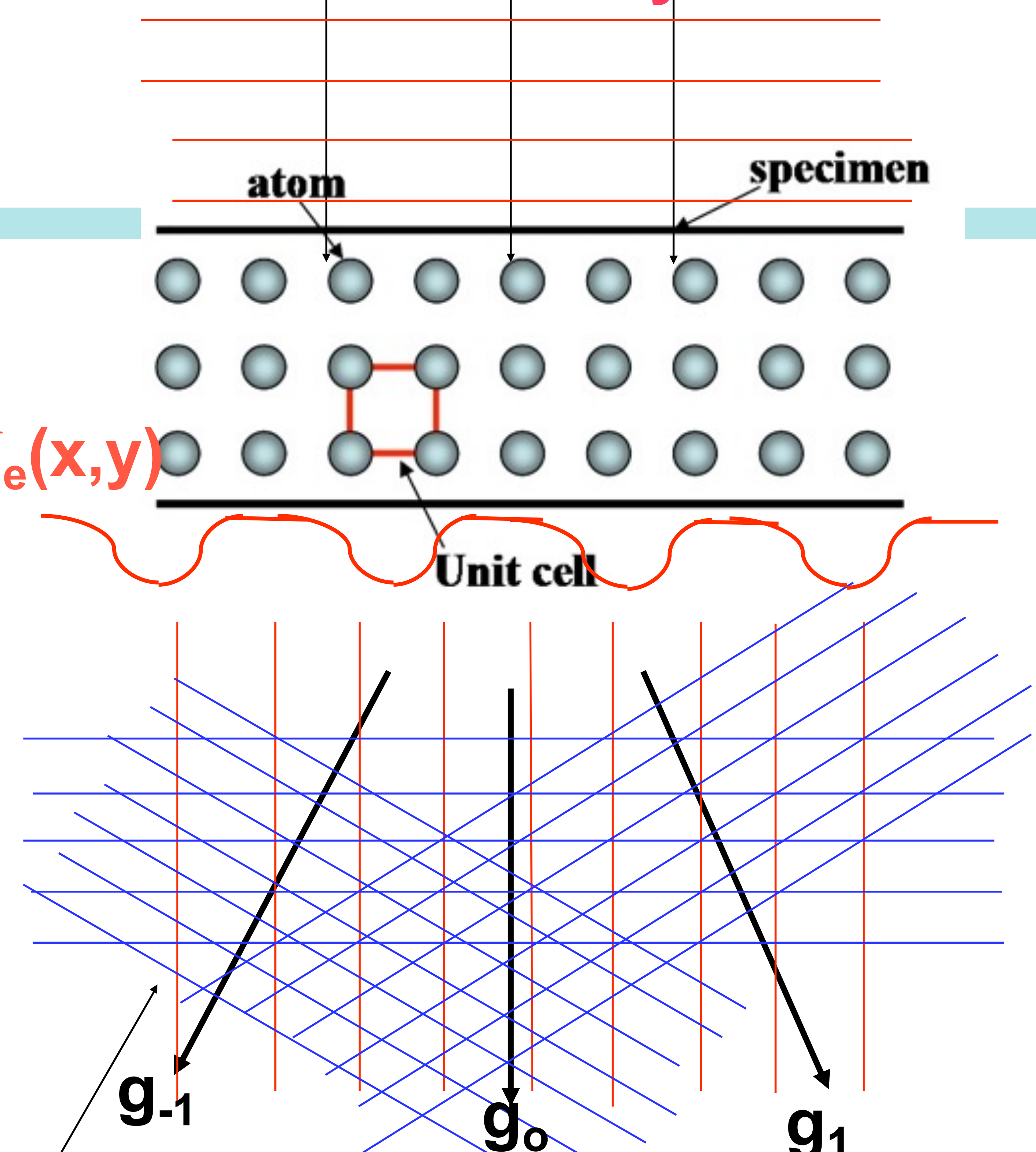
interference of 5 spherical waves

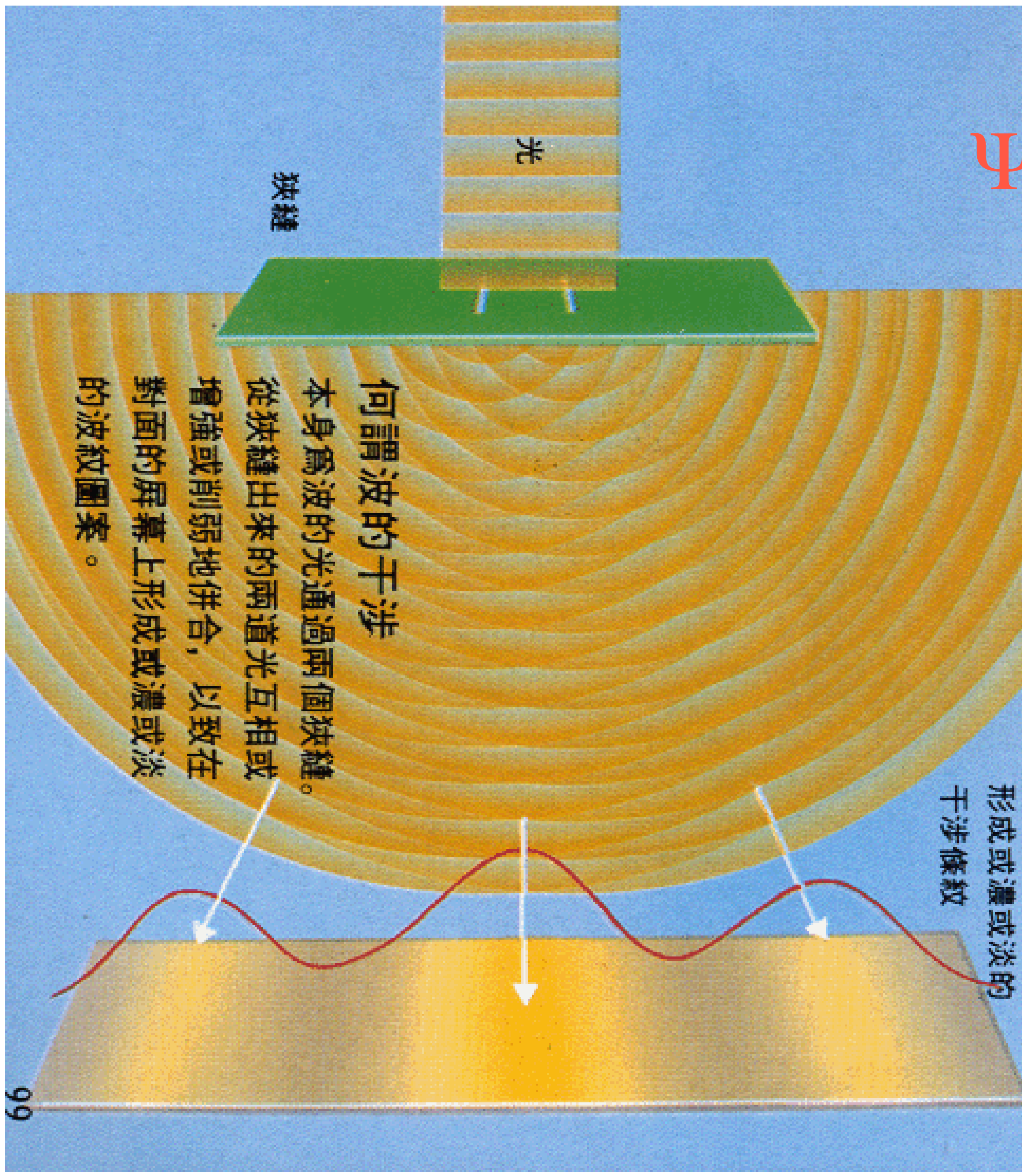


Fraunhofer Diffraction

Fourier Transform of 5 flat hat functions

6.3 Interaction of Electron Wave with Crystal





Ψ_e is composed of many Fourier components

$$\Psi_e(x,y) = \sum_{H=-g}^{g} F(H)\exp(-2\pi H \bullet r)$$

亮線位置不一定與原子柱位置重疊

TEM CENTER

Fourier Synthesis

NTHU

$$f(x) = F(0) + \sum_n F(H_n)\exp(-2\pi nx/a)$$

$$H_n = 2\pi n/a$$

$$f(x) = F(0) + \sum_n F(H_n)\exp(-H_n x)$$

Amplitude — Phase

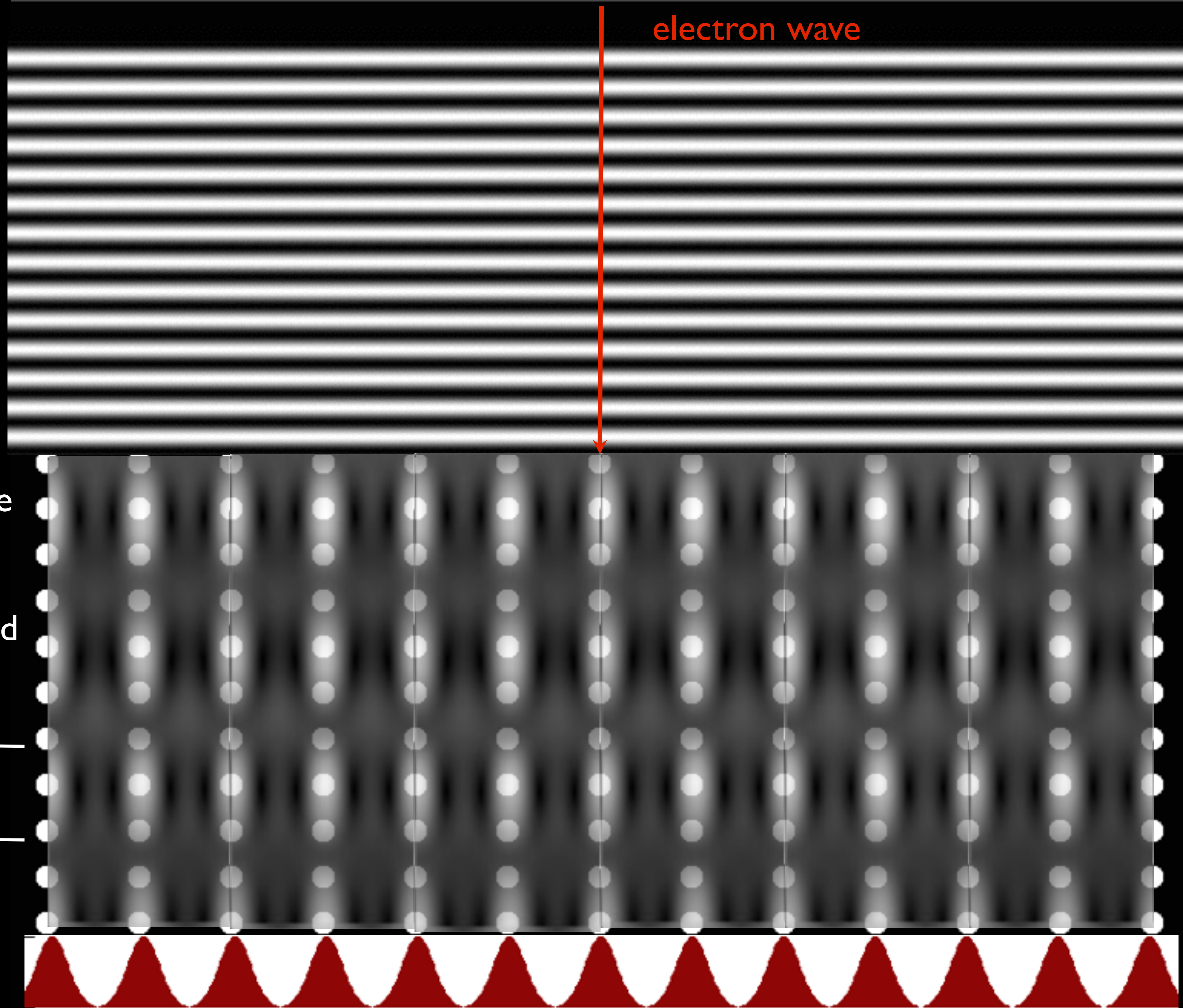
So, the f(x) can be regarded as a summation of a series of “WAVE”

Electron Channeling

wave propagates inside crystal

~ electrons are trapped along the atomic columns

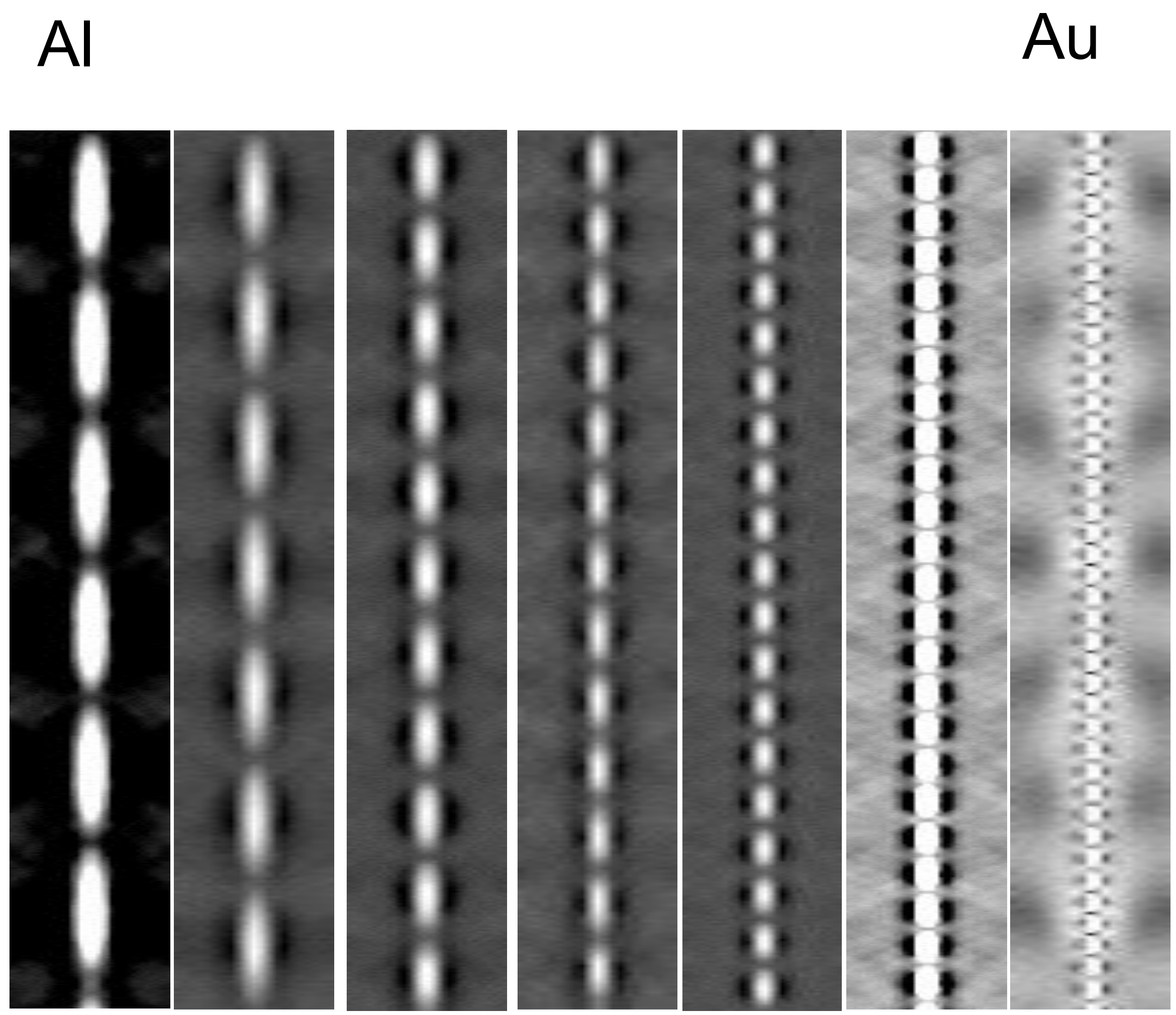
depends on z

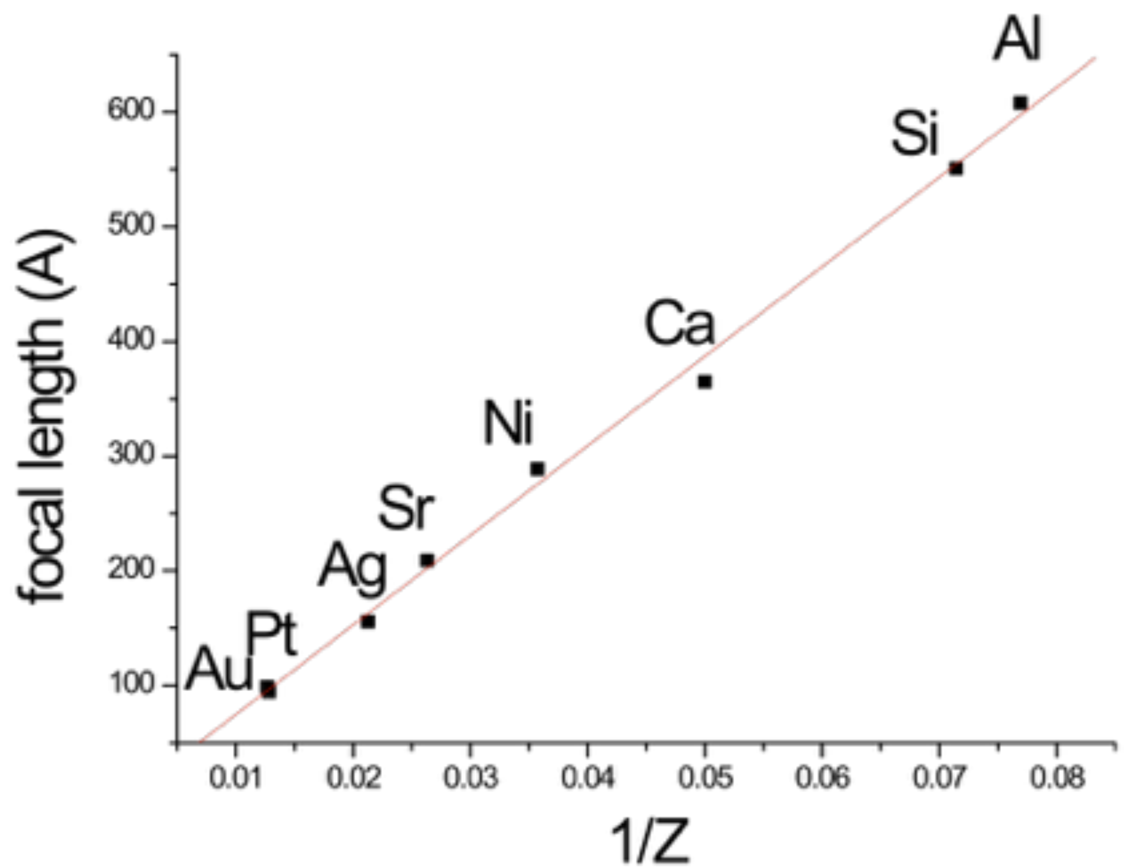


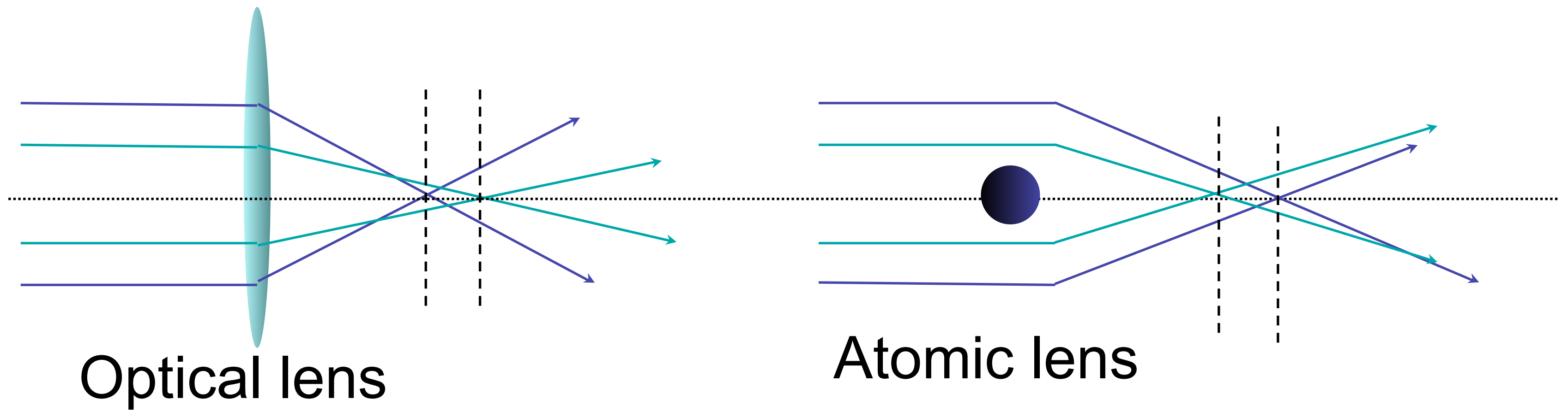
Exit Wave

6.3 Wave Propagates inside Crystal

Channeling Theory



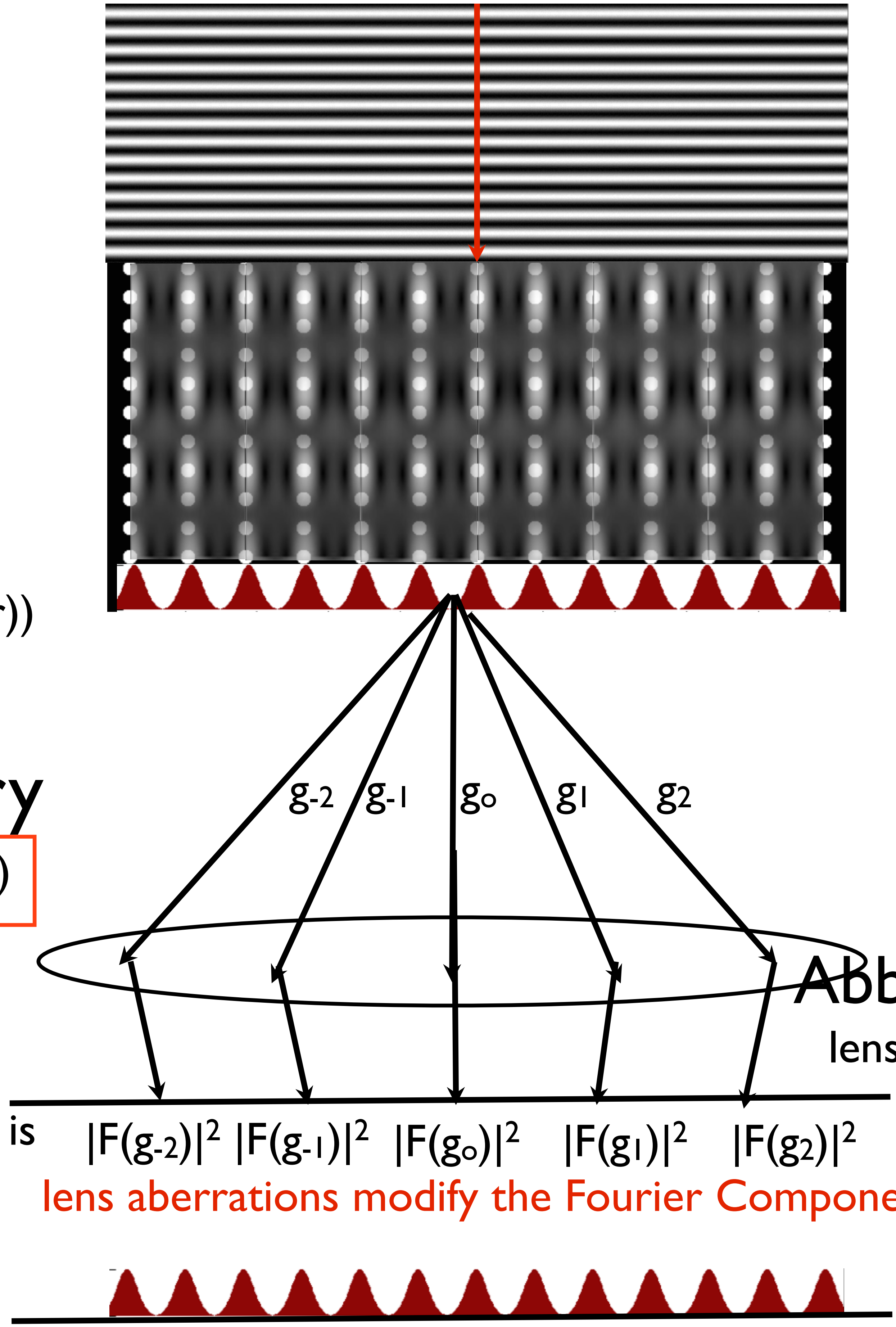




electron wave

exit wave

$\psi_e(r)=A(r)\exp(i\varphi(r))$



Fourier Theory

$\psi_e(x,y)=\Sigma F(g)\exp(2\pi gr)$

Abbe Microscopy Theory

lens does two Fourier transforms

Physics

Focal plane

each Fourier component is called diffracted wave

image plane

$I=|A(r)|^2$, Phase lost

6.4 Fourier Synthesis

NTHU

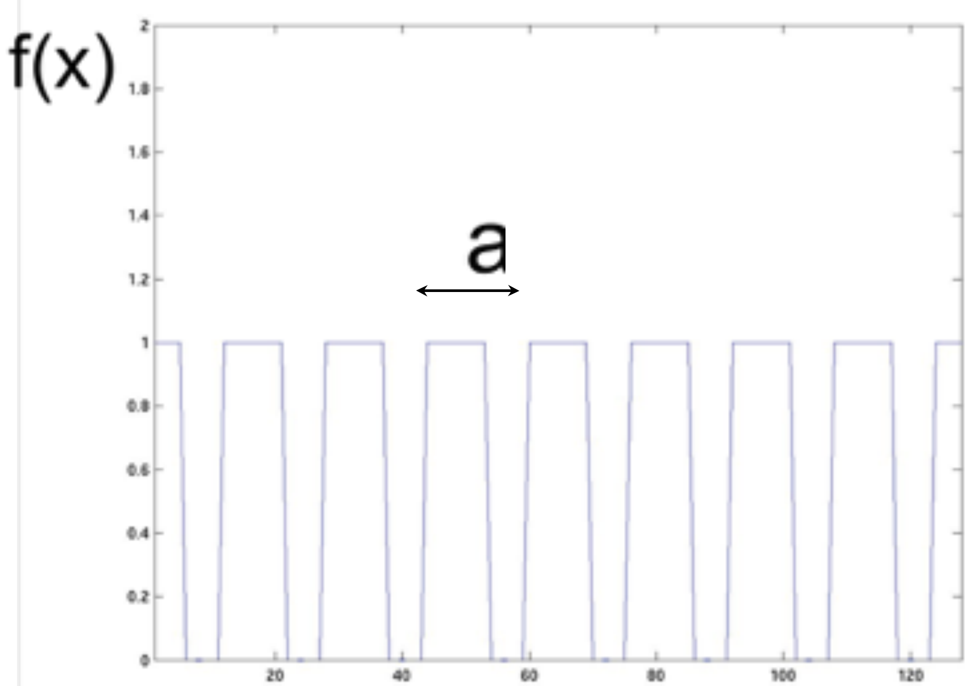
An function f(x) can be expressed in terms of sum of a series of Fourier coefficients F(H) multiply by the sine (or cosine, or exponential) functions

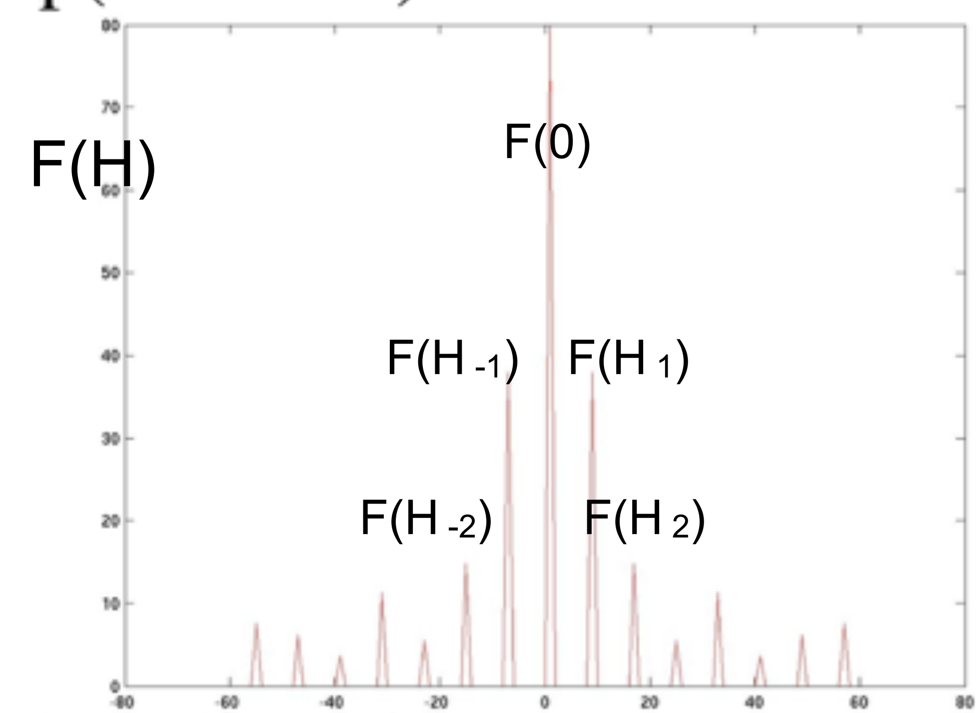
Periodicity
(real space, Crystal)

Frequency
(reciprocal space,Fourier Space, Diffraction space)

Inverse Fourier Transform

$$f(x) = F(0) + \sum_n F(H_n)\exp(-2\pi nx/a)$$





$$F(H) = f(0) + \sum_n f(x_n)\exp(2\pi nx/a)$$

Fourier Transform

H

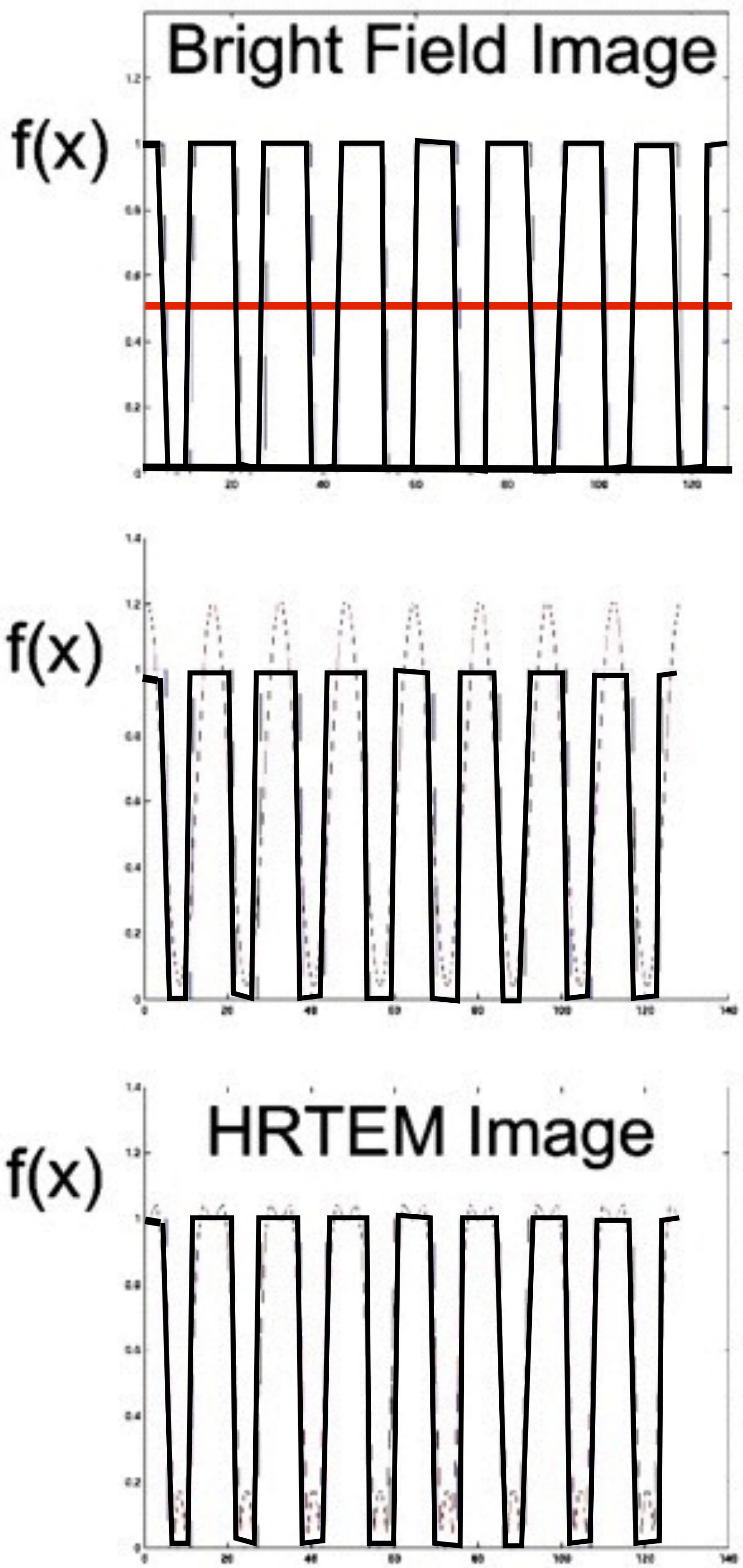
low frequency

high frequency

Fourier Synthesis

Periodicity
(real space, Crystal)

Frequency
(reciprocal space, Fourier Space, Diffraction space)

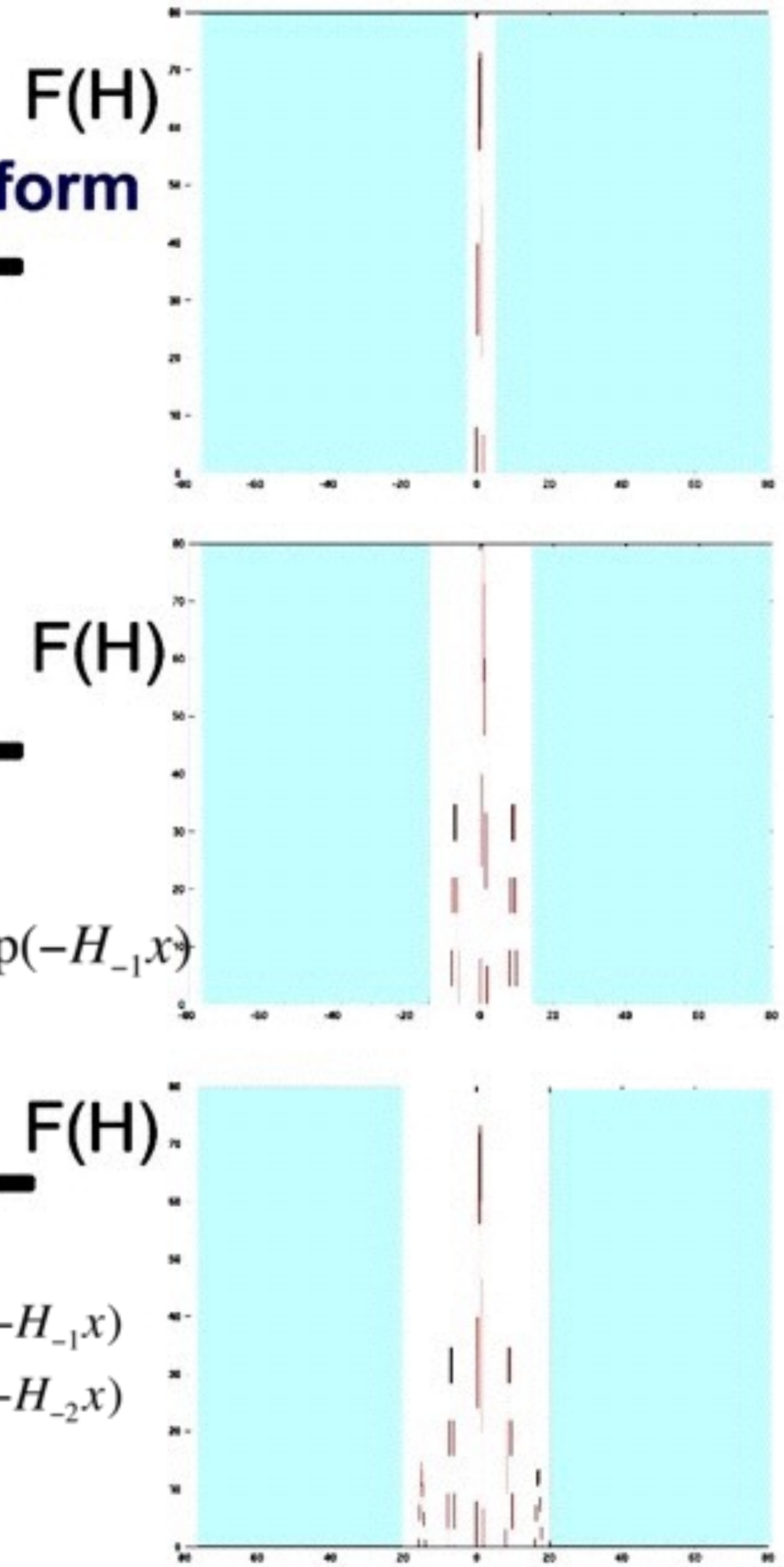


Inverse Fourier Transform

$$f(x) = F(0)\exp(-0.x)$$

$$f(x) = F(0) + F(H_1)\exp(-H_1x) + F(H_{-1})\exp(-H_{-1}x)$$

$$f(x) = F(0) + F(H_1)\exp(-H_1x) + F(H_{-1})\exp(-H_{-1}x) + F(H_2\exp(-H_2x) + F(H_{-2})\exp(-H_{-2}x)$$

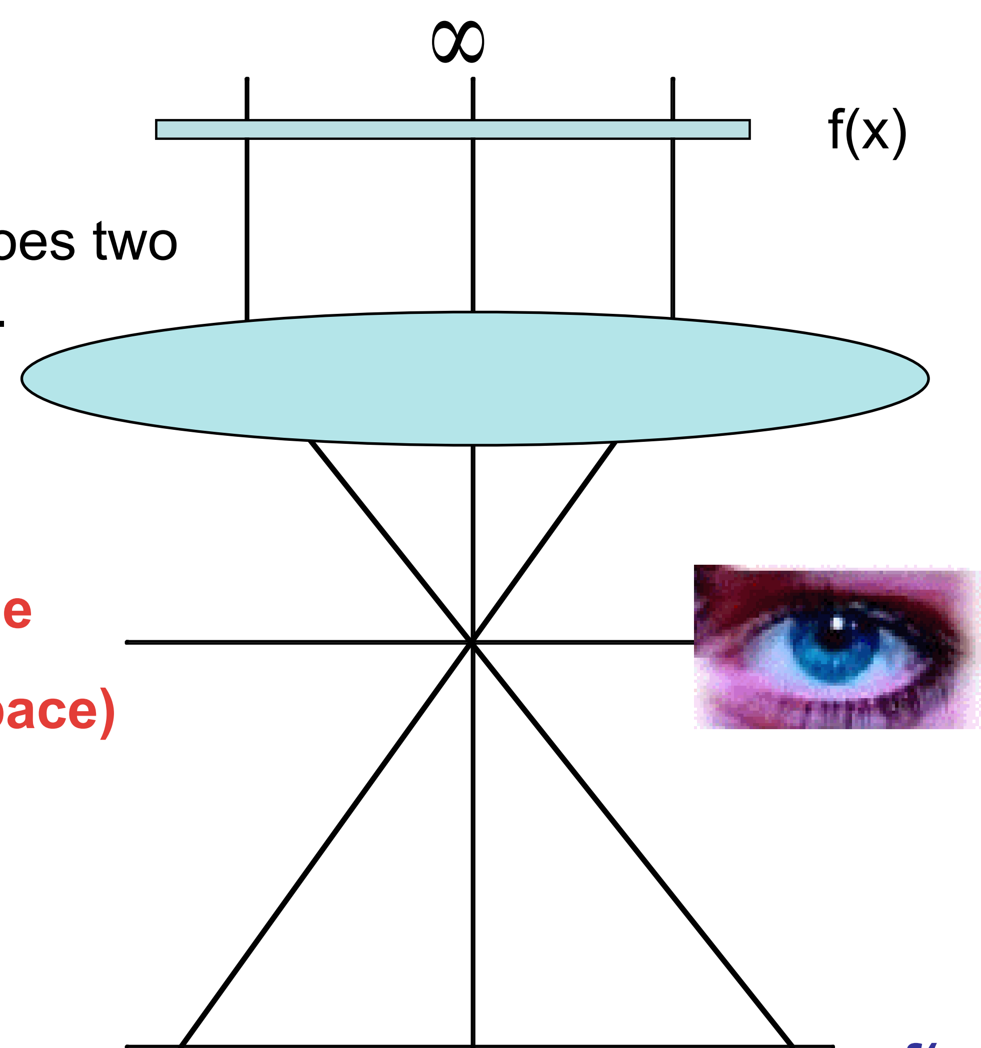


Low Frequ

High Freque

6.5 Abbe Theory of Microscopy

A perfect microscope does two Fourier transformations.



One at **back focal plane**

(Fourier, reciprocal space)

For an observer at the focal plane, the beam comes from infinite. So he observes a **Fraunhofer Diffraction** pattern $F(H)=\mathcal{F}(f(x))$

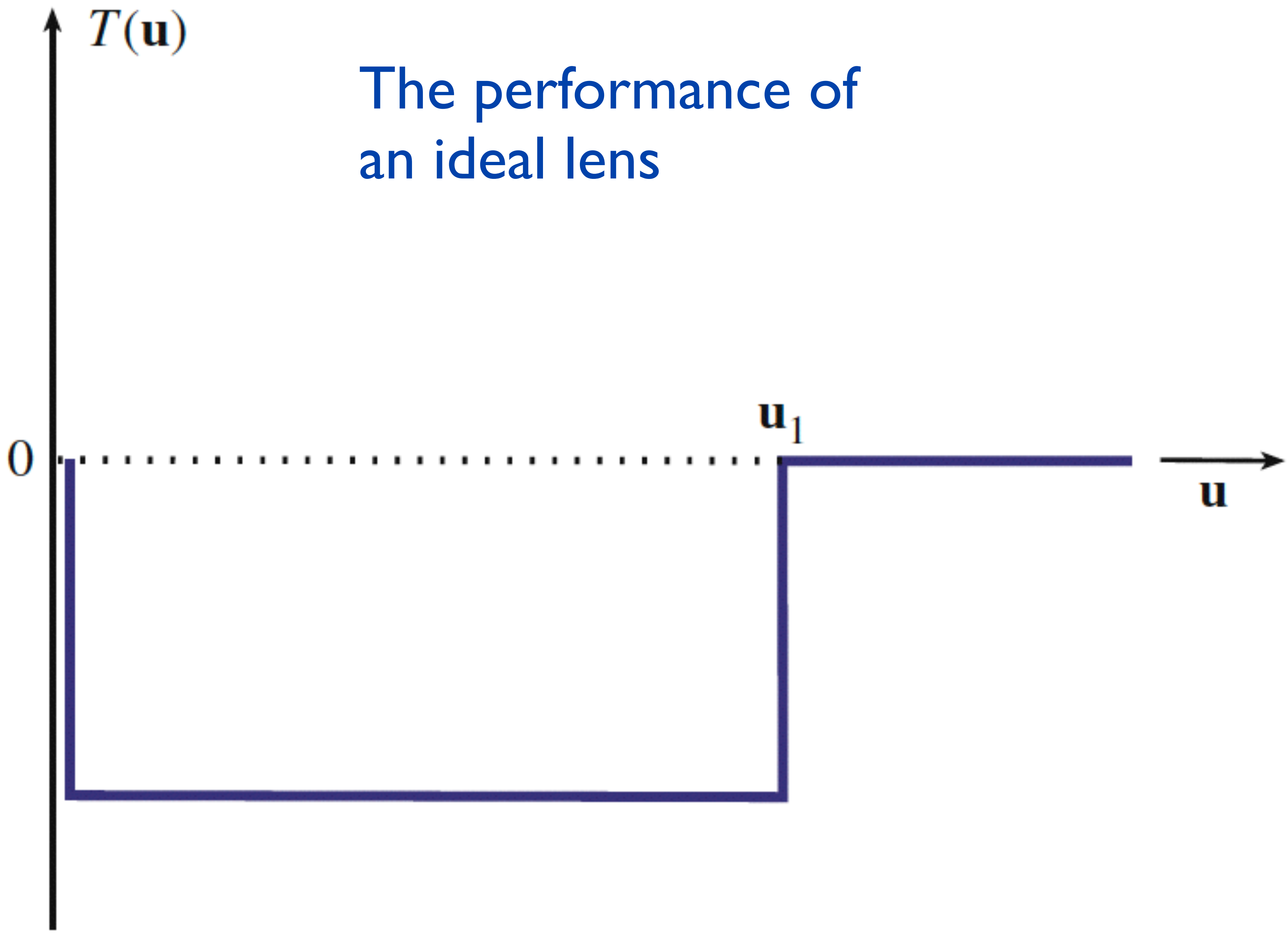
One at **image plane**

$f(-x/M)= \mathcal{F}^{-1}(\mathcal{F}(f(x)))$

Inverted and Real Image

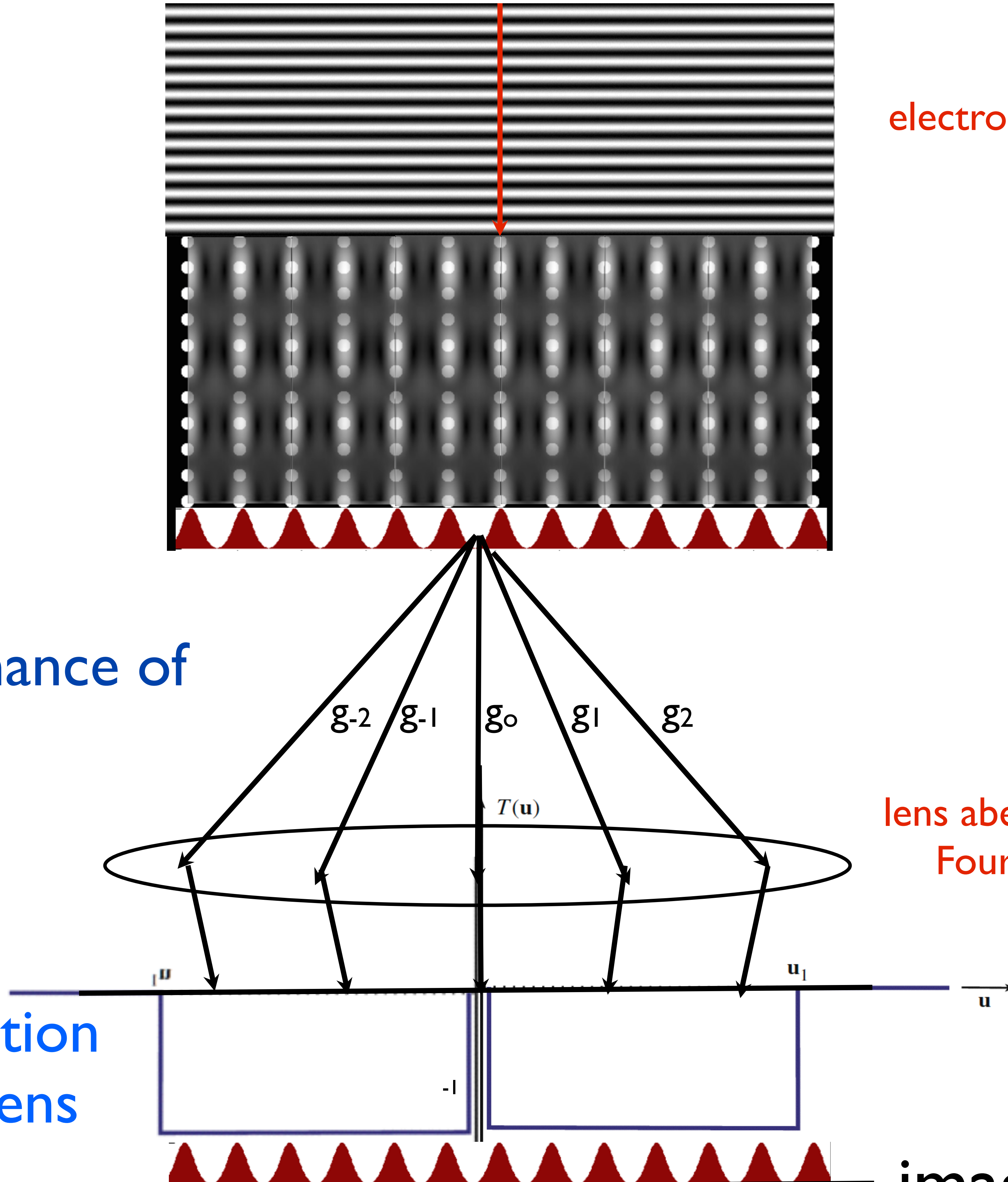
Ideal Transfer function

The performance of
an ideal lens



electron wave

The performance of an ideal lens



lens aberrations modify the Fourier Components

transfer function for an ideal lens

image plane

$I=|A(r)|^2$, Phase lost

6.6 Lens Aberrations

TEM CENTER

NTHU

- A.Defocus (correctable)

  -- The wave propagates a finite distance from the position of exact focus (Change phase of Fourier waves)

- B.Spherical aberration (correctable)

  --lens has different focus power to beam from different angles。(Change phase of Fourier waves)

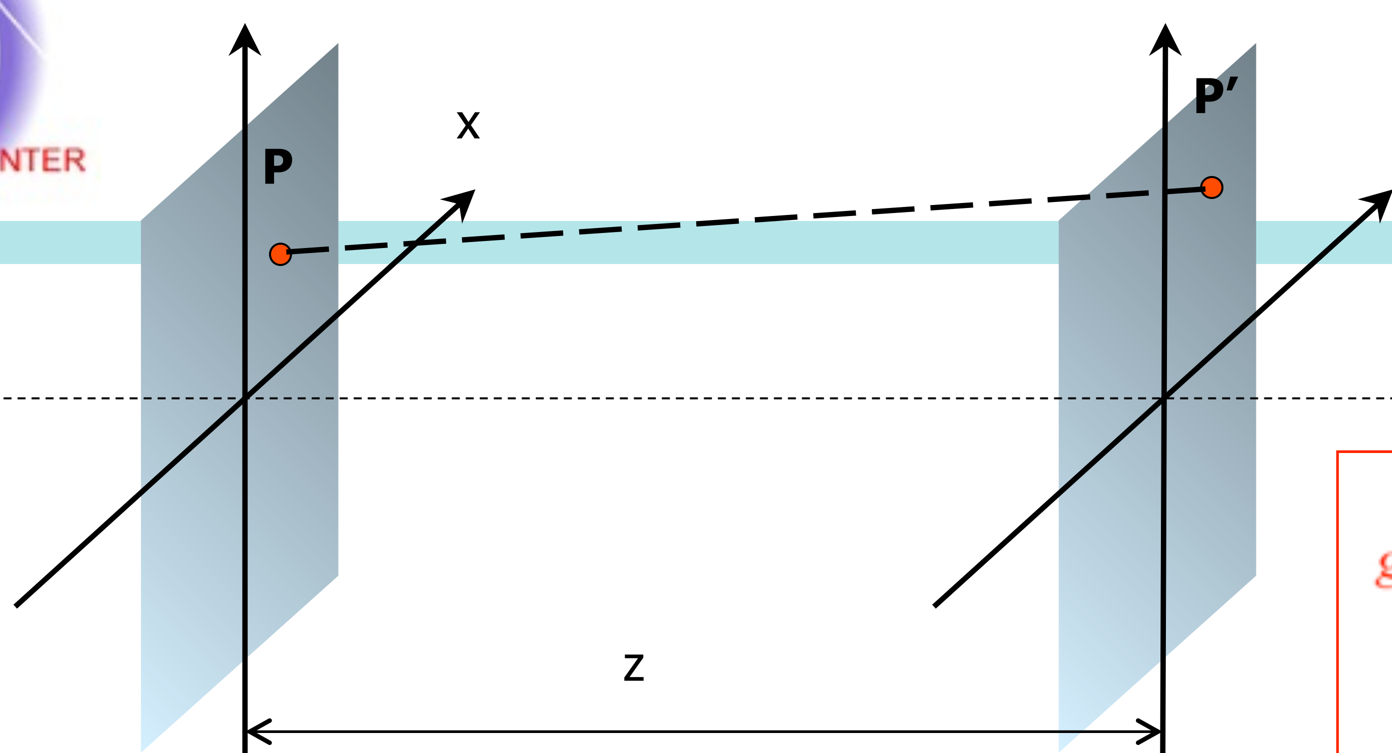
- C. Chromatical aberration (correctable)

  -- lens has different focus power to beam with different wavelength (energy)(Change modulus of Fourier waves)

- D. Spatial Coherency (partially correctable)

  -- lens has different focus power to beam with different wavelength (energy)(Change modulus

Defocus and Fresnel Diffraction



$$g(x,y)=\int_{-\infty}^{\infty} f(x',y')\phi(x-x',y-y')dx'dy'$$
$$= f(x,y)*\phi(x,t)$$

$$\psi_1(x,y) \qquad\qquad \psi_2(x,y)$$

$$\psi_2(x,y)\approx\frac{i\exp(-2\pi iz/\lambda)}{\lambda z}\iint\psi_1(x,y)\exp\{-\frac{i\pi}{\lambda z}[(x-X)^2+(y-Y)^2]\}dXdY$$

$$=A\psi_1(x,y)\otimes\exp\{-\frac{i\pi}{\lambda z}[x^2+y^2]\}$$

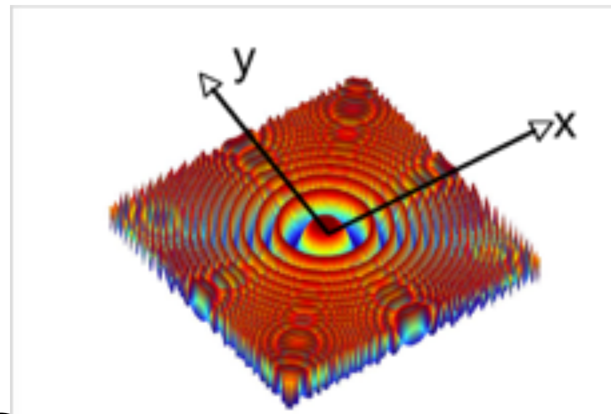
$$\psi_2(x,y)=\psi_1(x,y)\otimes P_z(x,y)$$

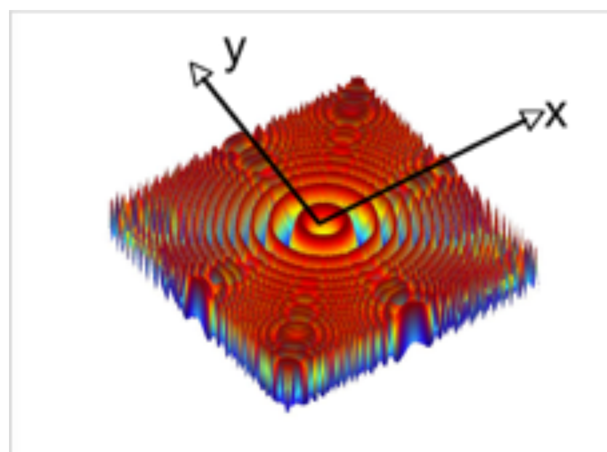
Convolution relates information between Real Space--> Real Space.

When a signal propagates to a finite distance z, the information will be modified by convolution with a propagator $P_z(x,y)$

Example of Fresnel Diffraction

$\otimes$

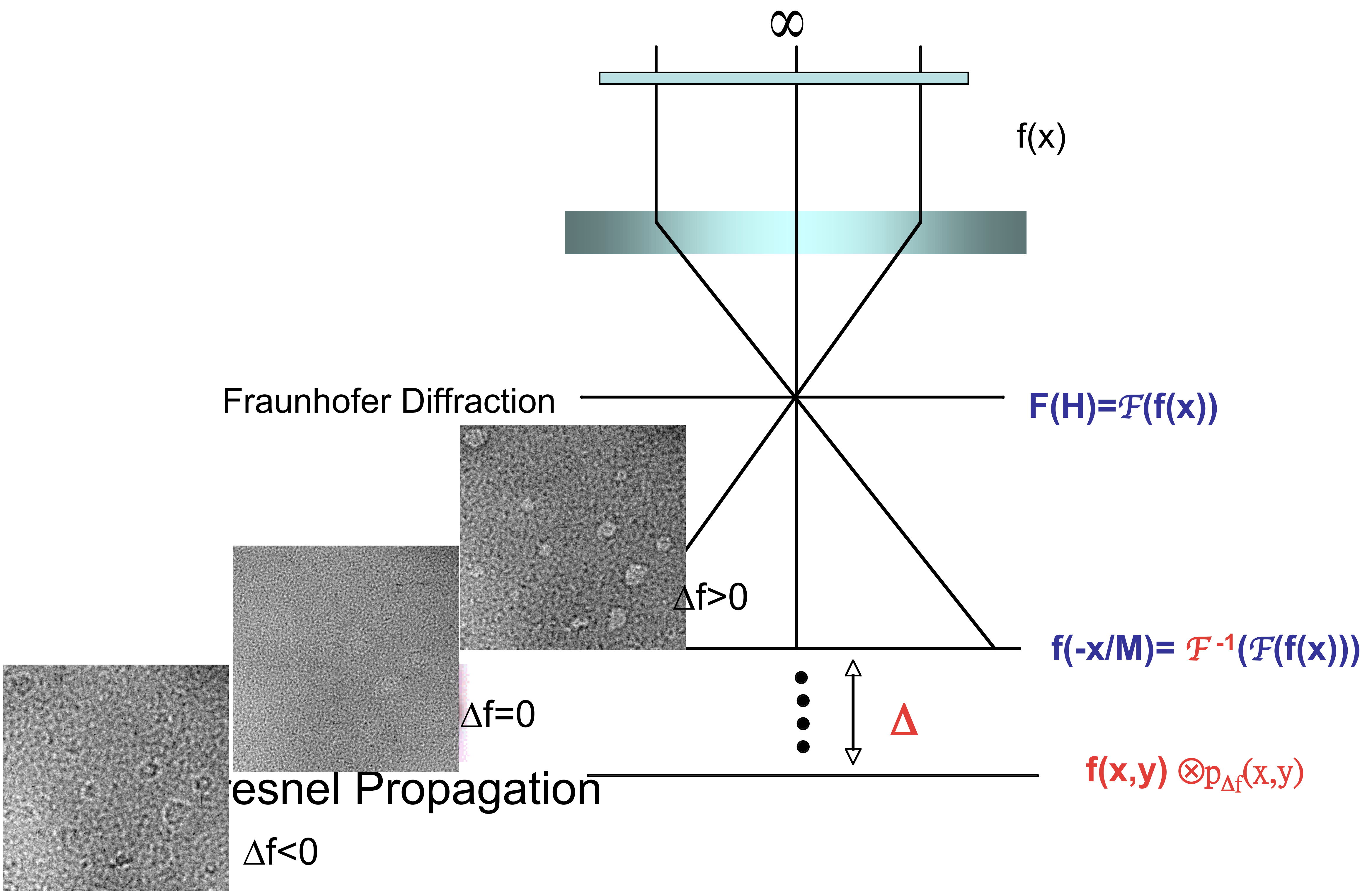




$$p_z(x,y)=\exp(-2\pi\iota\lambda(x^2+y^2)/2z)$$

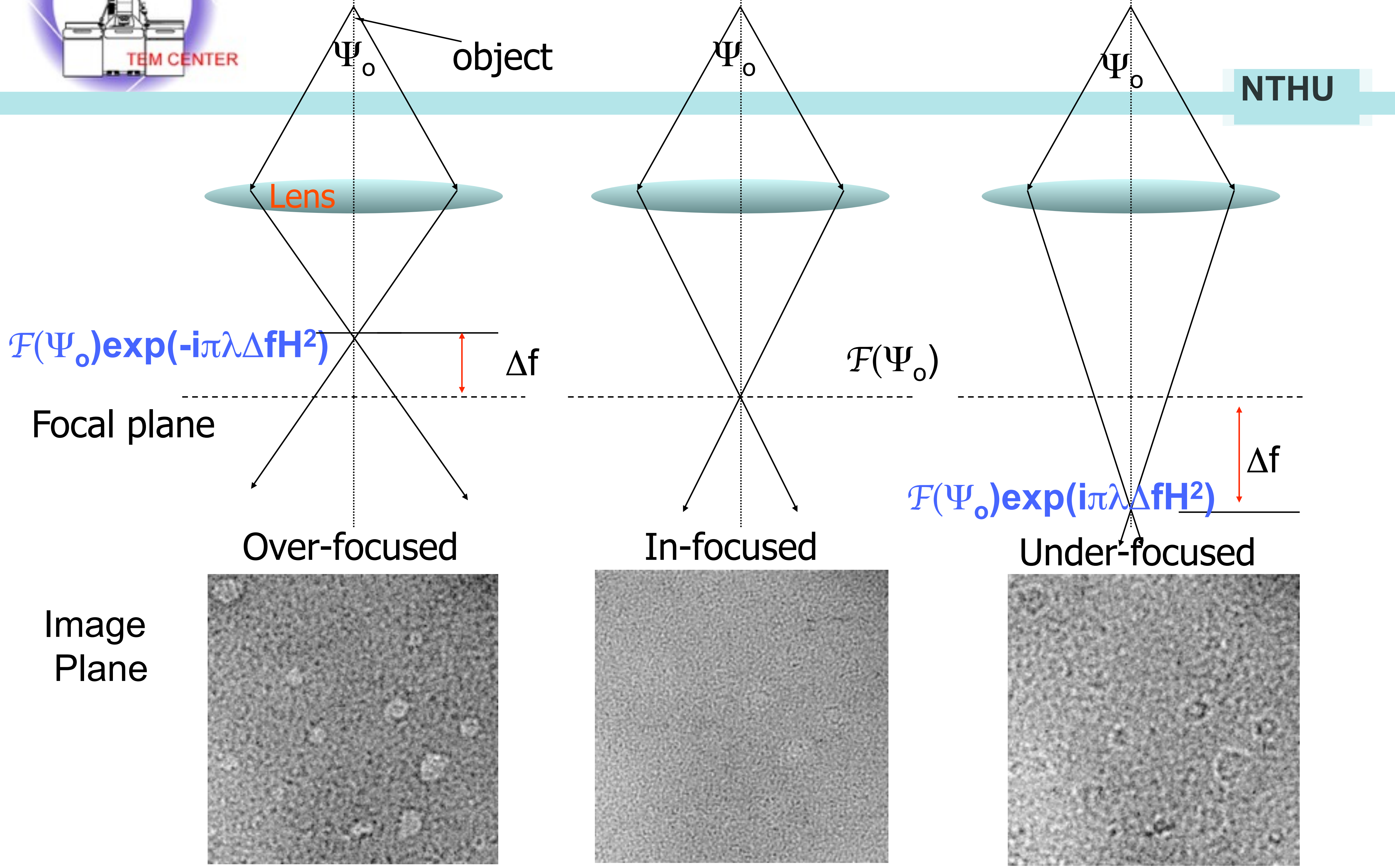
6.6.1 Fresnel Propagation in de-focus plane

NTHU



Aberration From Focus

(造成相位差: 越高頻修正越大)

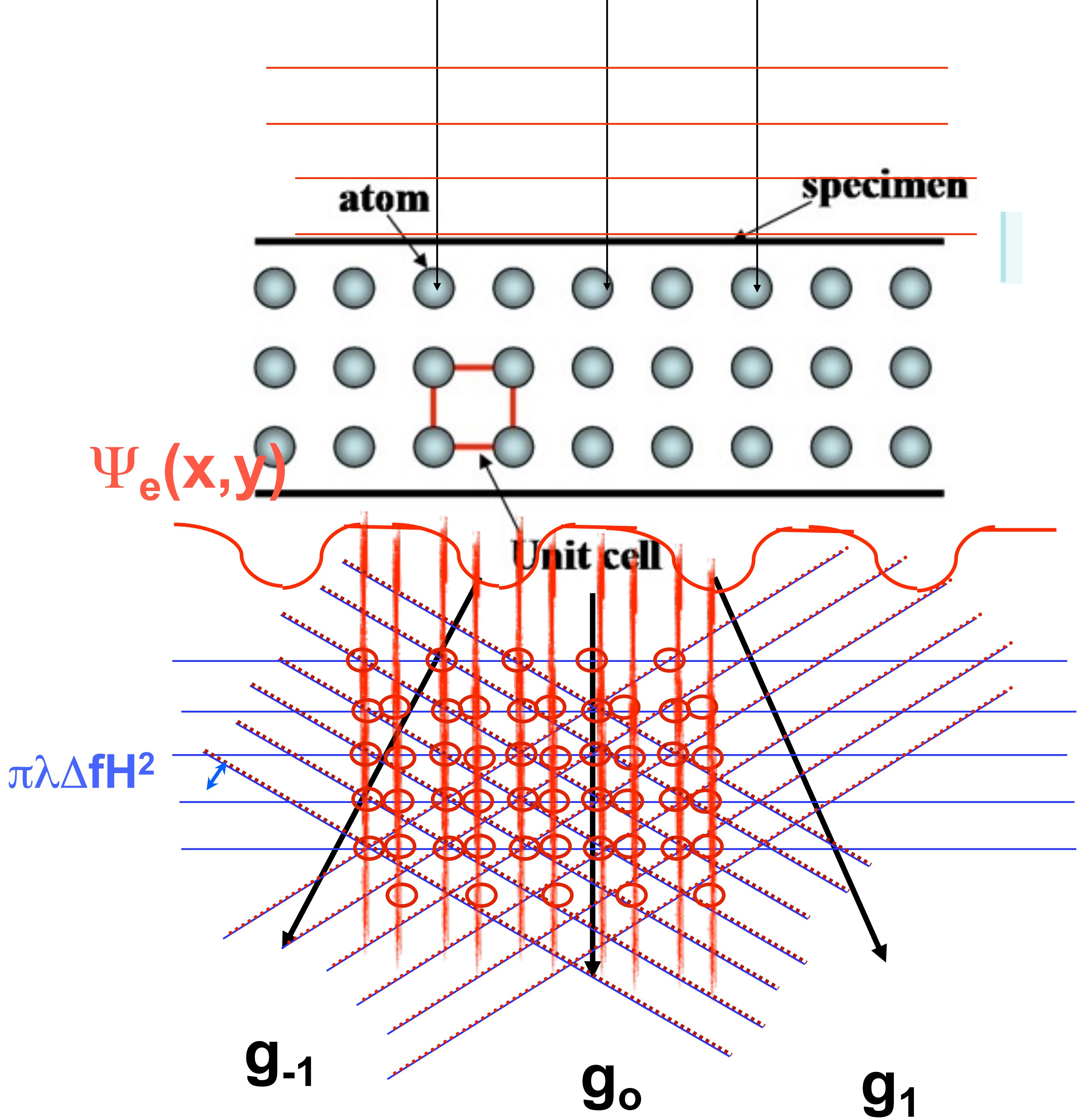


$\Psi_i = [\Psi_o \otimes \exp(-i\pi(x^2+y^2)/\lambda\Delta f)]$

$I = \Psi_i \Psi^*_i$

$\Psi_i = \Psi_o$

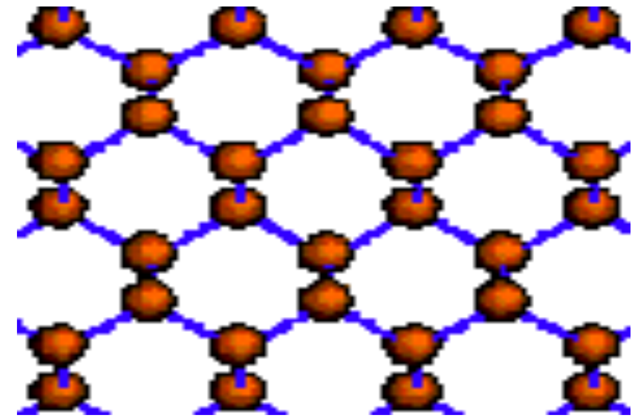
$\Psi_i = [\Psi_o \otimes \exp(i\pi(x^2+y^2)/\lambda\Delta f)]$

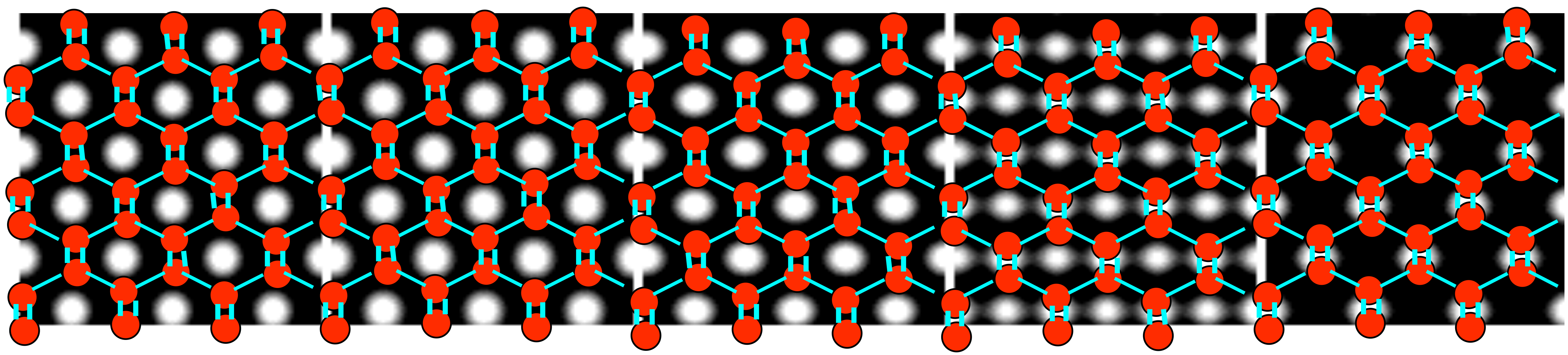


Ψ_e is composed of many Fourier components

高分辨影像之行為隨著欠焦而變

Si [110], 400keV





Δf= -16nm -32 nm -48nm -64nm -80nm

Scherzer focus =-48nm

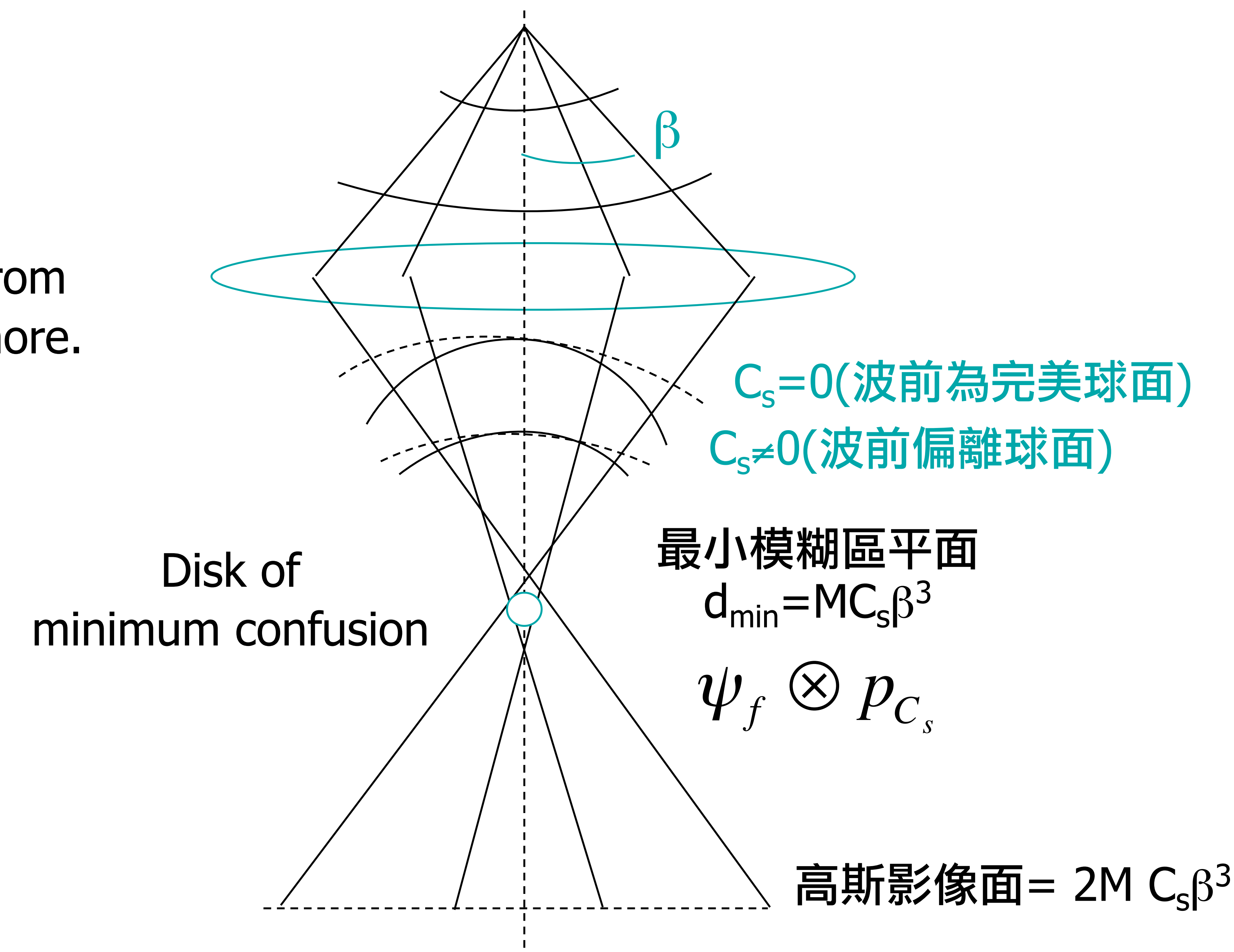
B. Spherical Aberration

1. lens has stronger focus power in the edge

2. electron beam enters from larger angle is refracted more.

- C_s : coefficient of sphical aberration

  ~ 1mm ~ 3mm
  much larger than the wavelength of electron



$$\psi_f \otimes p_{C_s} = \Im^{-1}[\Im(\psi_f) \bullet P_{C_s}]$$

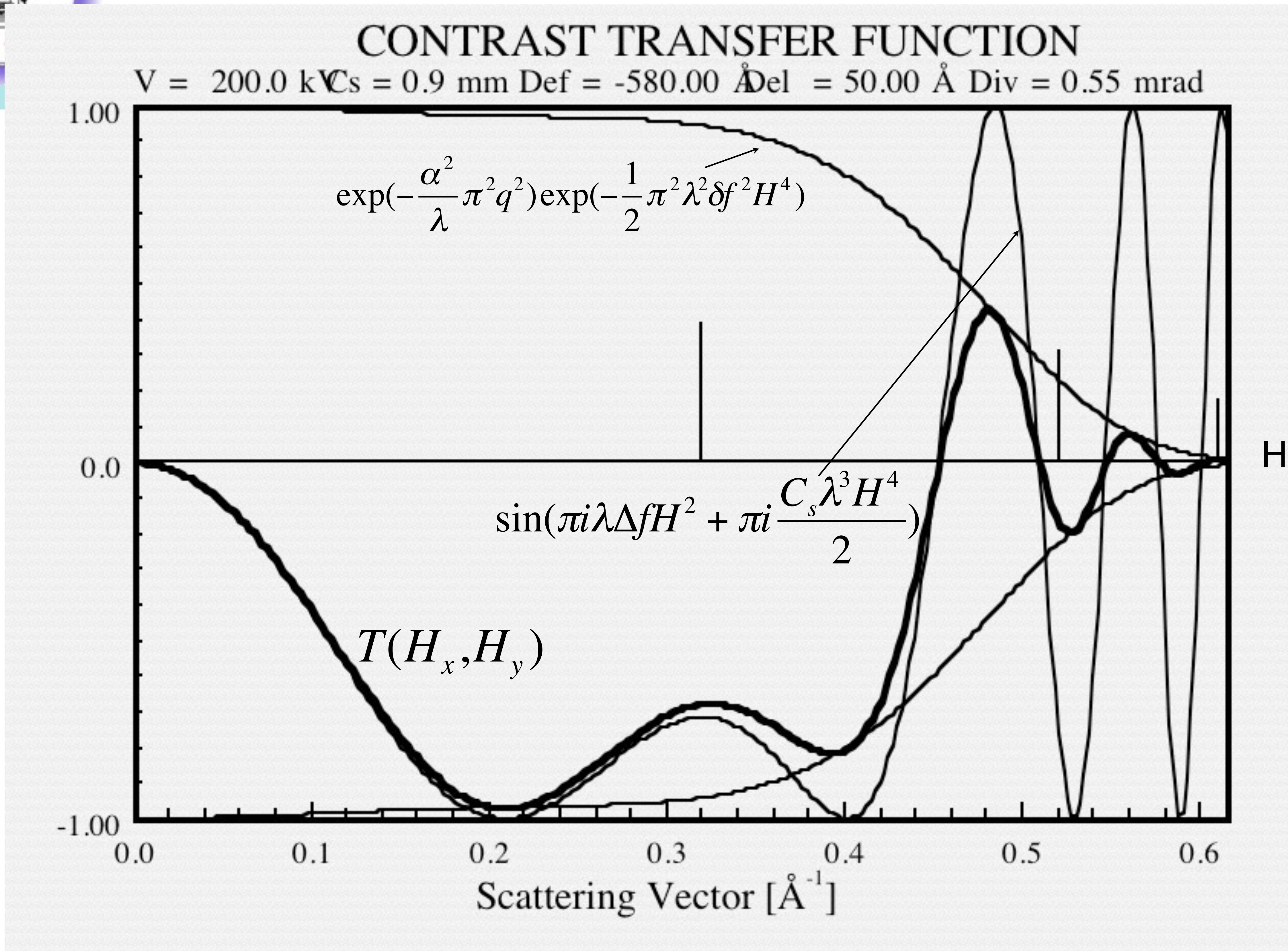
$$P_{C_s} = \exp(2\pi i \frac{C_s \lambda^3 H^4}{4}) = \exp(2\pi i \frac{C_s \lambda^3 (H_x{}^2 + H_y{}^2)^2}{4})$$

The spherical aberration introduces an extra "phase factor in reciprocal space expression. The signal of higher frequency is modified much more. (Change the position of wave peak)

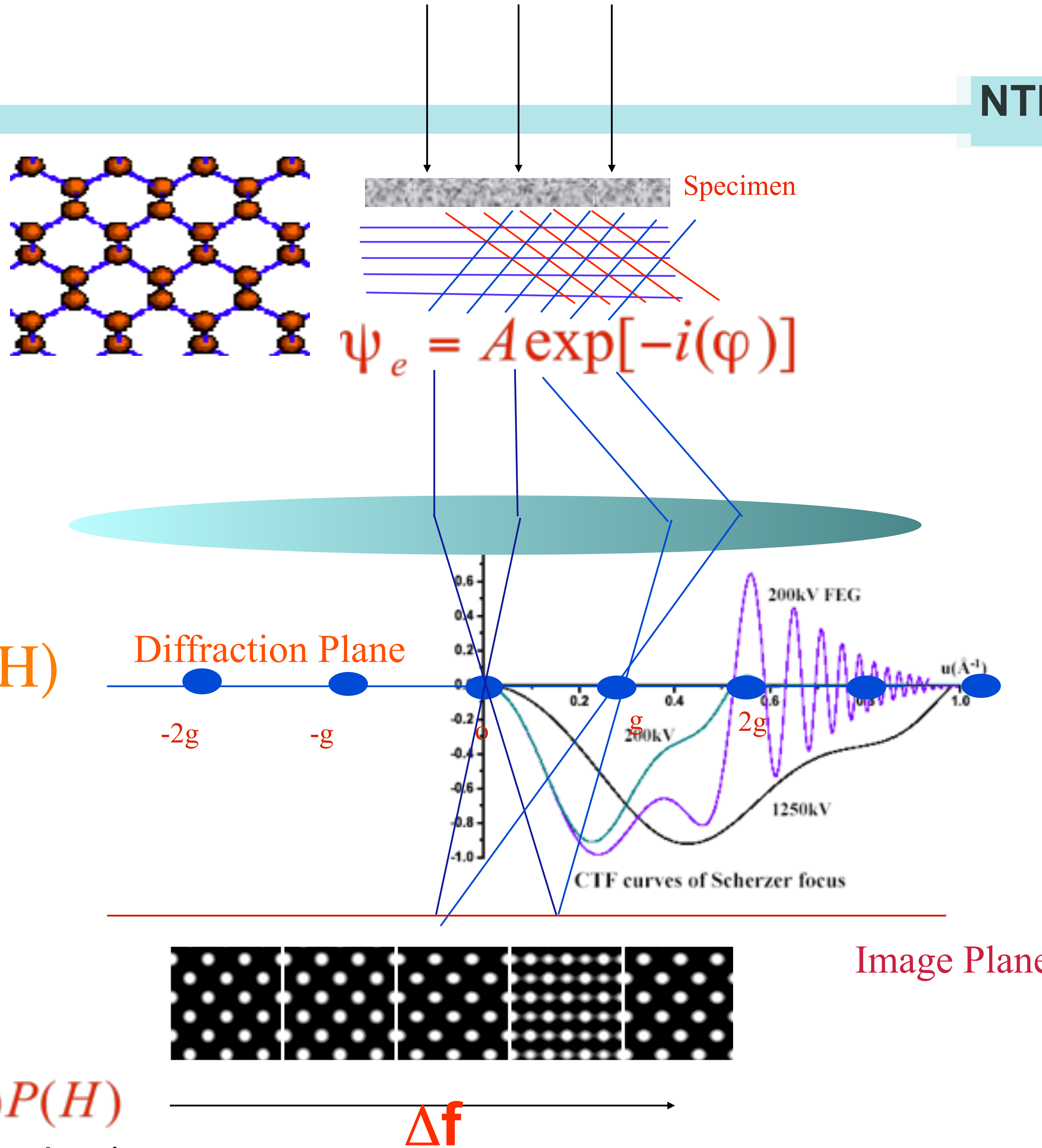
Total Phase Shift from Lens Aberration

$$\chi = \pi i \lambda \Delta f H^2 + \pi i \frac{C_s \lambda^3 H^4}{2}$$

defocus spherical aberration


CONTRAST TRANSFER FUNCTION
V = 200.0 kV Cs = 0.9 mm Def = -580.00 Å Del = 50.00 Å Div = 0.55 mrad
$\exp(-\frac{\alpha^2}{\lambda}\pi^2 q^2)\exp(-\frac{1}{2}\pi^2\lambda^2\delta f^2 H^4)$
$\sin(\pi i\lambda\Delta f H^2 + \pi i \frac{C_s\lambda^3 H^4}{2})$
$T(H_x, H_y)$
1.00
0.0
-1.00
0.0
0.1
0.2
0.3
0.4
0.5
0.6
Scattering Vector [Å^{-1}]
H

Transfer Function of Aberrated Lens



$$\Psi_g = F(\Psi_e)\exp(i\chi)P(H)$$

$$\psi_i \psi_i^* = I$$

$$\psi_i = \psi_e \otimes \Im^{-1}\exp(i\chi)P(H)$$

(phase lost)

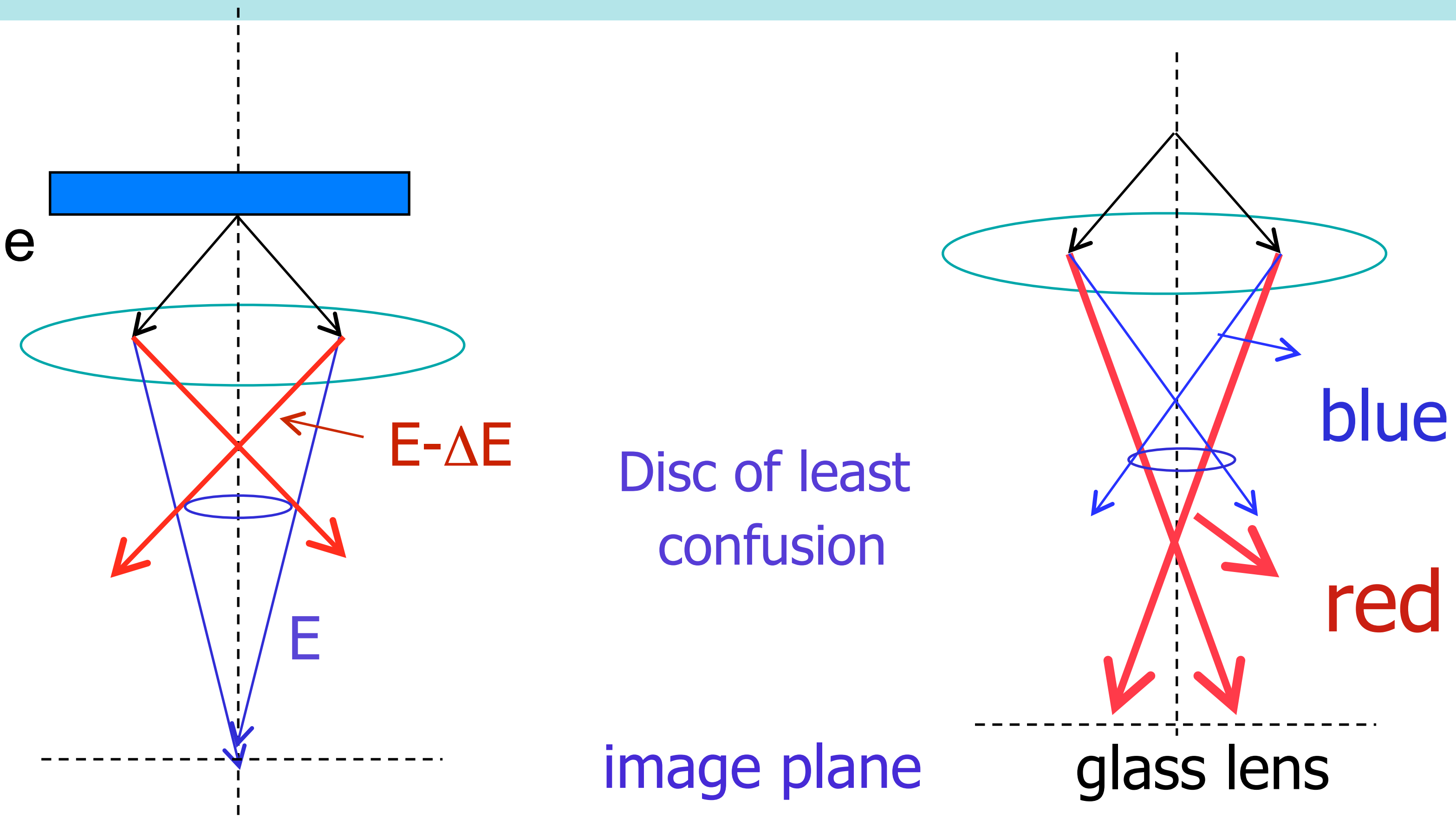
C. Chromatic Aberration

$$\Gamma_{chr} = C_c \frac{\Delta E}{E_o} \beta$$

$$C_c = 1mm \sim 3mm$$

instability of the lens current

$$\frac{\delta i}{i}$$



electro-magnetic lens

Lower energy electron is easier to be focused

Higher energy electron is more difficult to be focused

$$\frac{\delta f}{f} = \frac{\delta V}{V} + \frac{\delta i}{i}$$

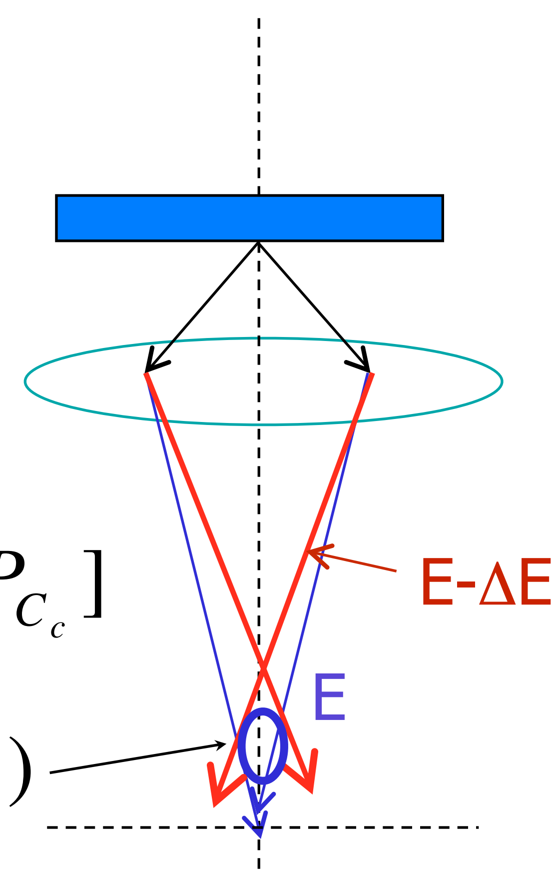
focal spread; instability of applied voltage; instability of lens current

$$\delta f = C_c\{(\frac{\delta V}{V})^2 + 4(\frac{\delta i}{i})^2\}^{1/2}$$

Since the energy of electrons is different in the image plane, they do not coherently interfere each other. i.e. As a result, they do not cause a shift shift as the “spherical aberration” and “de-focus” effect, instead they damping down the amplitude of the image wave.

$$\psi_f \otimes p_{Cc} = \Im^{-1}[\Im(\psi_f) \bullet P_{C_c}]$$

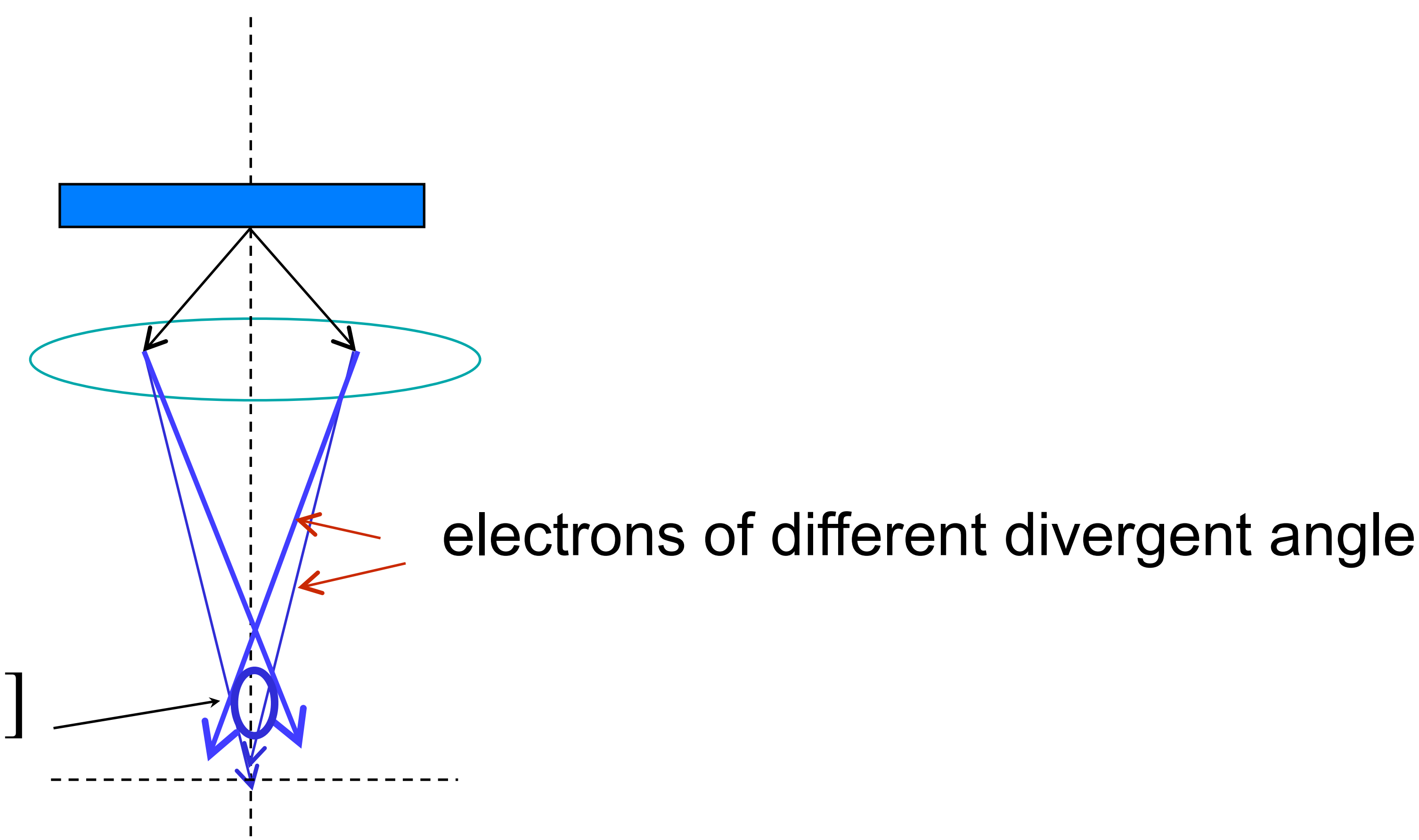
$$P_{C_c} = \exp(-\frac{1}{2}\pi^2\lambda^2\delta f^2 H^4)$$



The signal of high frequency damps more than the lower frequency part.

D. Spatial Coherency

Since the electrons do not coherently interfere each other. i.e. As a result, they do not cause a phase shift as the “spherical aberration” and “de-focus” effect, instead they damping down the amplitude of the image wave.



$$\psi_f \otimes p_C = \Im^{-1}[\Im(\psi_f) \bullet P_C]$$

$$P_C = \exp(-\frac{\alpha^2}{\lambda}\pi^2 q^2), where\ q = (\pi\lambda\Delta f H + \pi C_s \lambda^3 H^3)$$

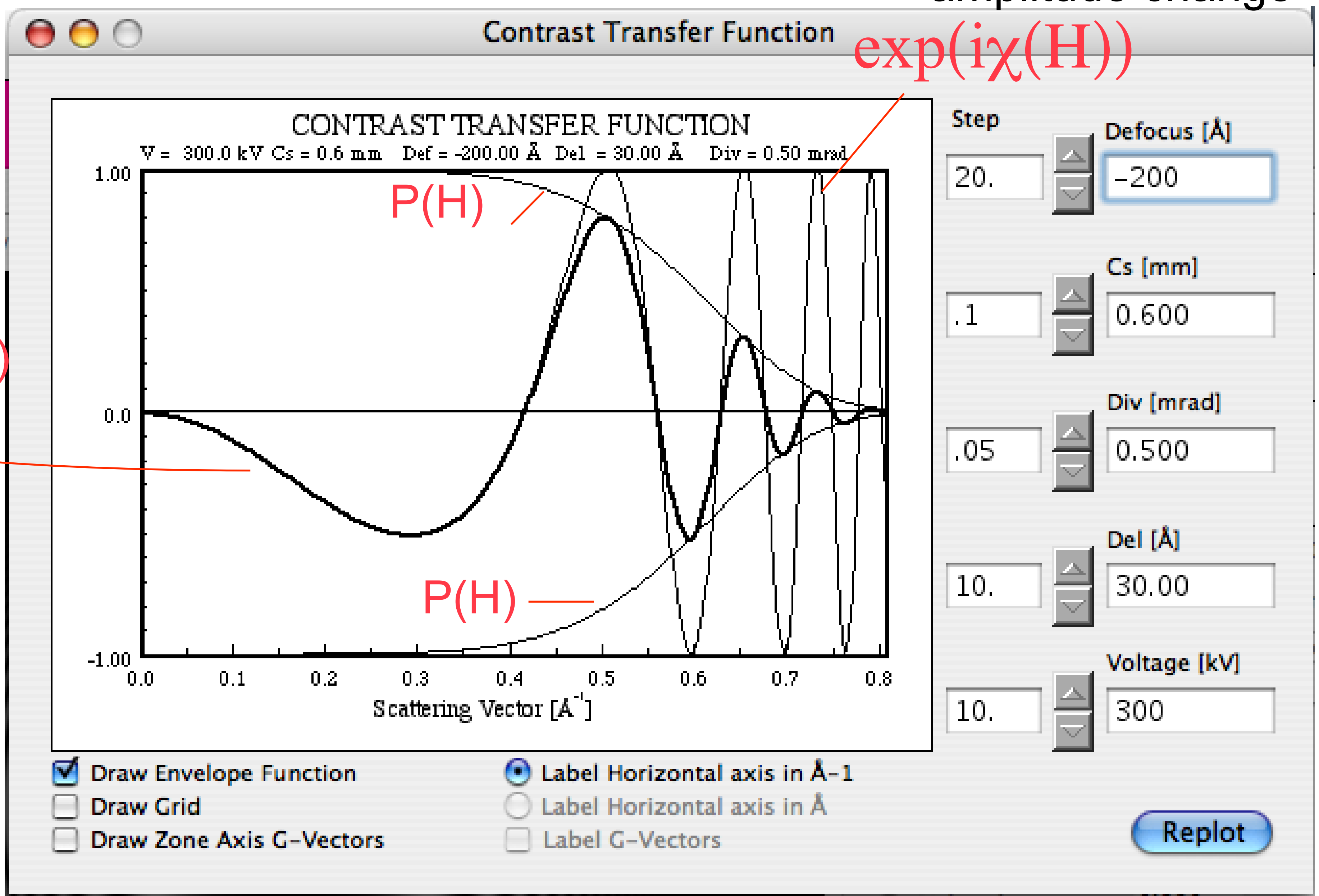
(lens contrast transfer function)

NTHU

$$T(H)=\exp(i\pi\lambda\Delta f H^2)\,\exp(i(\pi/2)C_s\lambda^3H^4)\,\exp(-\pi^2\Delta^2\lambda^2H^2/2)\,\exp(-\pi^2(\alpha/\lambda)^2q/\ln(2))$$

$\exp(i\chi(H))$ — defocus phase shift, spherical aberration

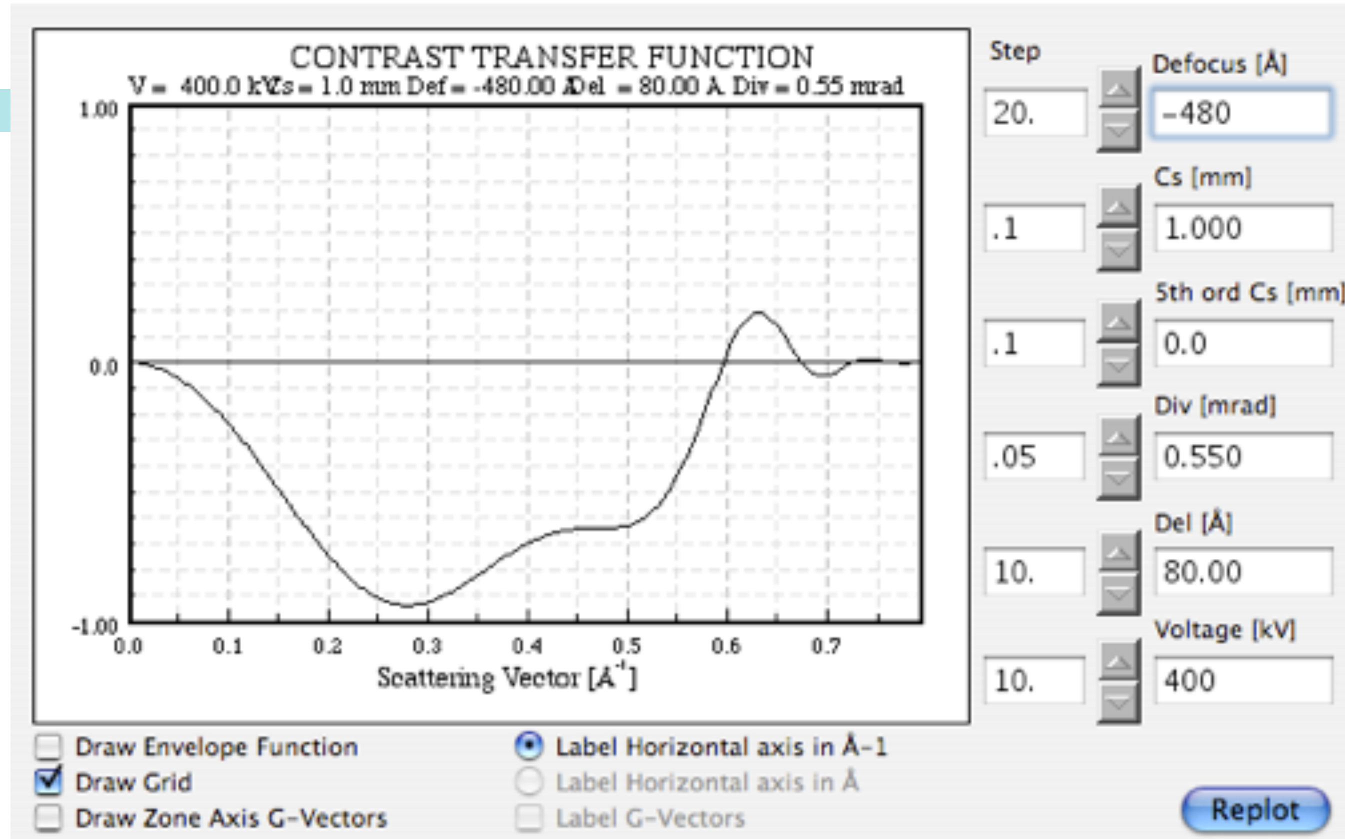
chromatic aberration, spatial coherency — amplitude change — P(H)



$\exp(i\chi(H))P(H)$

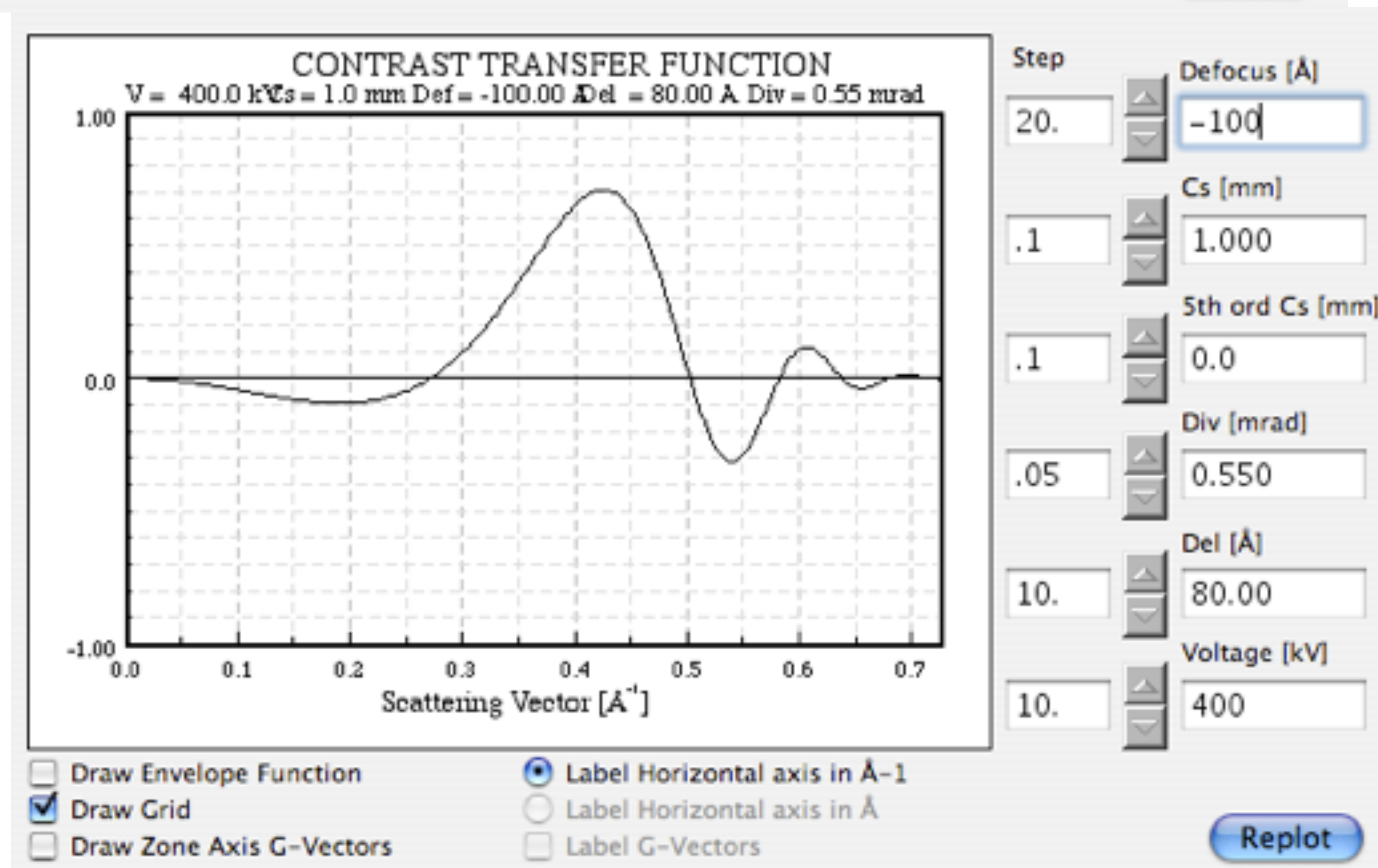
Optimum Focus and Minimum Contrast Focus

Optimum Focus: The focus value to make largest plateau in CTF



Scherzer focus value= $-1.22(C_s\lambda)^{1/2}$

Minimum Contrast Focus: (Gaussian focus)
The focus value to make largest plateau=0 in CTF



Gaussian focus value= $-0.3(C_s\lambda)^{1/2}$

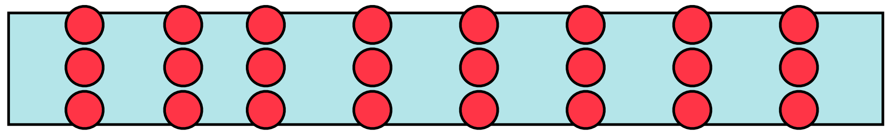
TEM CENTER

Weak Phase Object

NTHU

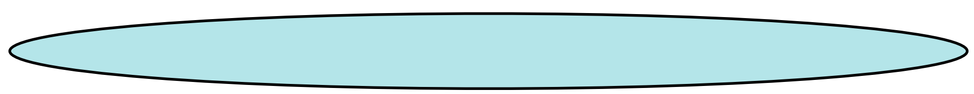
Assuming the object is a weak phase object

$$\psi_o = 1$$



$$\psi_e = \exp(i\varphi(x,y))$$
$$= 1 + i\varphi(x,y)$$

Only the phase change involved
Amplitude does not change



$$\Im(\psi_e) = \delta + i\Im[\varphi(x,y)]$$

B.F.P.

$$\Im(\psi_e) \bullet T(H)$$

$$T(H_x,H_y) = \exp(\pi i\lambda\Delta f H^2)\exp(\pi i\frac{C_s\lambda^3H^4}{2})\exp(-\frac{\alpha^2}{\lambda}\pi^2q^2)\exp(-\frac{1}{2}\pi^2\lambda^2\delta f^2H^4)$$

defocus — spherical aberration — spatial coherency — chromatic aberration

$$\Im^{-1}[\Im(\psi_e) \bullet T(H)] = \psi_e \otimes t(r)$$

In diffraction Plane

$$\Im(\psi_e) \bullet T(H) = \{\delta + i\Im[\varphi(x,y)]\}\{\exp(i\chi(H))\}P(H)$$

$$= \{\delta + i\Im[\varphi(x,y)]\}\{\cos(\chi(H)) + i\sin(\chi(H))\}P(H)$$

$$= \{\delta + 0 + i\Im[\varphi(x,y)]\cos(\chi(H)) - \Im[\varphi(x,y)]\sin(\chi(H))\}P(H)$$

In Image Plane

$$\psi_i = \Im[\Im(\psi_e) \bullet T(H)] = \{1 - \varphi(\frac{-x}{M},\frac{-y}{M}) \otimes \Im(\sin(\chi(H)) + i\varphi(\frac{-x}{M},\frac{-y}{M}) \otimes \Im(\cos(\chi(H))\} \otimes P(H)$$

$$I = \psi_f \psi_f^*$$

$$= \{1 - \varphi(\frac{-x}{M},\frac{-y}{M}) \otimes \Im(\sin(\chi(H))\}^2 \otimes P^2(H) + \{[i\varphi(\frac{-x}{M},\frac{-y}{M}) \otimes \Im(\cos(\chi(H))\}^2 \otimes P^2(H)$$

if we neglect the second order terms

$$\sim 1 - 2\varphi(\frac{-x}{M},\frac{-y}{M}) \otimes \Im(\sin(\chi(H)) \otimes P^2(H)$$

This is so called phase contrast

Two Resolutions: How to Improve Resolution

NTHU

$d=\frac{\lambda}{2n\sin\alpha}$

幾何光學
分辨率

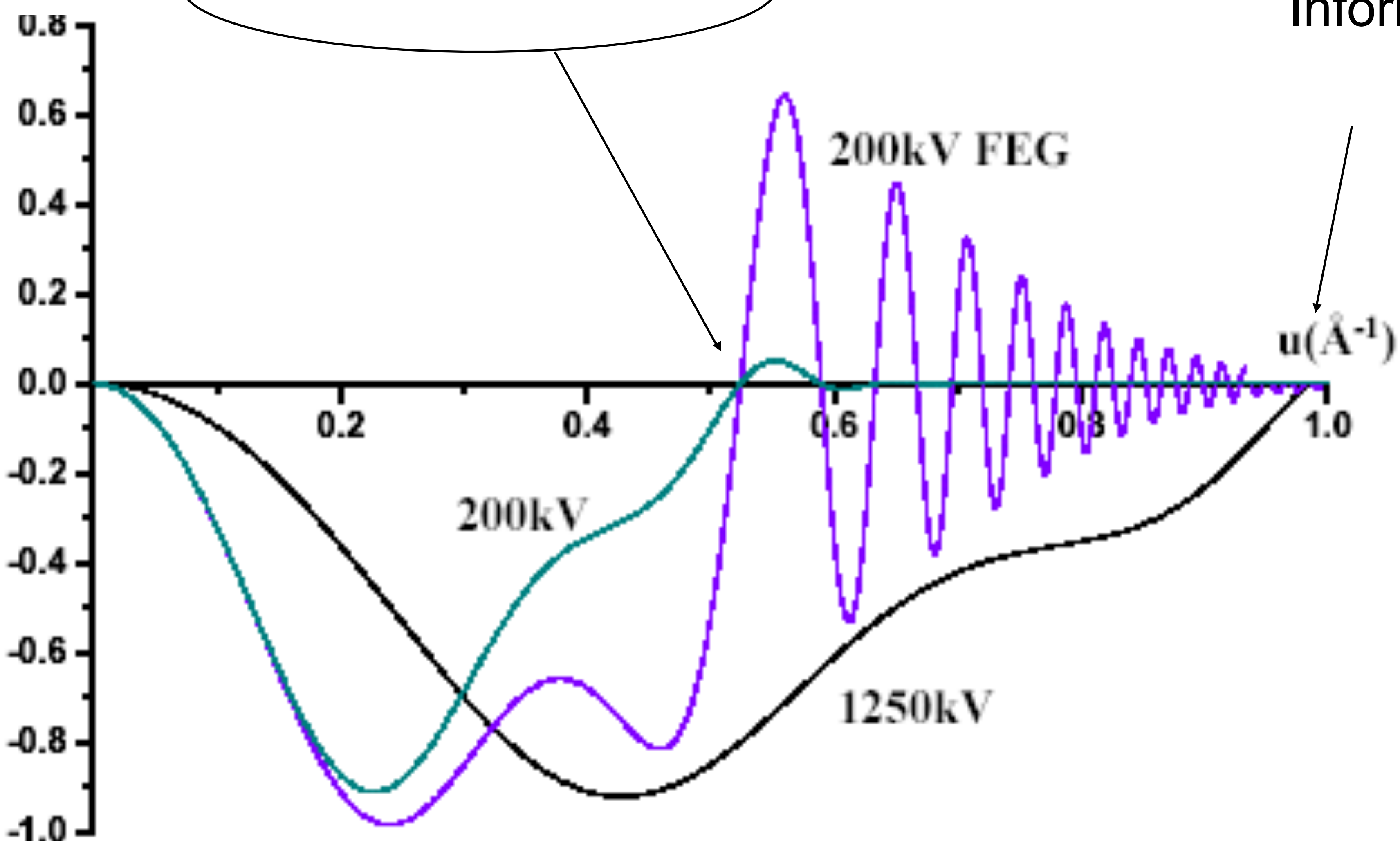
Scherzer Resolution
Point-point resolution
$d=0.66C_s^{1/4}\lambda^{3/4}$

C_s ↓ λ ↓ **(high voltage TEM
Cs corrected TEM)**

Information limit

C_c ↓ α ↓

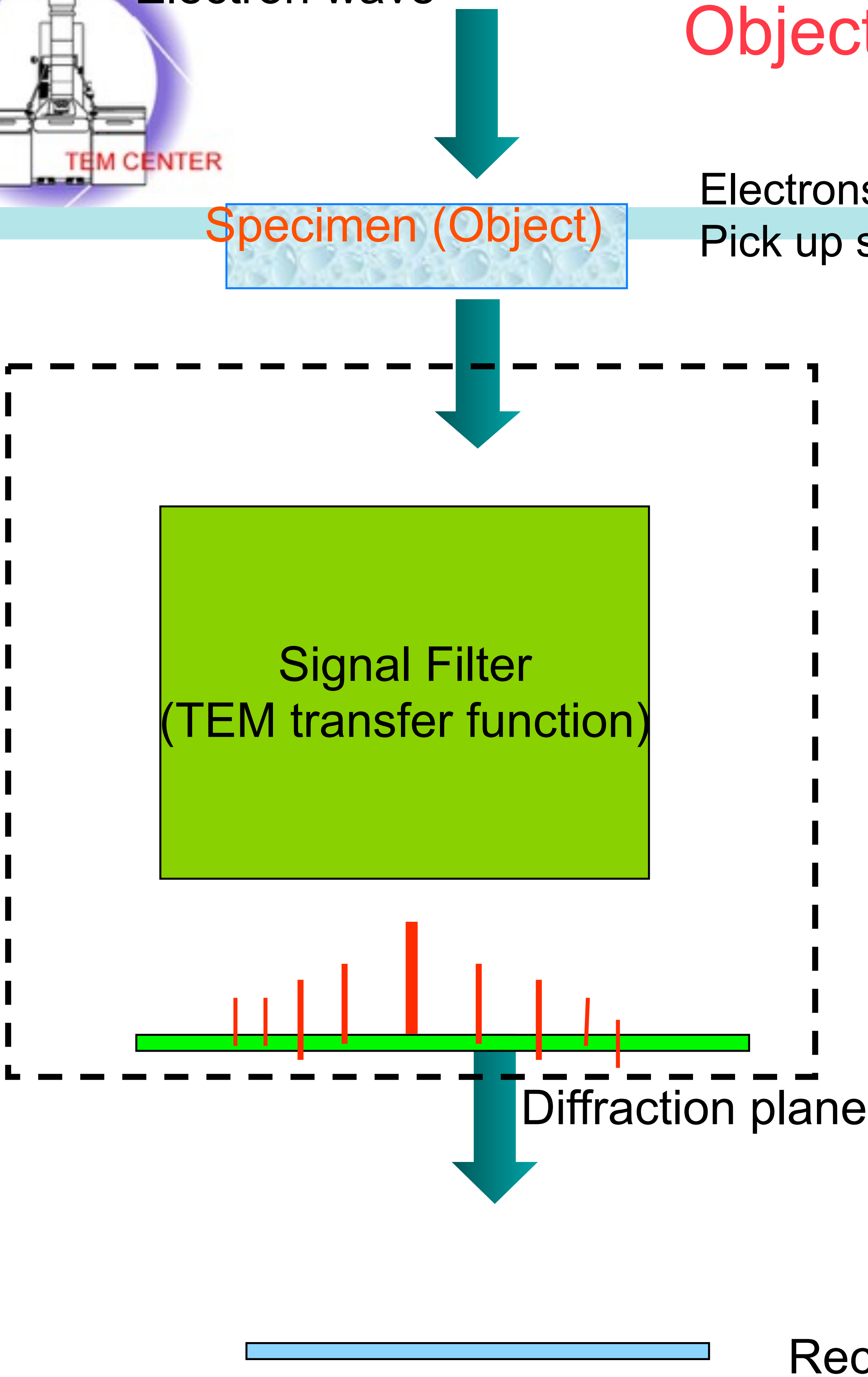
Coherency ↑
(**FEG Gun
Monochromator
Cc corrector
Cs corrector**)



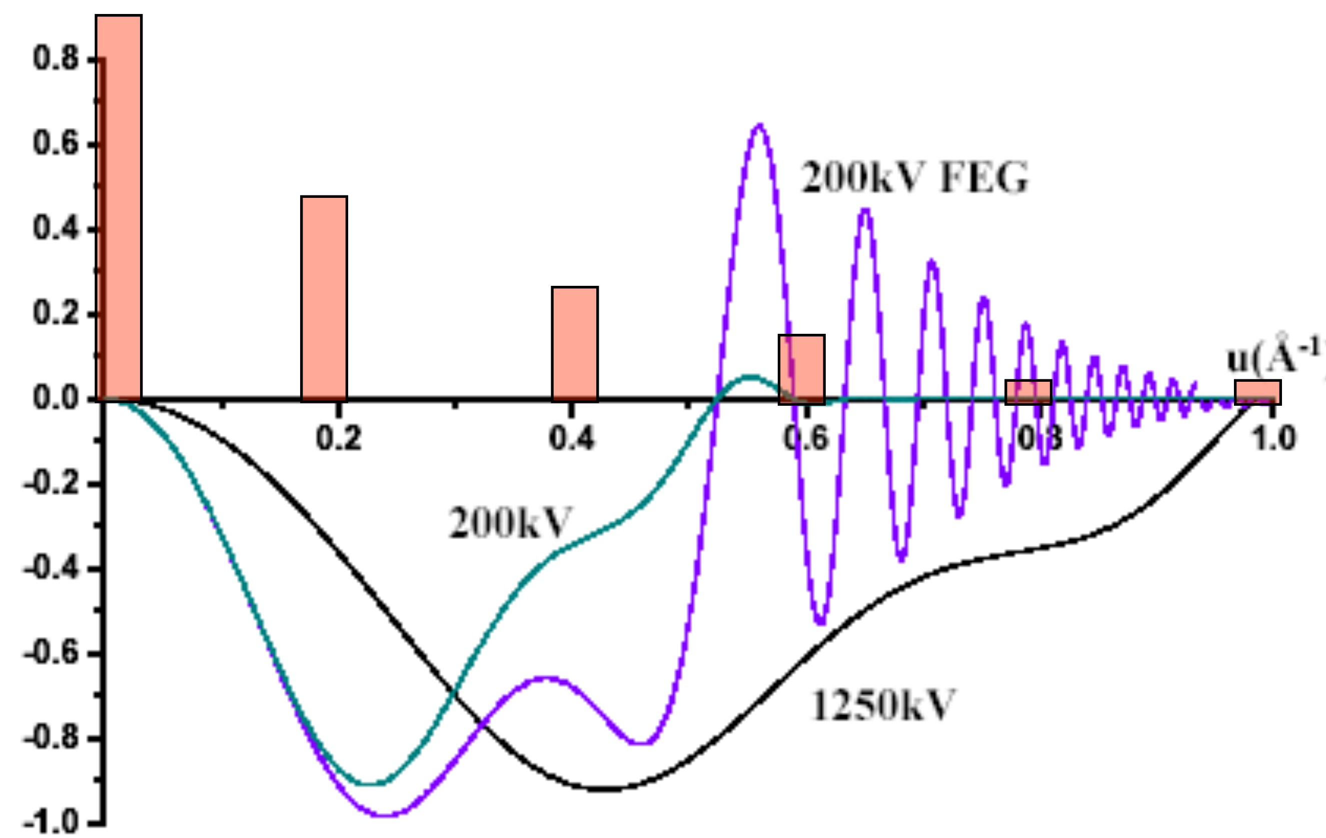
CTF curves of Scherzer focus $= -1.22(C_s\lambda)^{1/2}$

CTF有很寬之通帶

Objective lens acts as a signal filter



Electrons interact with atoms
Pick up structure information



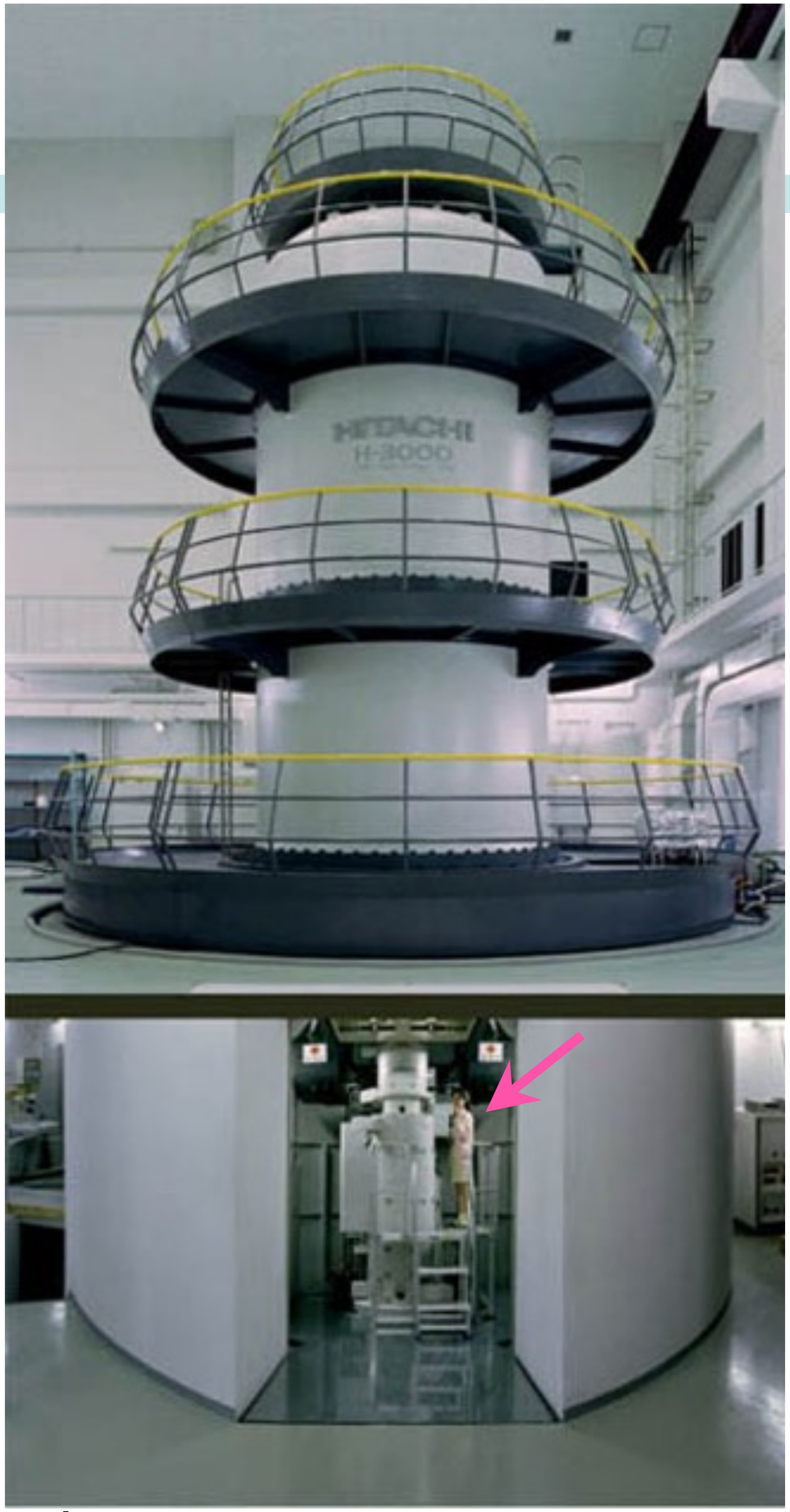
CTF curves of Scherzer focus

Recorded image (Observer)

Using Ultra-High Voltage TEM

- 1. Electron Wave Length
  - ➢ Decreasing the electron wavelength
  - ➢ Develop ultra higher accelerating voltage up to 1MeV ~0.1 nm

- 2. Coherence of electron wave
  - ➢ Using a field emission gun (FEG), the temporal incoherence can be reduce, information limit extend to 0.1nm



Osaka University, Japan

Lens Aberration Correction

Spherical aberration C_s, Chromatical aberration C_c Astigmatism etc.

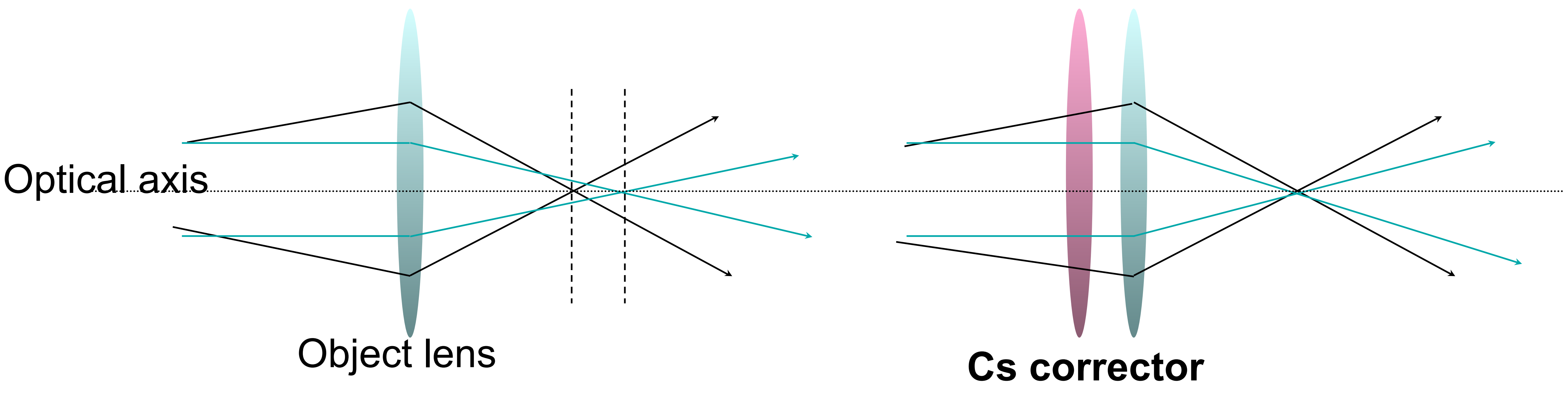
NTHU

- Simplest, a better lens design yielding lower spherical aberration at intermediate voltages

  ~0.17 nm is reached at 300kV
- Develop Cs corrector in intermediate voltages

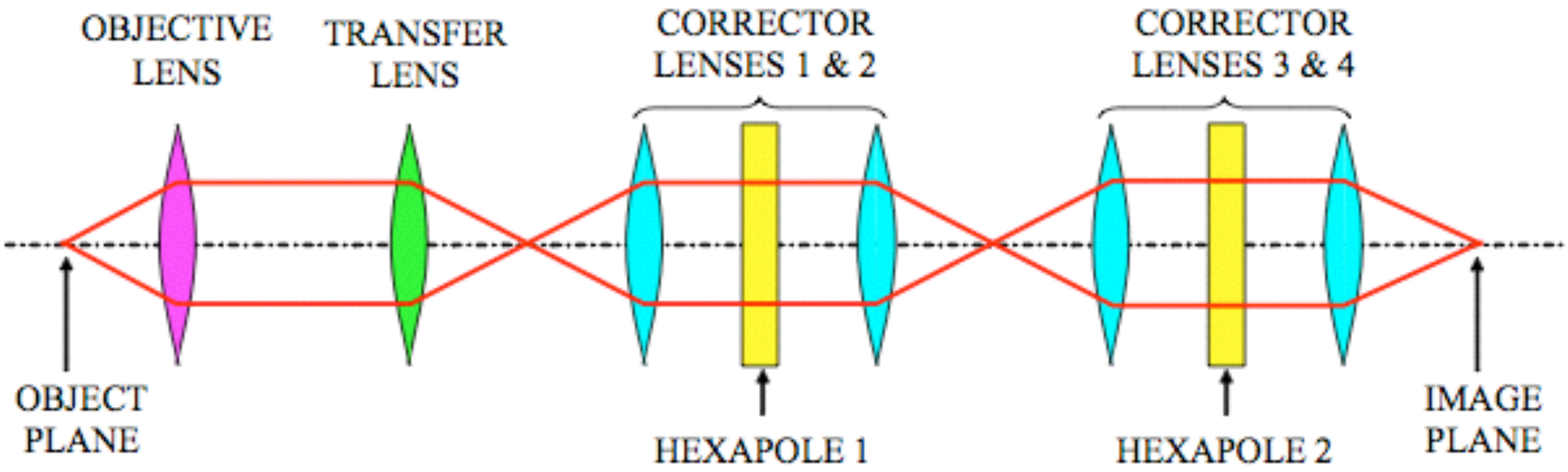
  ~0.1 nm
- Develop Monochromator in intermediate voltage

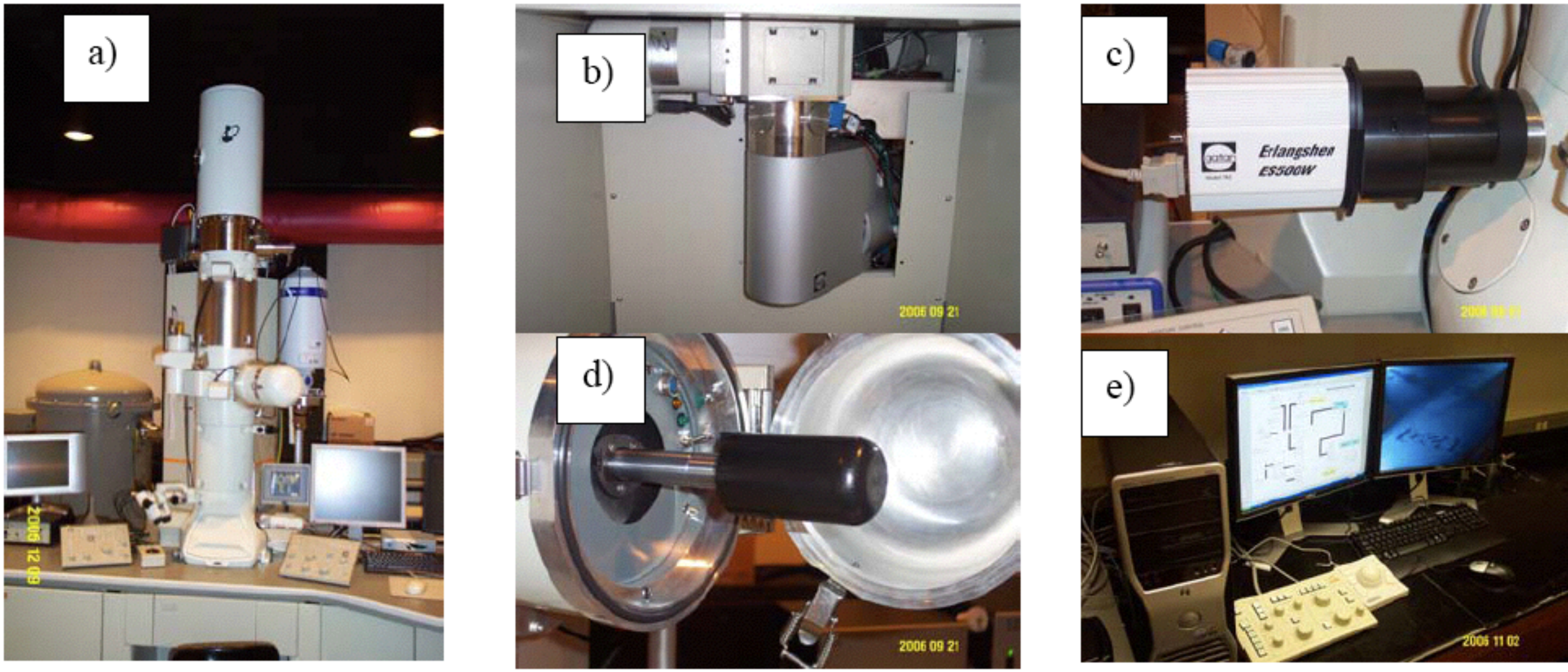
Spherical aberration Cs



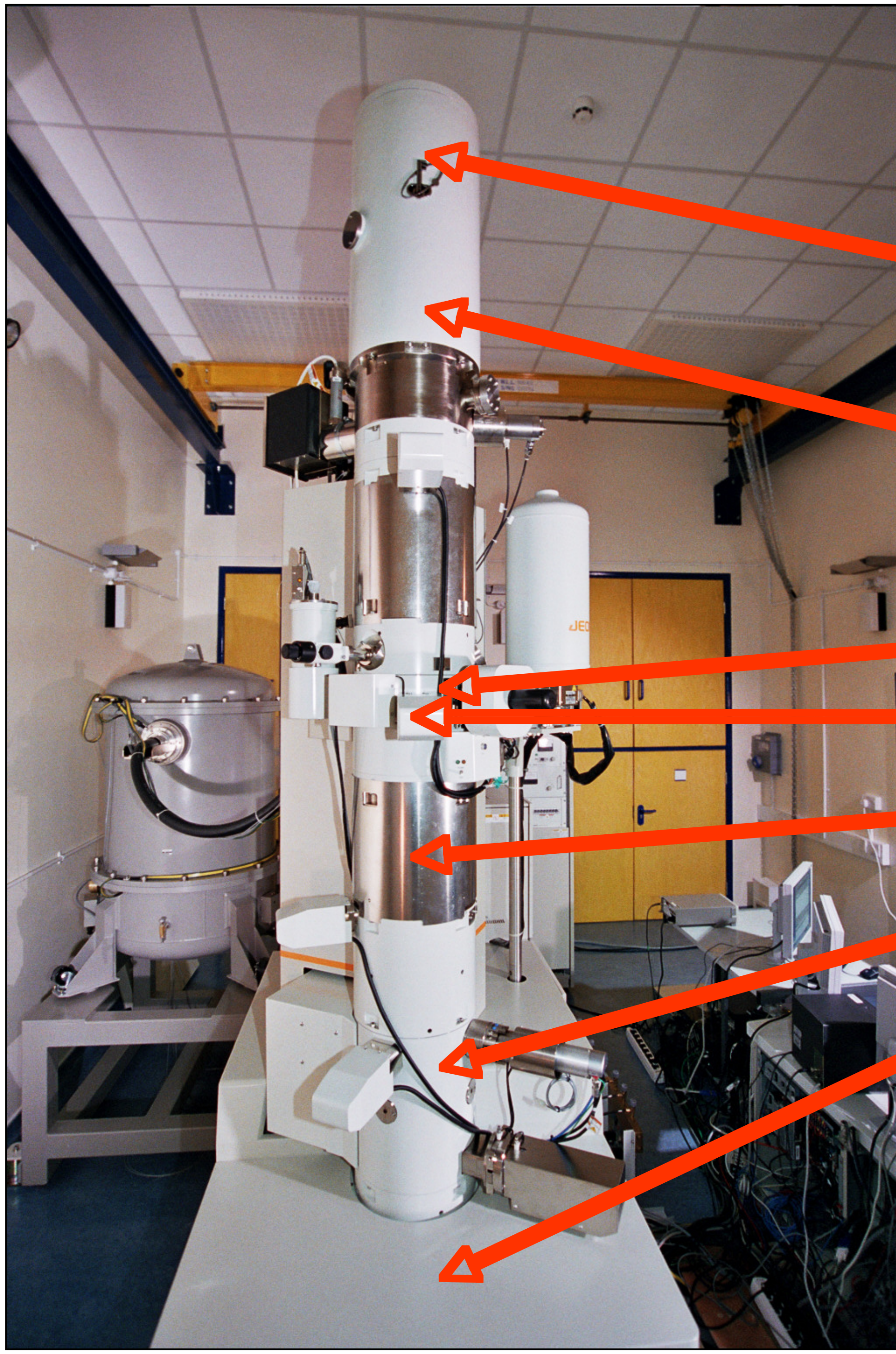
Hardware Correctors

- Probe forming corrector
- Objective Lens Corrector


OBJECTIVE LENS
TRANSFER LENS
CORRECTOR LENSES 1 & 2
CORRECTOR LENSES 3 & 4
OBJECT PLANE
HEXAPOLE 1
HEXAPOLE 2
IMAGE PLANE


a)
b)
c)
d)
e)
Erlangshen
ES500W
2006 12 09
2006 09 21
2006 09 21
2006 11 02

HREM - initial JEOL 2200FS



FEG

200kV HT

X-Y piezo stage

URP polepiece

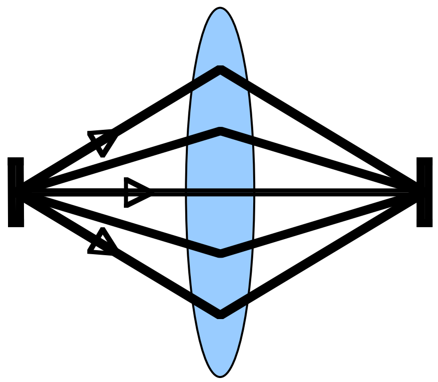
CEOS TEM corrector

Omega filter

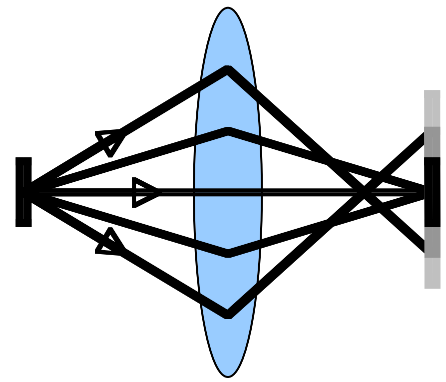
2k x 2k camera

purpose-built room

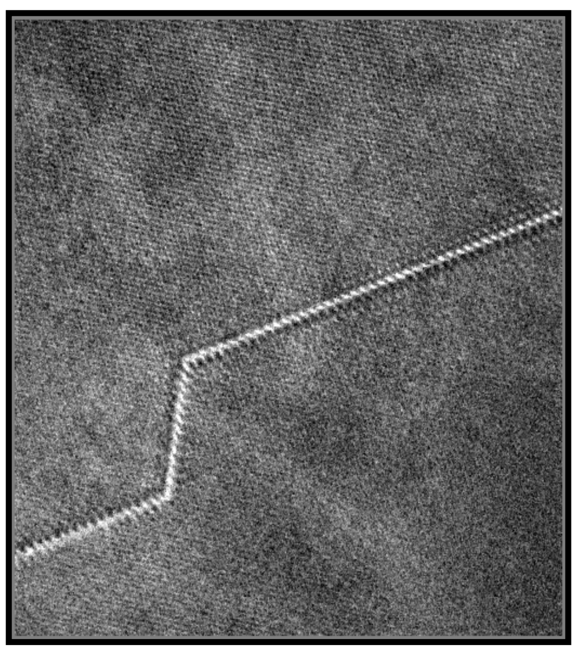
delocalisation



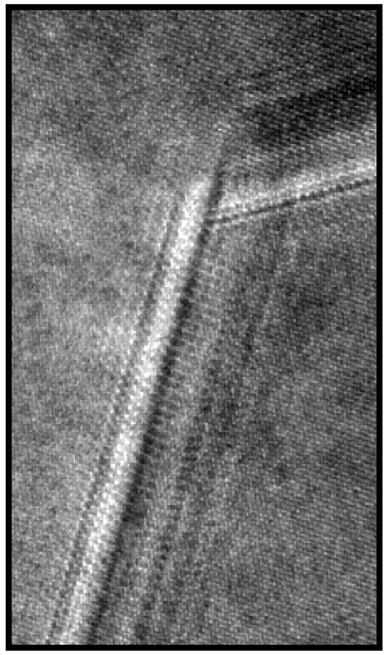
(a)



(b)



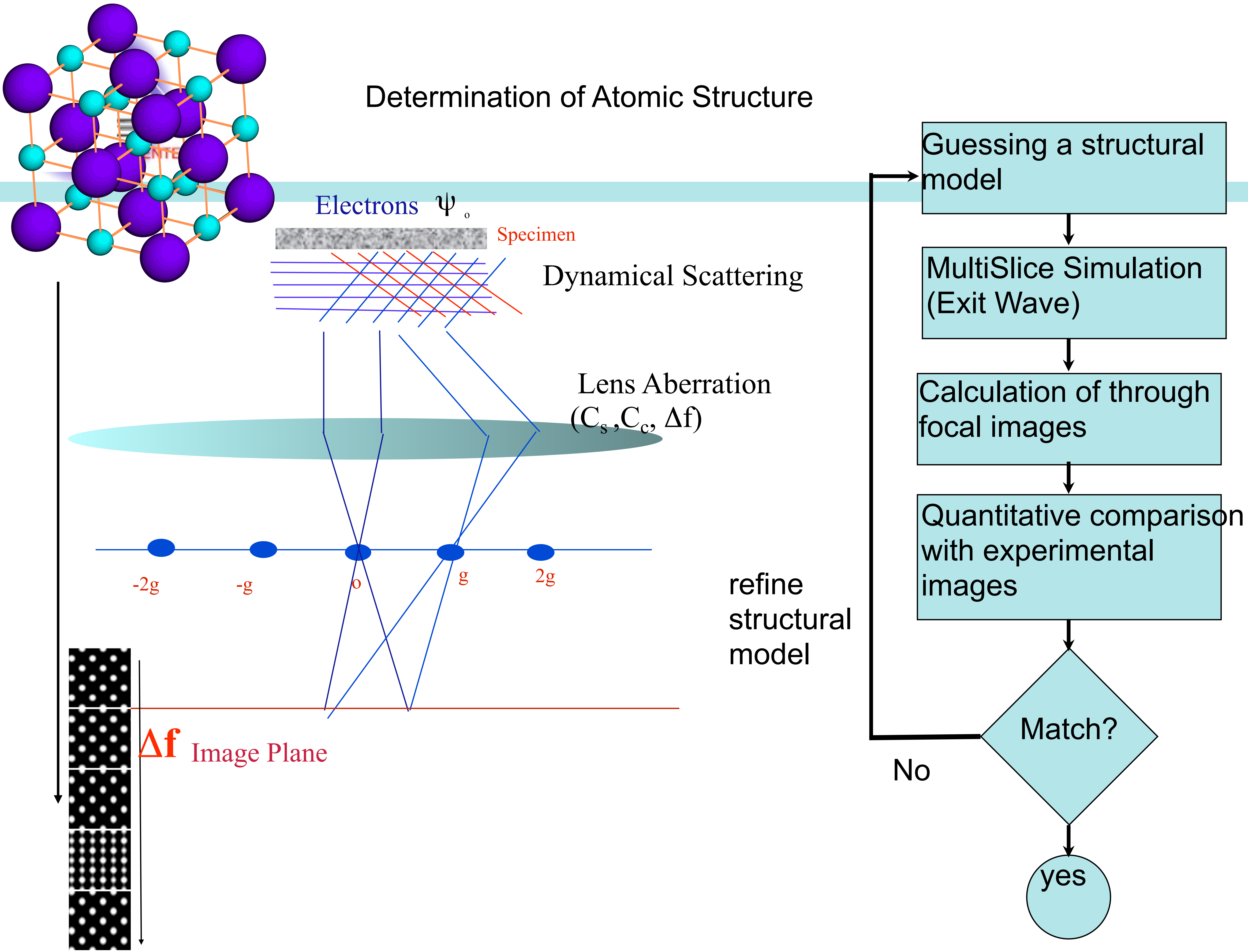
zero Cs



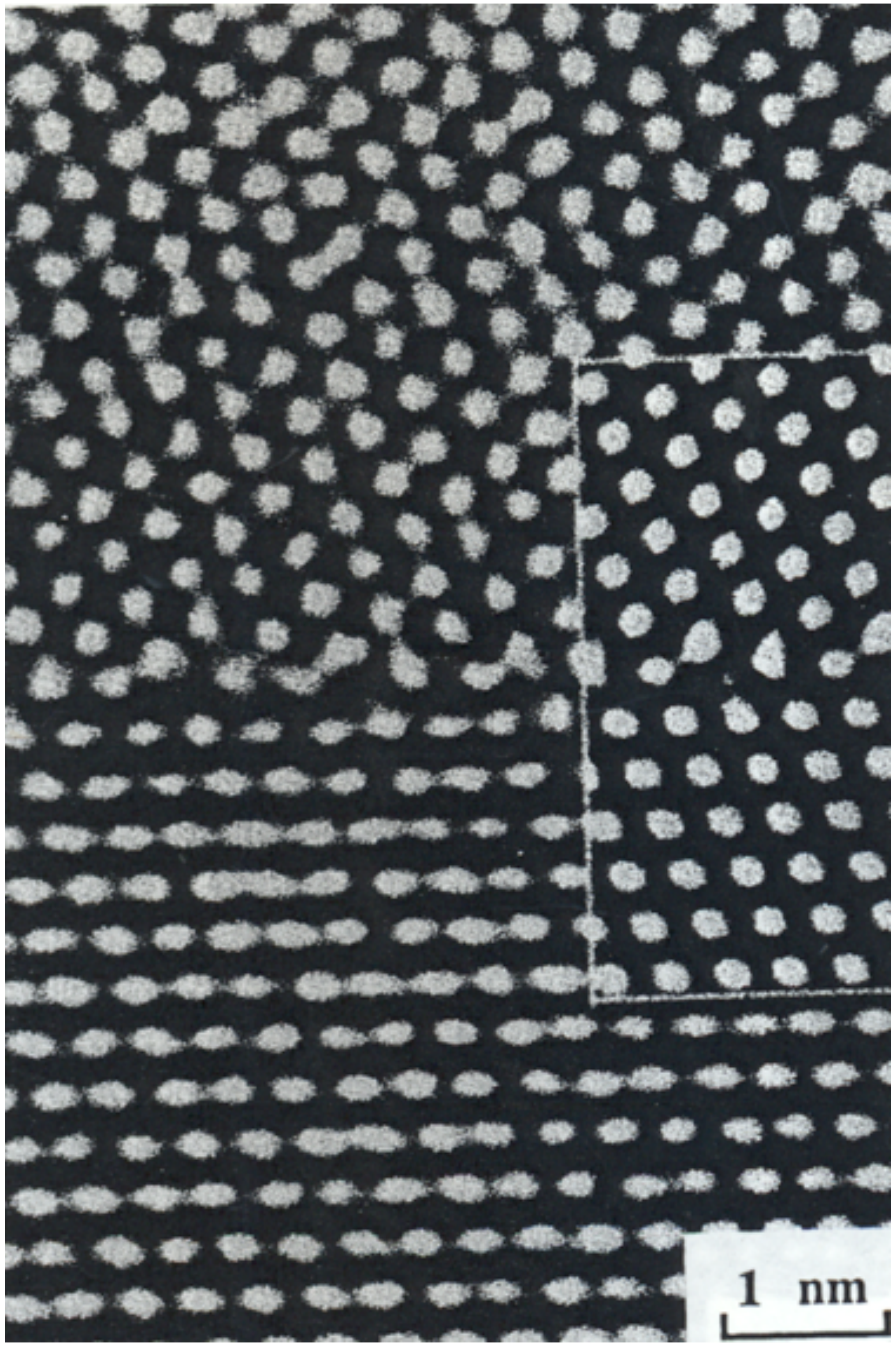
with Cs

twin boundary in gold
111 zone
0.144nm fringes
(200kV)

Determination of Atomic Structure

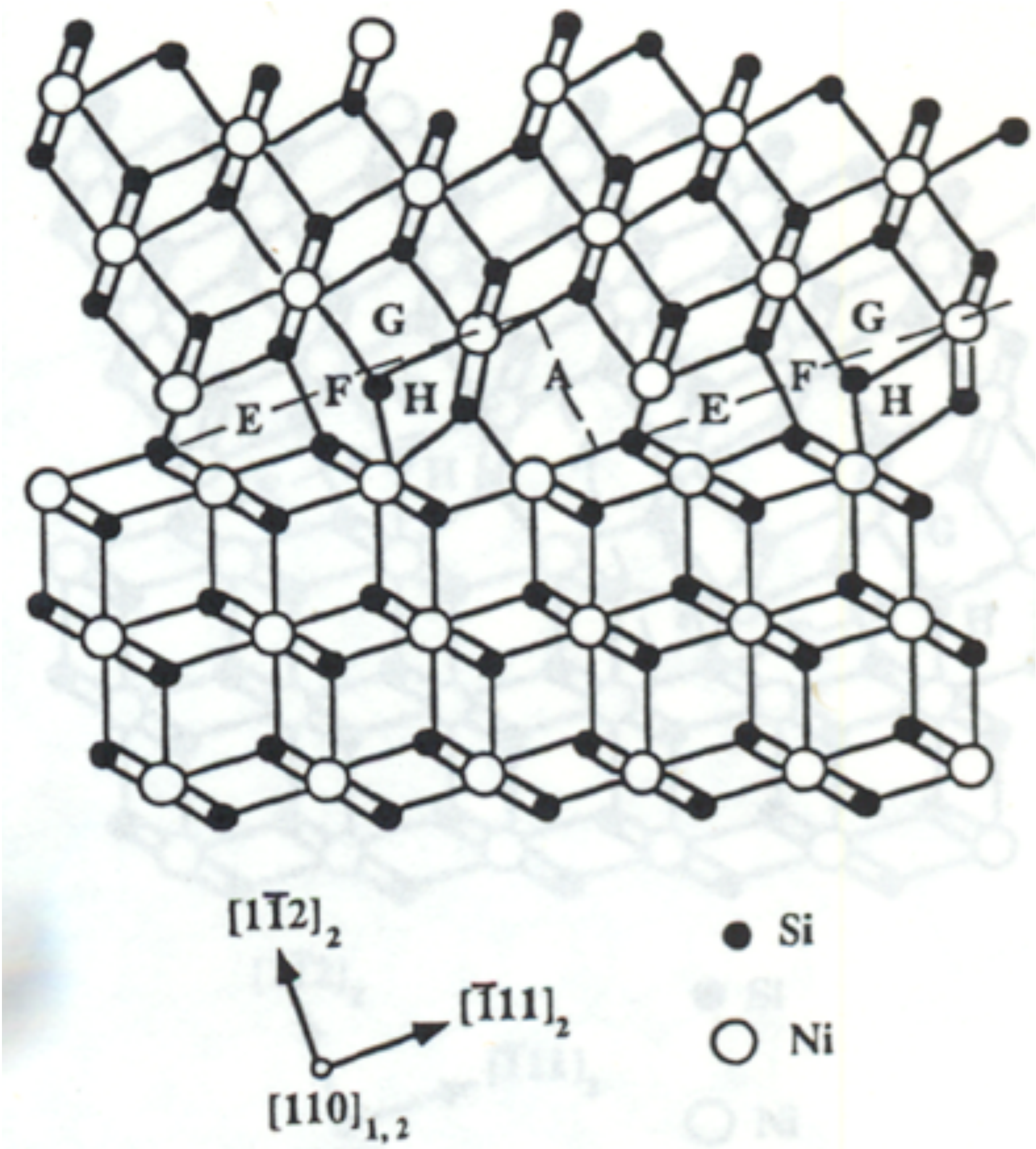


Example: $NiSi_2$ {115}/{111} Twin Boundary

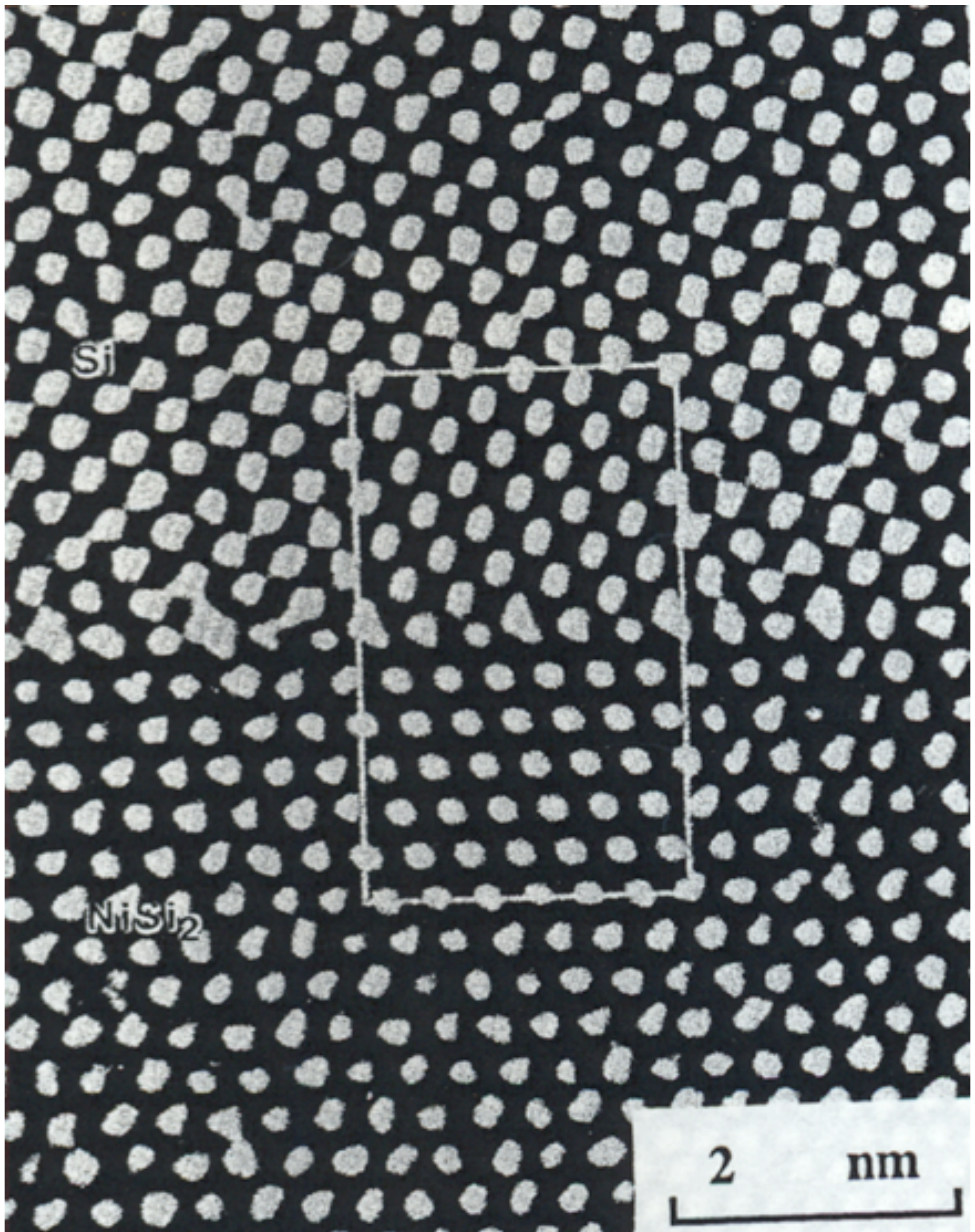


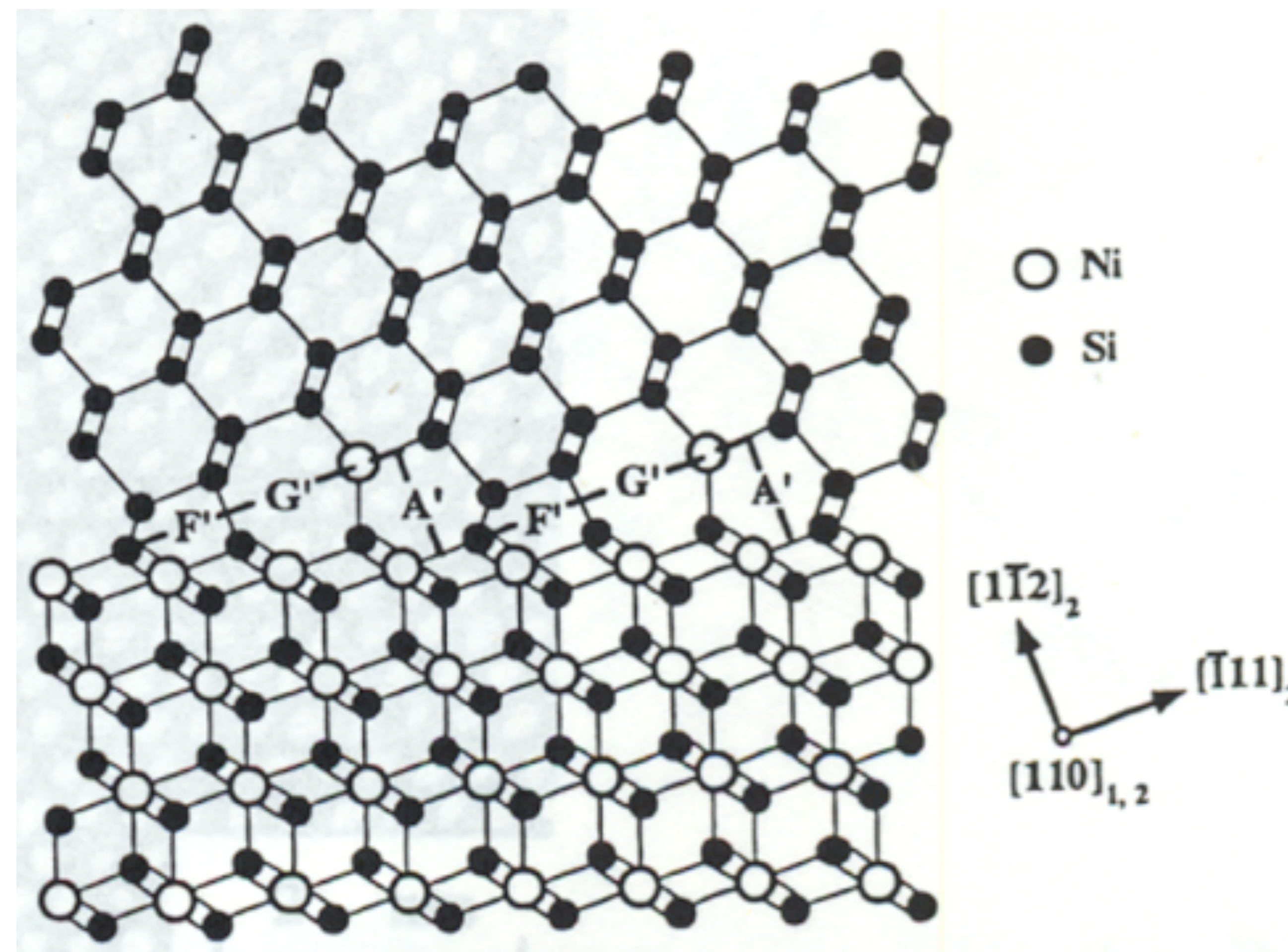
{115}

{111}

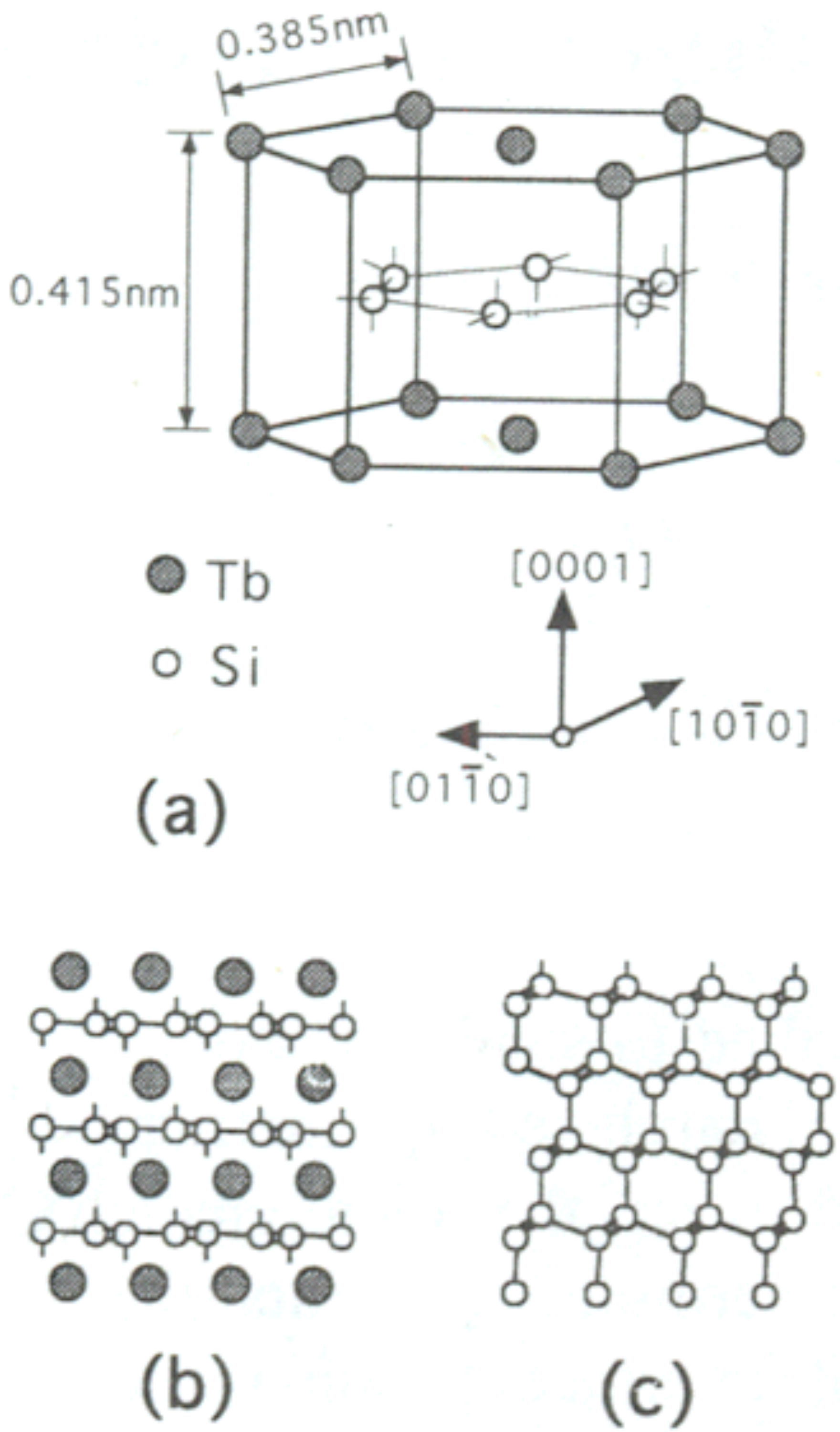


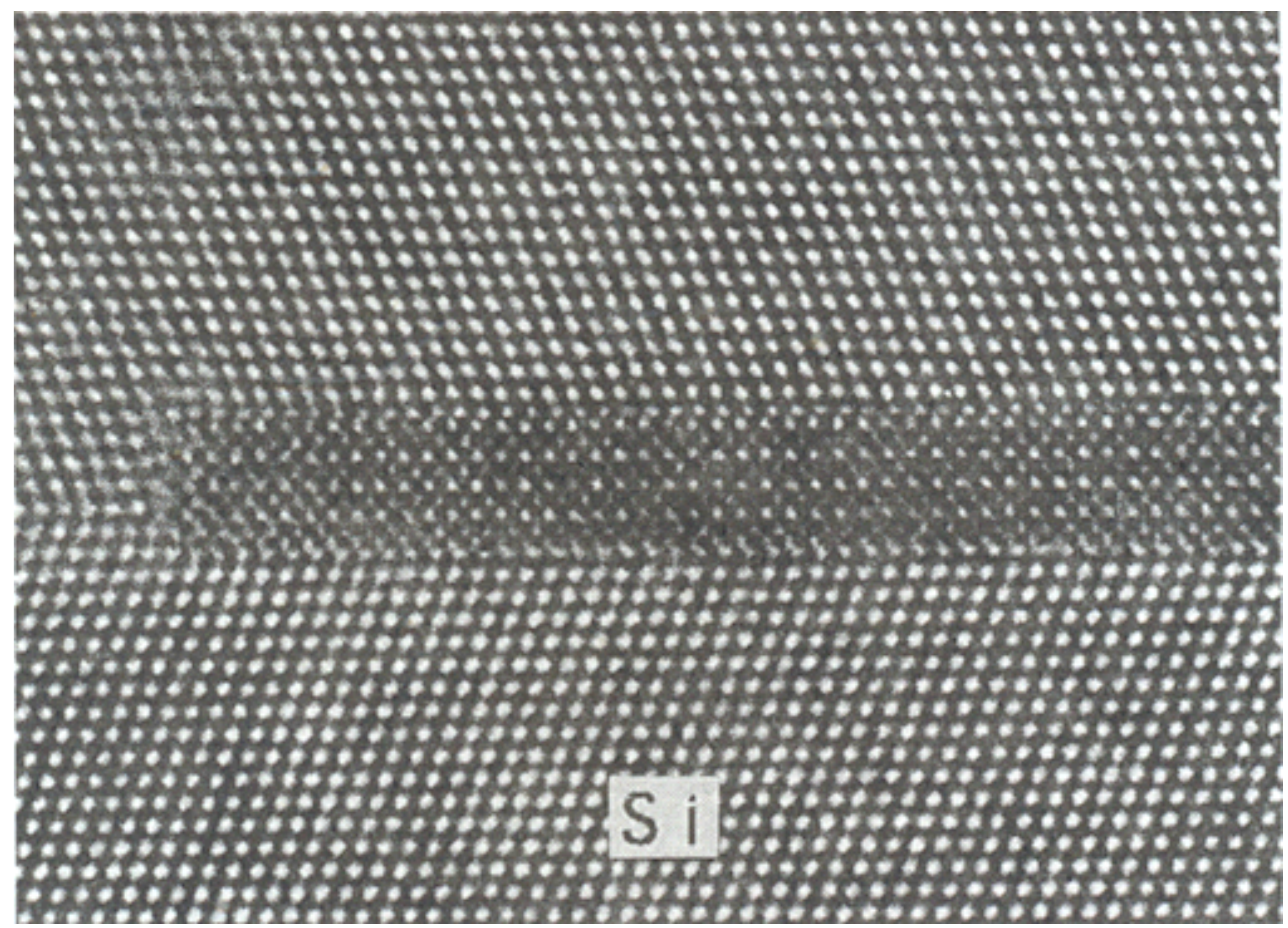
Example: Si{115}/ $NiSi_2$ {111} Twin Boundary





Example: $TbSi_2$/ Si Interface





Analysis of Variations in Structure from High Resolution Electron Microscope Images by Combining Real Space and Fourier Space Information

Martin J. Hÿtch

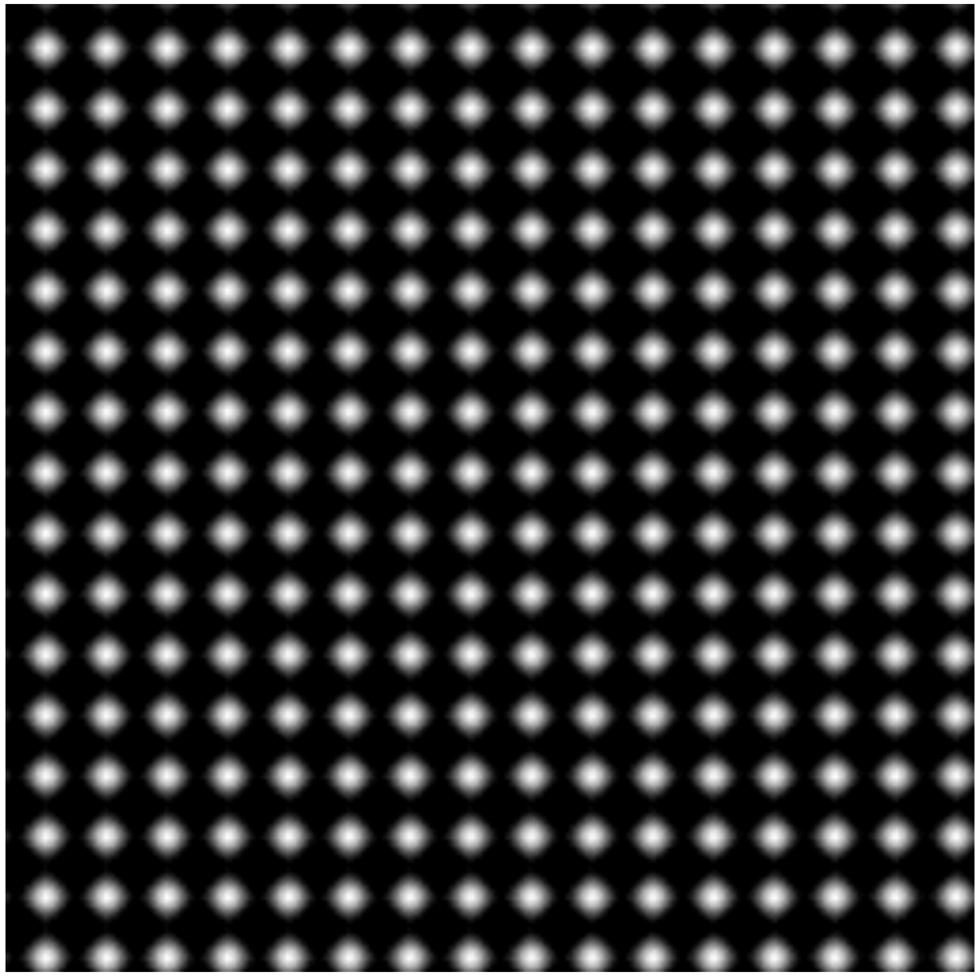
Microsc. Microanal. Microstruct. 8 (1997) 41–57

Quantitative measurement of displacement and strain fields from HREM micrographs

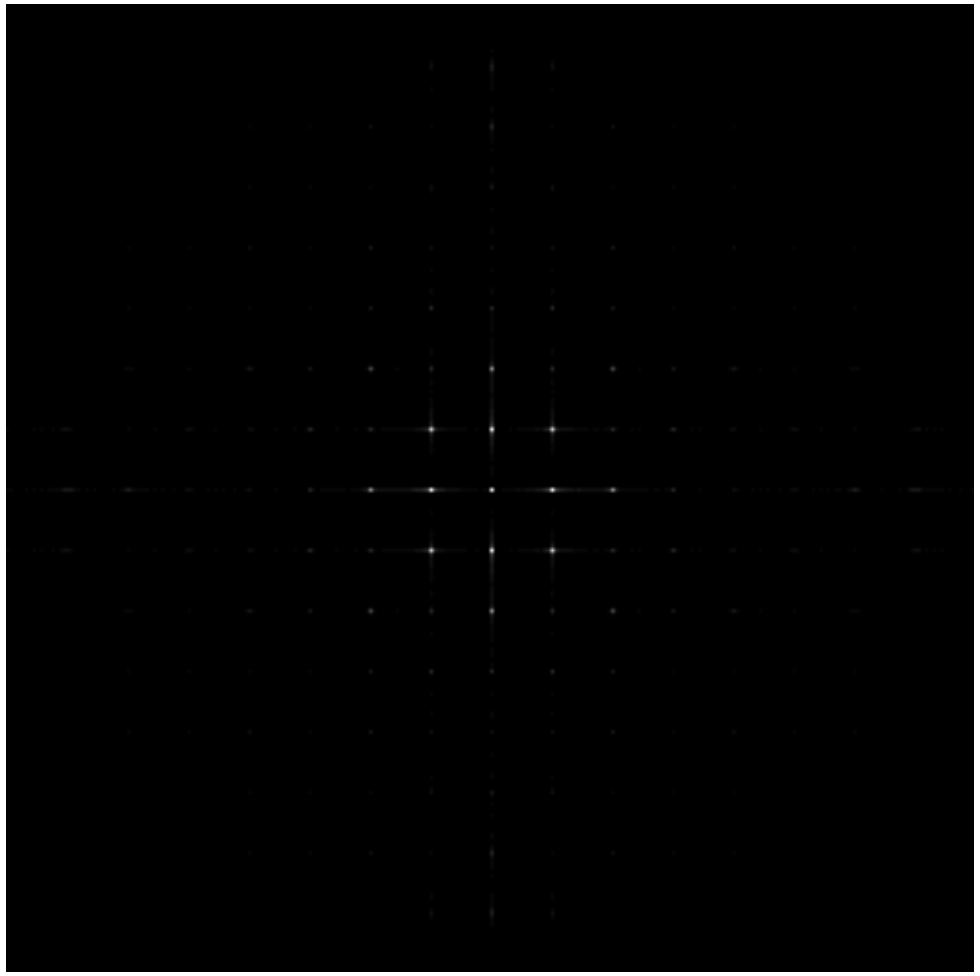
Ultramicroscopy 74 (1998) 131–146

M.J. Hÿtch[a,*], E. Snoeck[b], R. Kilaas[c]

Background on Geometric Phase

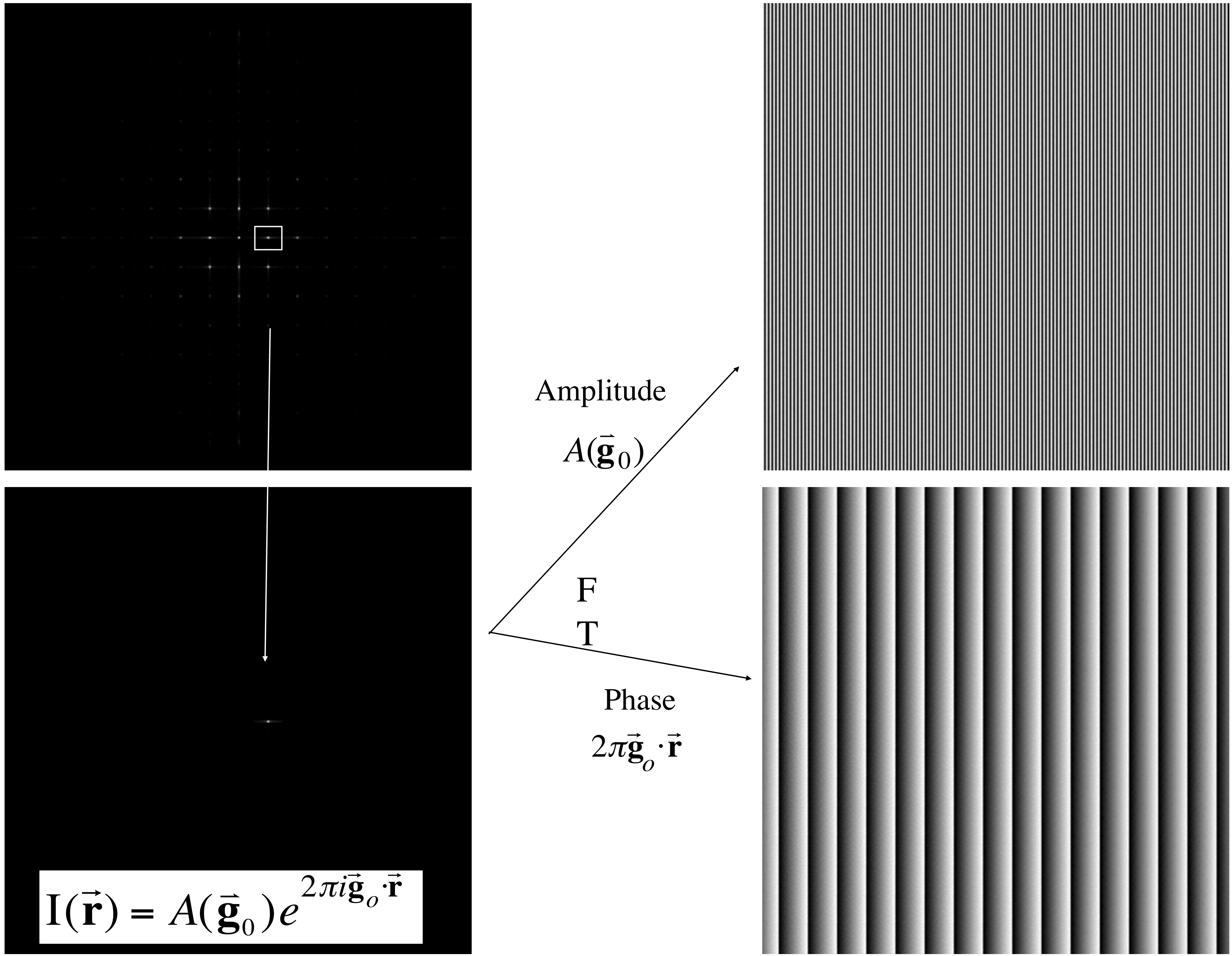


Fourier
Transform

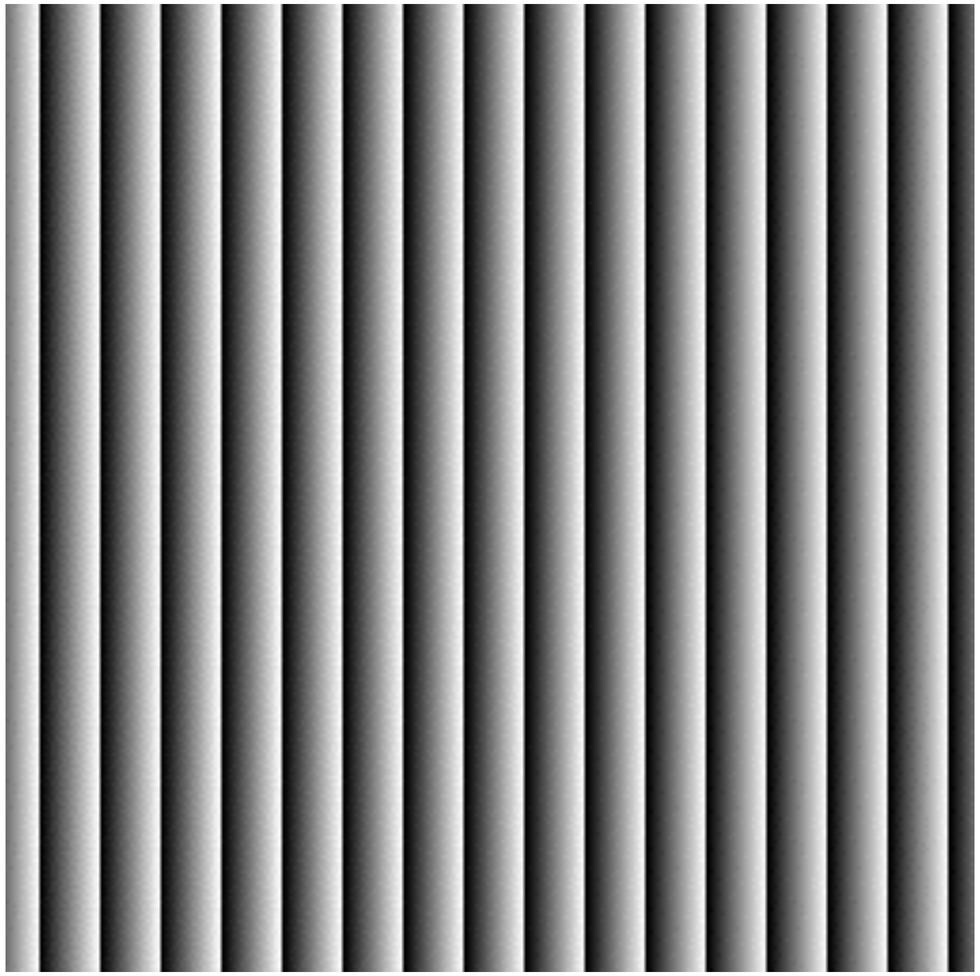


$$I(\vec{\mathbf{r}}) = \sum_{\mathbf{g}} A(\vec{\mathbf{g}}) e^{2\pi i \vec{\mathbf{g}} \cdot \vec{\mathbf{r}}}$$

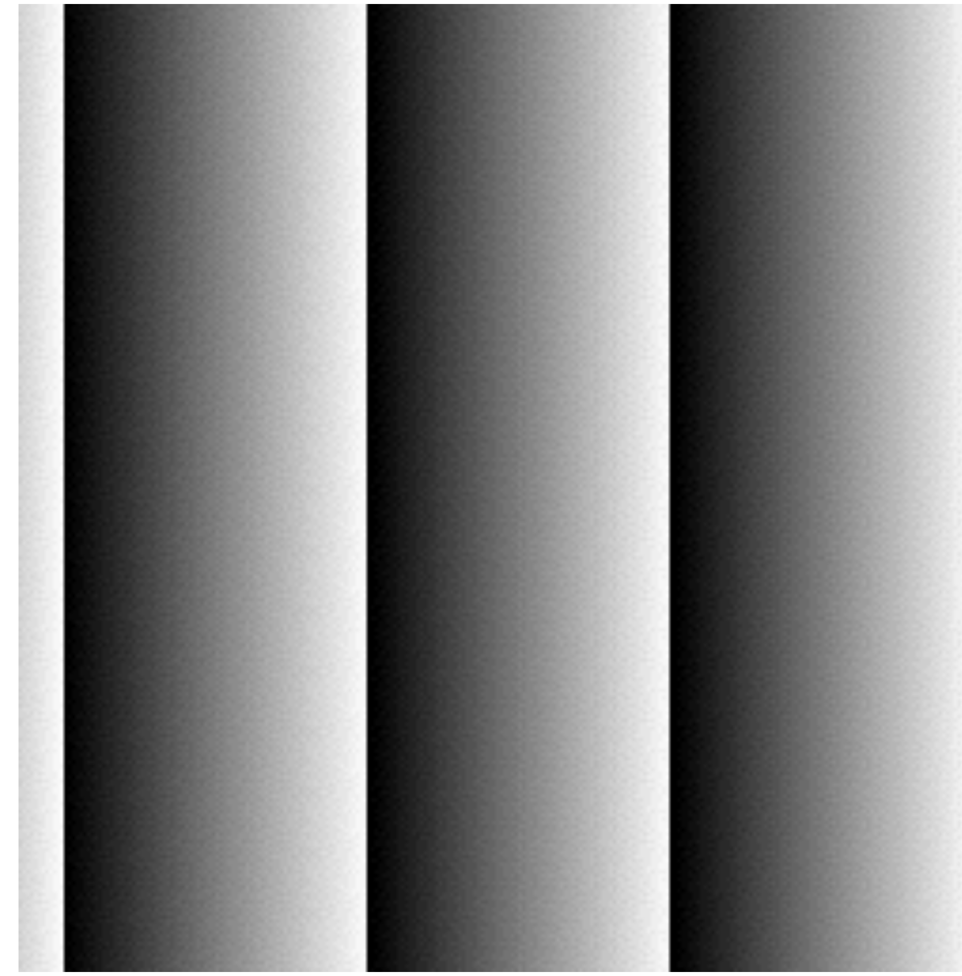
By Dr. Roar Kilaas


Amplitude
$A(\vec{\mathbf{g}}_0)$
F
T
Phase
$2\pi\vec{\mathbf{g}}_o\cdot\vec{\mathbf{r}}$
$\mathrm{I}(\vec{\mathbf{r}}) = A(\vec{\mathbf{g}}_0)e^{2\pi i\vec{\mathbf{g}}_o\cdot\vec{\mathbf{r}}}$

Digital Moire Images



$$\frac{2\pi\vec{\mathbf{g}}_o\cdot\vec{\mathbf{r}}}{M} \quad ; \qquad M = 1$$



$$\frac{2\pi\vec{\mathbf{g}}_o\cdot\vec{\mathbf{r}}}{M} \quad ; \qquad M = 5$$

Higher and higher magnification M is equivalent to shifting the reciprocal lattice vector closer and closer to the center of the Fourier transform. The phase image used for the displacement calculation is equivalent to M -> ∞ , where subtracting off the term $2\pi\mathbf{g}_0\bullet\mathbf{r}$ has the same effect as shifting the origin of the FT to the position of the reciprocal frequency $\mathbf{g}_0$

- Non perfect crystal - Small deviations from perfect lattice spacings

$$\mathrm{I}(\vec{\mathbf{r}}) = A(\vec{\mathbf{r}})e^{2\pi i \vec{\mathbf{g}}(\vec{\mathbf{r}})\cdot\vec{\mathbf{r}}} = A(\vec{\mathbf{r}})e^{2\pi i(\vec{\mathbf{g}}_0 + \Delta\vec{\mathbf{g}}(\vec{\mathbf{r}}))\cdot\vec{\mathbf{r}}}$$

- Displacement Field description

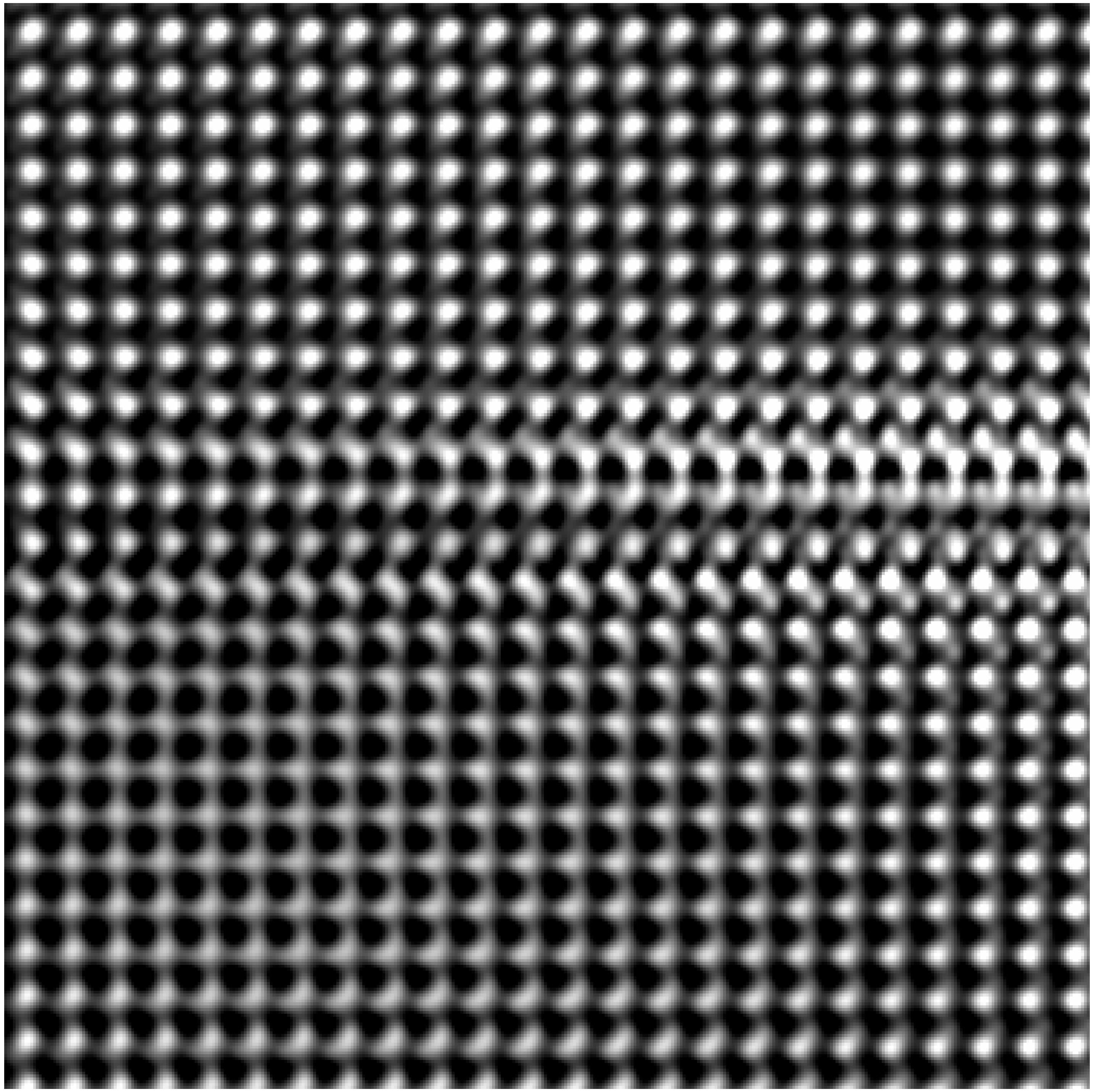
$$\vec{\mathbf{g}}(\vec{\mathbf{r}})\cdot\vec{\mathbf{r}} = \frac{1}{u_0 + \delta(\vec{\mathbf{r}})}\hat{\mathbf{g}}_0\cdot\vec{\mathbf{r}} =$$

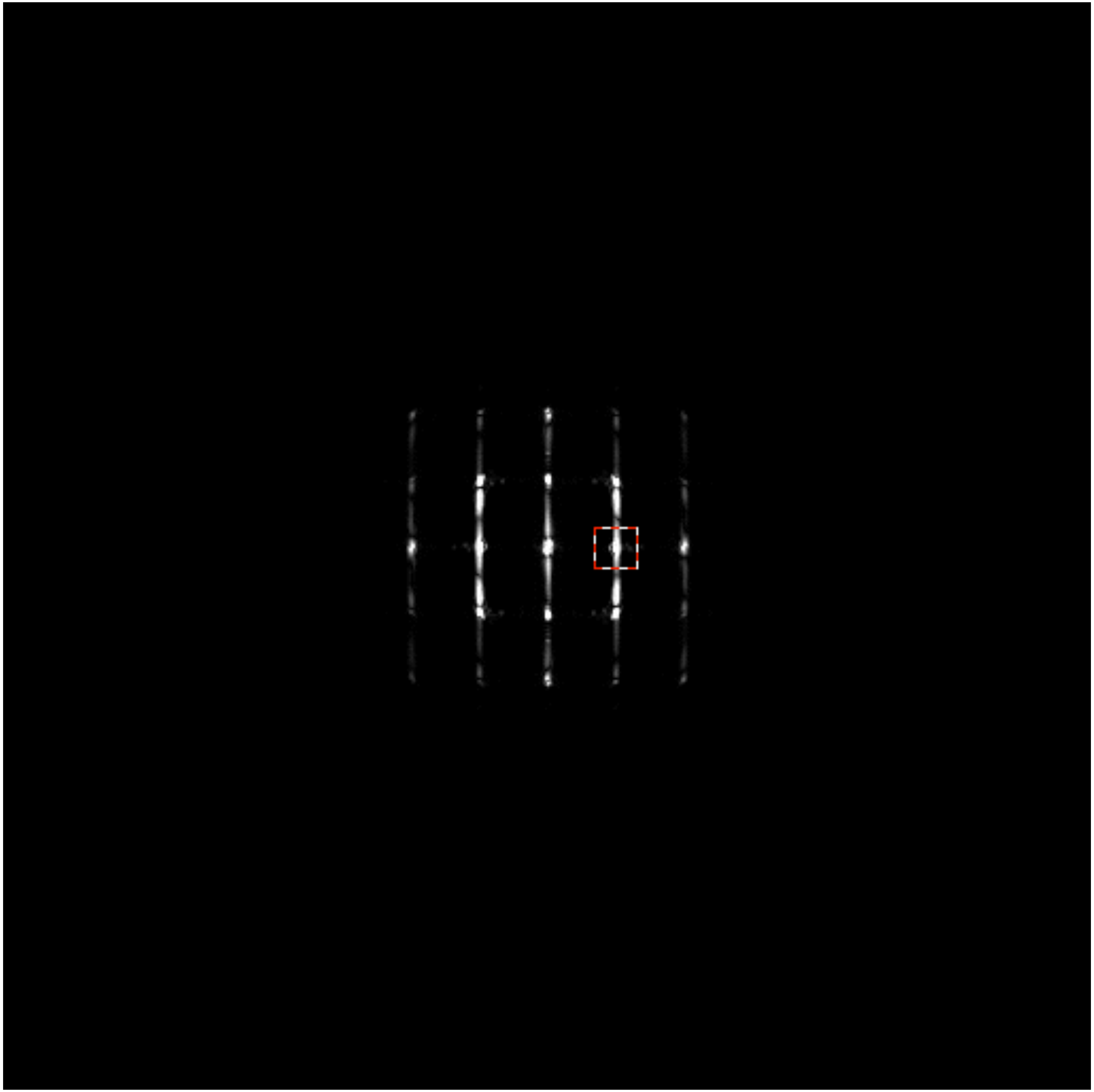
$$\frac{1}{u_0}\hat{\mathbf{g}}_0\cdot\vec{\mathbf{r}} - \frac{1}{u_0}\hat{\mathbf{g}}_0\cdot\frac{\delta(\vec{\mathbf{r}})}{u_0}\vec{\mathbf{r}} = \vec{\mathbf{g}}_0\cdot\vec{\mathbf{r}} - \vec{\mathbf{g}}_0\cdot\Delta\vec{\mathbf{u}}(\vec{\mathbf{r}})$$

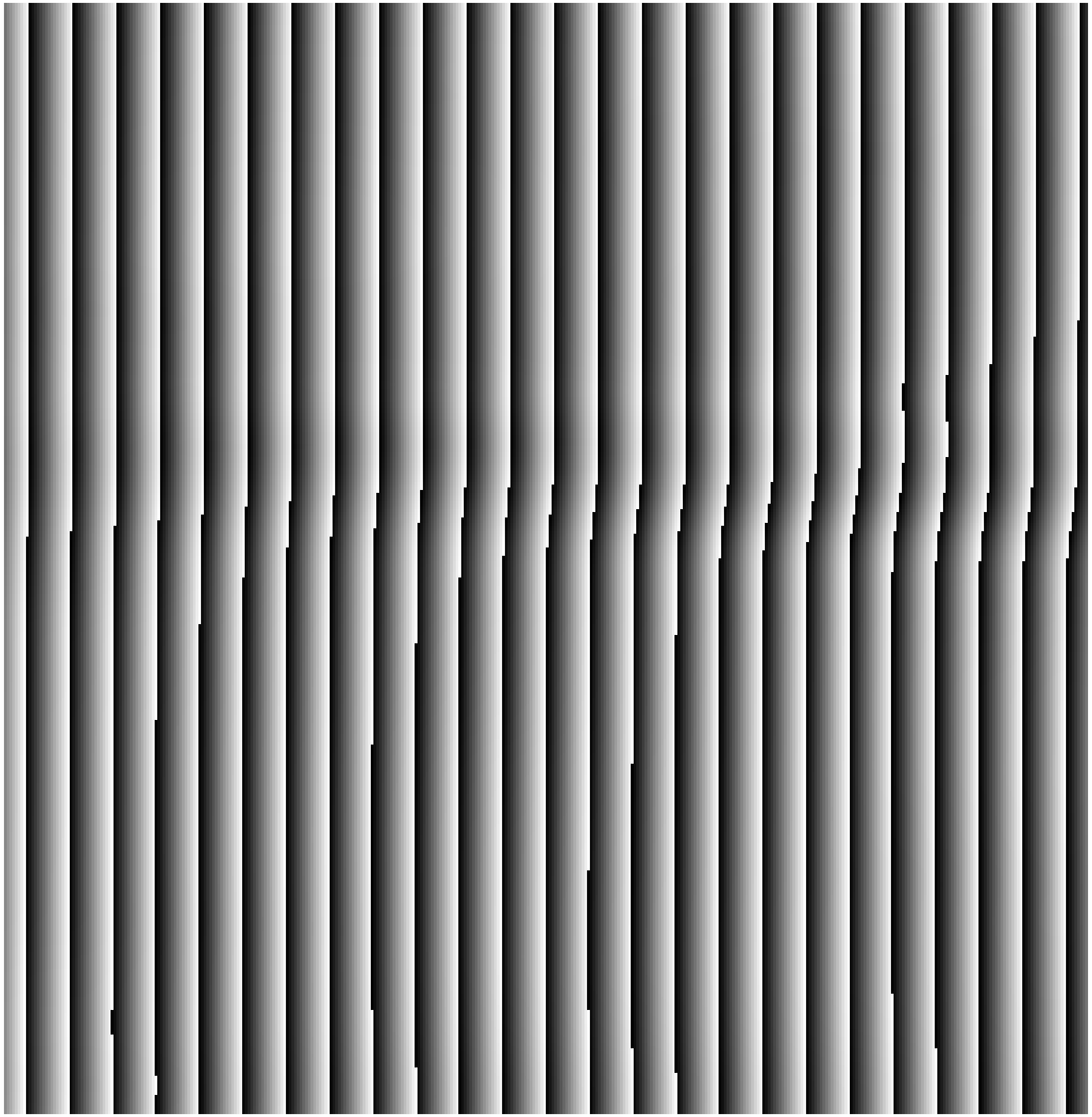
- Amplitude and Phase

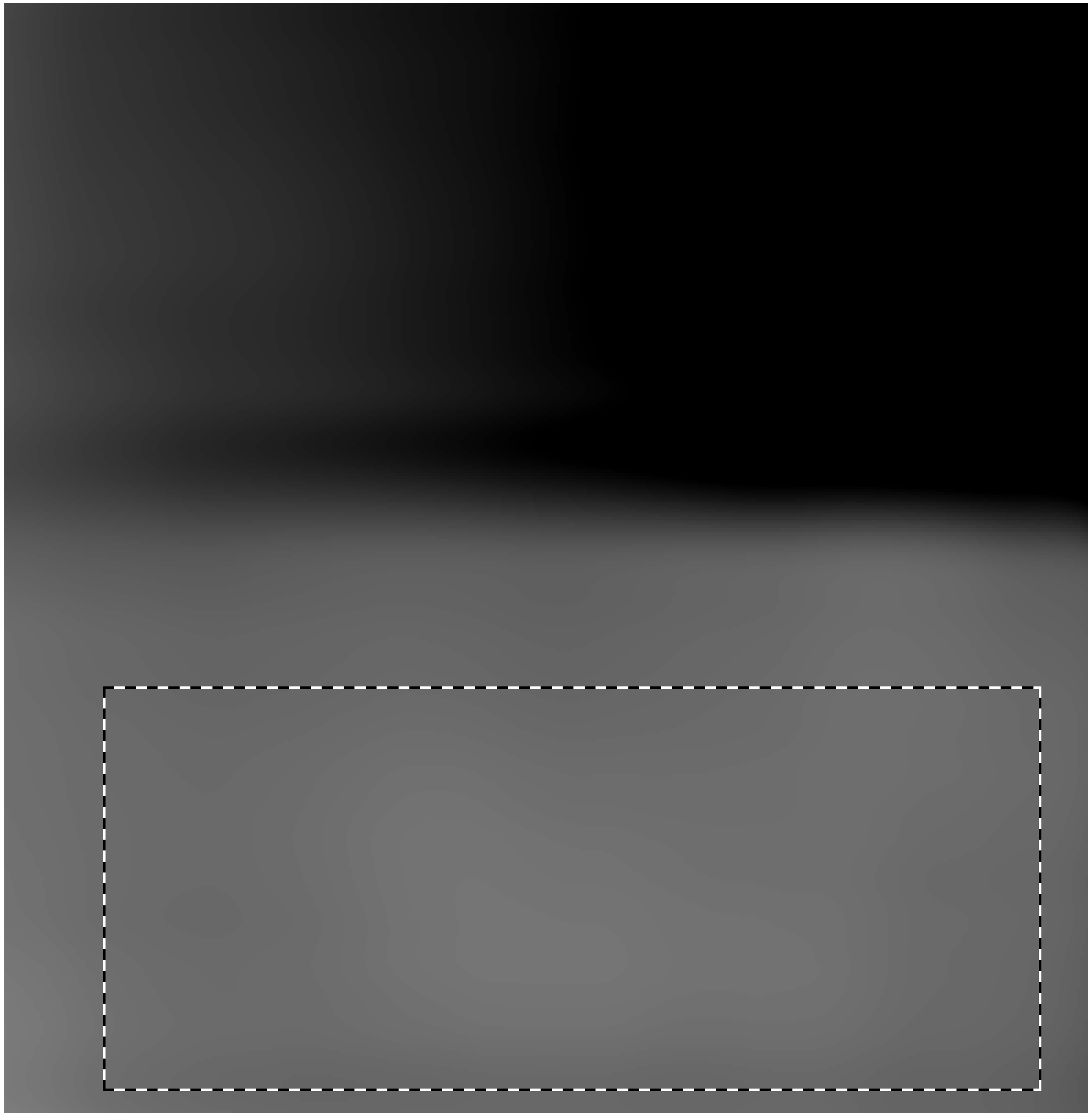
$$\mathrm{I}(\mathbf{r}) = A(\mathbf{r})e^{2\pi i\mathbf{g}(\mathbf{r})\cdot\mathbf{r}} = A(\mathbf{r})e^{2\pi i(\mathbf{g}_0 + \Delta\mathbf{g}(\mathbf{r}))\cdot\mathbf{r}}$$

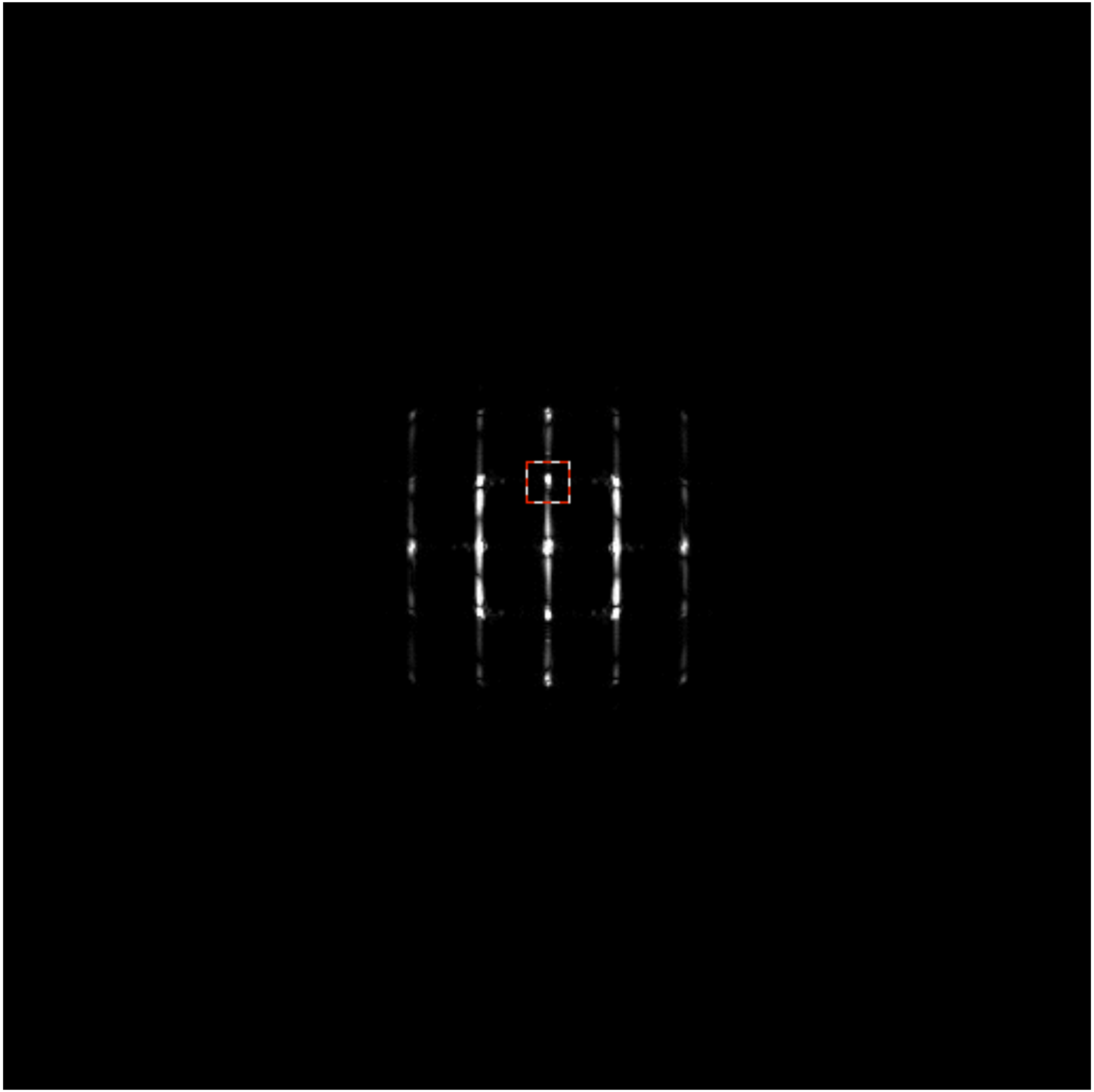
$$= A(\mathbf{r})e^{2\pi i(\mathbf{g}_0\cdot\mathbf{r} + \mathbf{g}_0\cdot\Delta\mathbf{u}(\mathbf{r}))} = A(\mathbf{r})\exp(iP(\mathbf{r}))$$

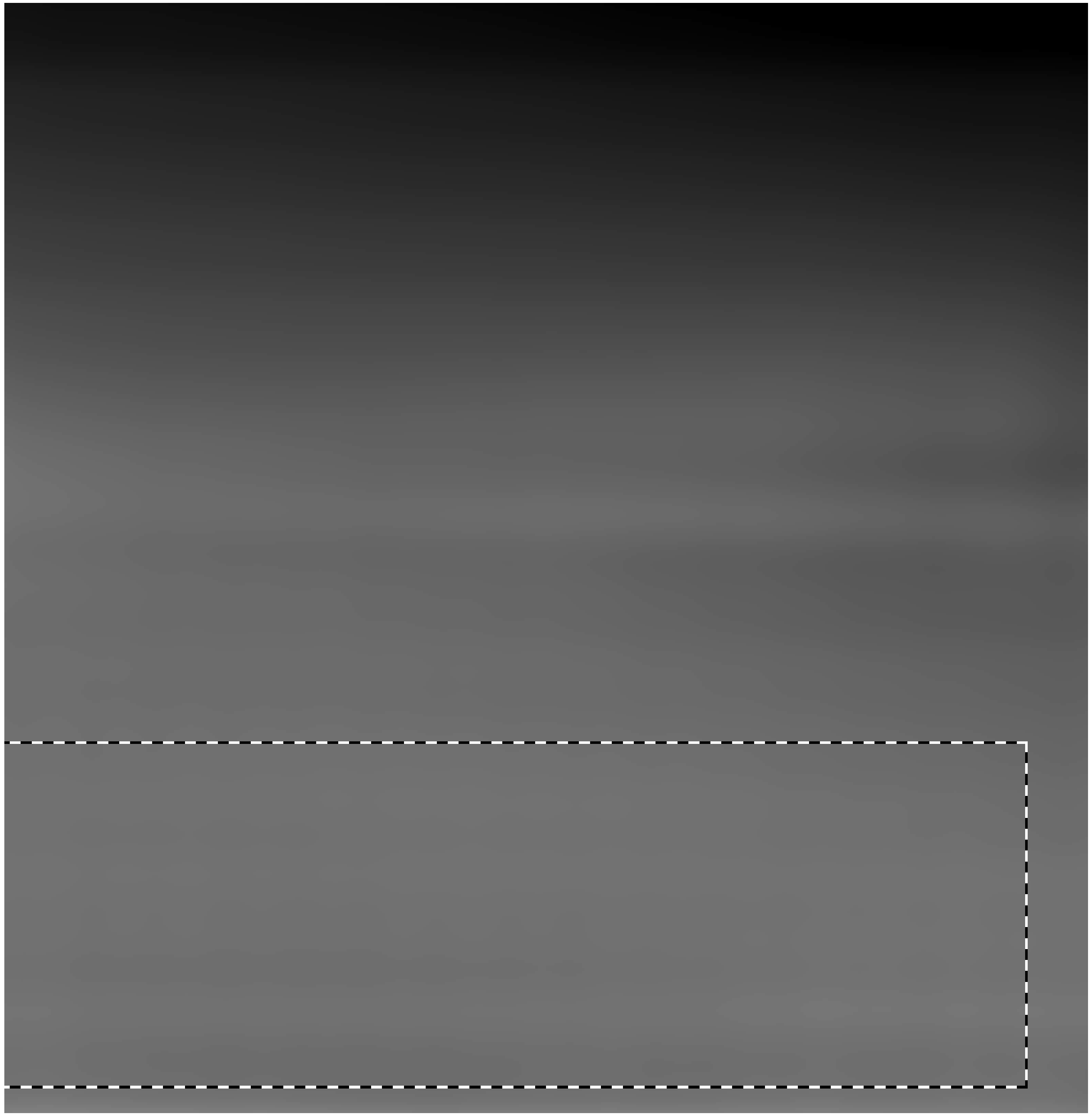












Displacement Field Calculation

- Requires 2 phase images from 2 different reflections

- Implicit definition of a reference lattice

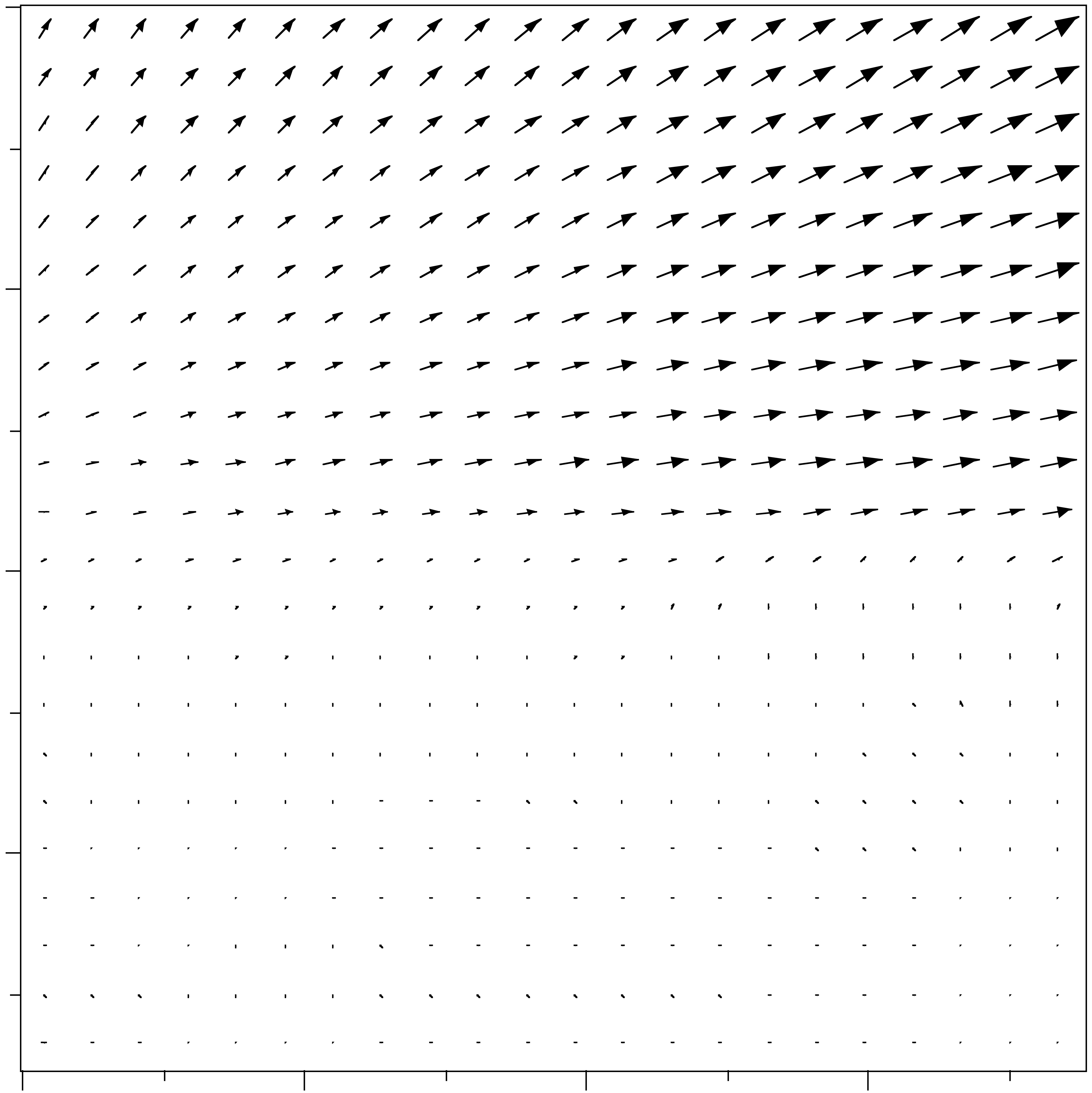
$$P_{g1}(\vec{r}) = 2\pi\ \vec{g}_1 . \vec{u}(\vec{r}) = 2\pi(g_{1x}.u_x(\vec{r}) + g_{1y}.u_y(\vec{r}))$$

$$P_{g2}(\vec{r}) = 2\pi\vec{g}_2 . \vec{u}(\vec{r}) = 2\pi(g_{2x}.u_x(\vec{r}) + g_{2y}.u_y(\vec{r}))$$

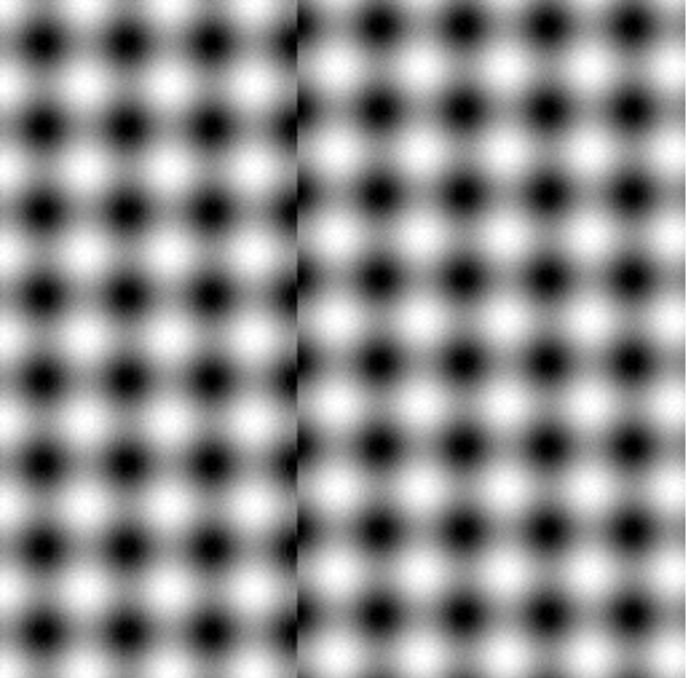
- Solution for the displacements with respect to the reference lattice

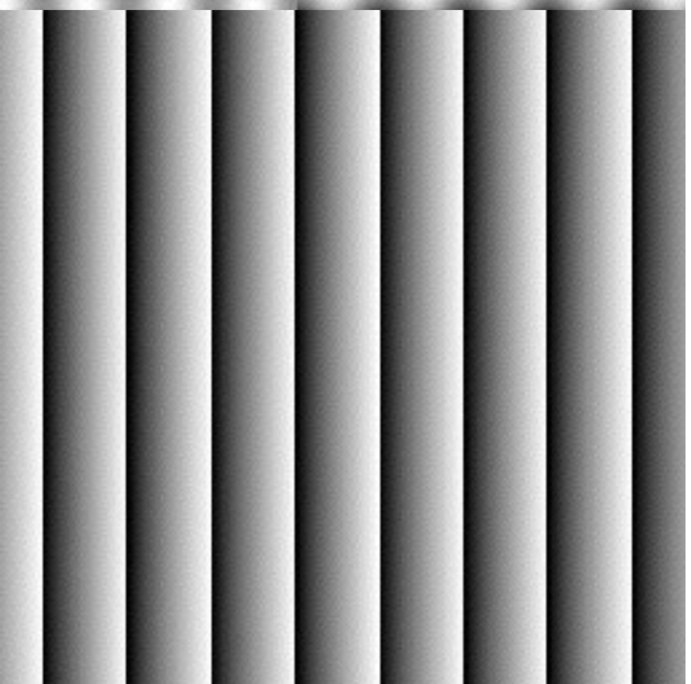
$$u_x(\vec{r}) = \frac{1}{2\pi}\left(\frac{P_{g1}(\vec{r}).g_{2y} - P_{g2}(\vec{r}).g_{1y}}{g_{1x}.g_{2y} - g_{1y}.g_{2x}}\right)$$

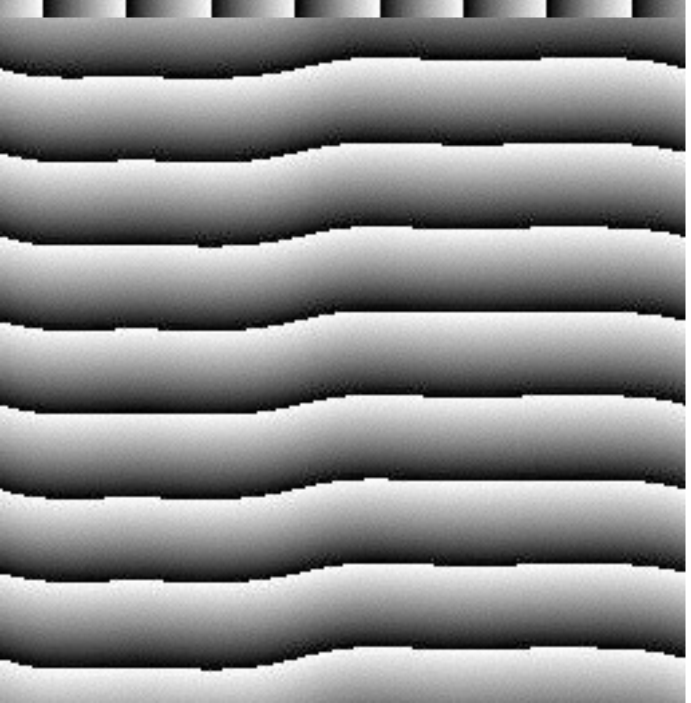
$$u_y(\vec{r}) = \frac{1}{2\pi}\left(\frac{P_{g2}(\vec{r}).g_{1x} - P_{g1}(\vec{r}).g_{2x}}{g_{1x}.g_{2y} - g_{1y}.g_{2x}}\right)$$

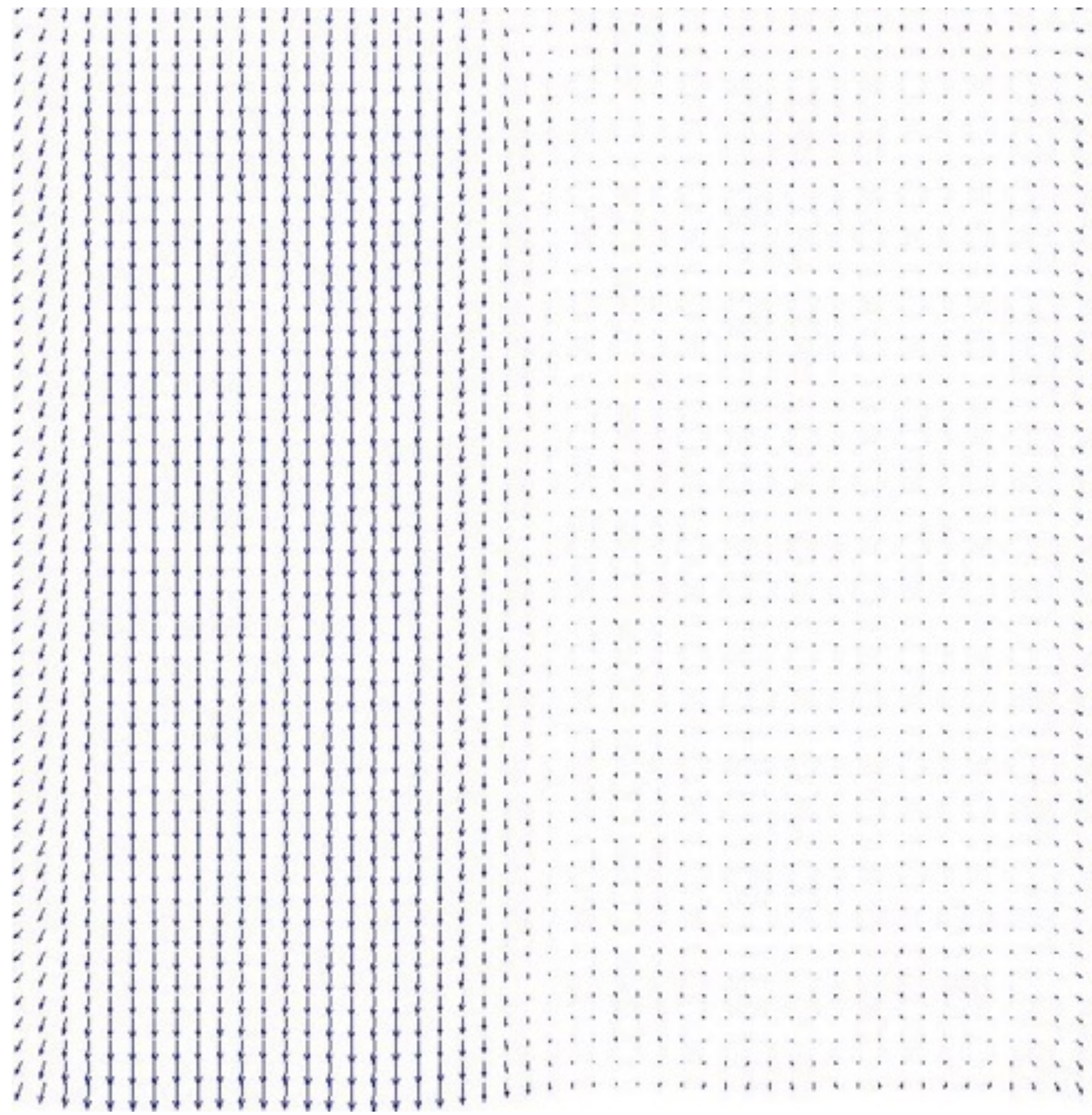


Shift Case

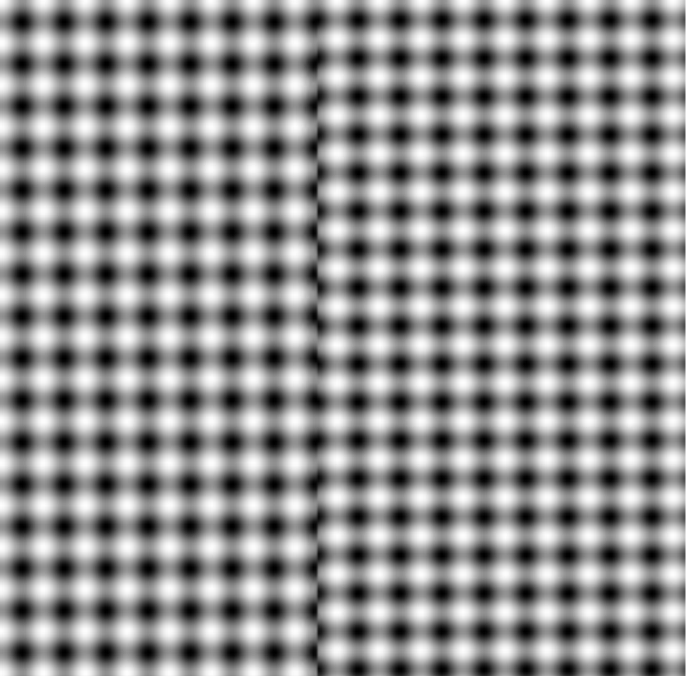

object


phase1

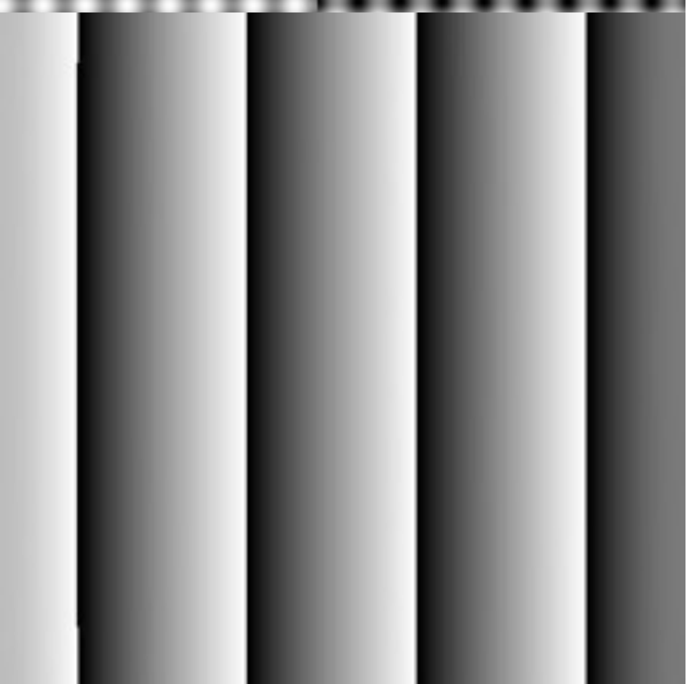

phase2


Displacement map

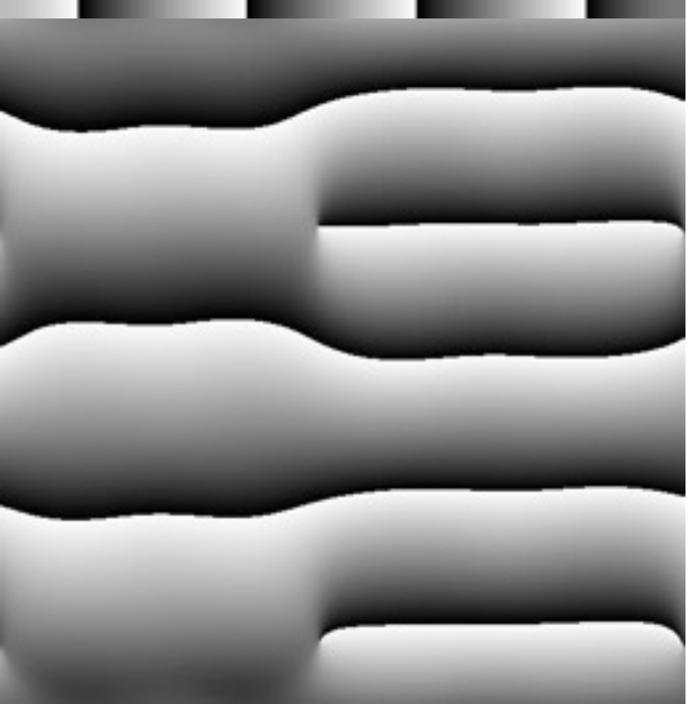
Dilatation Case



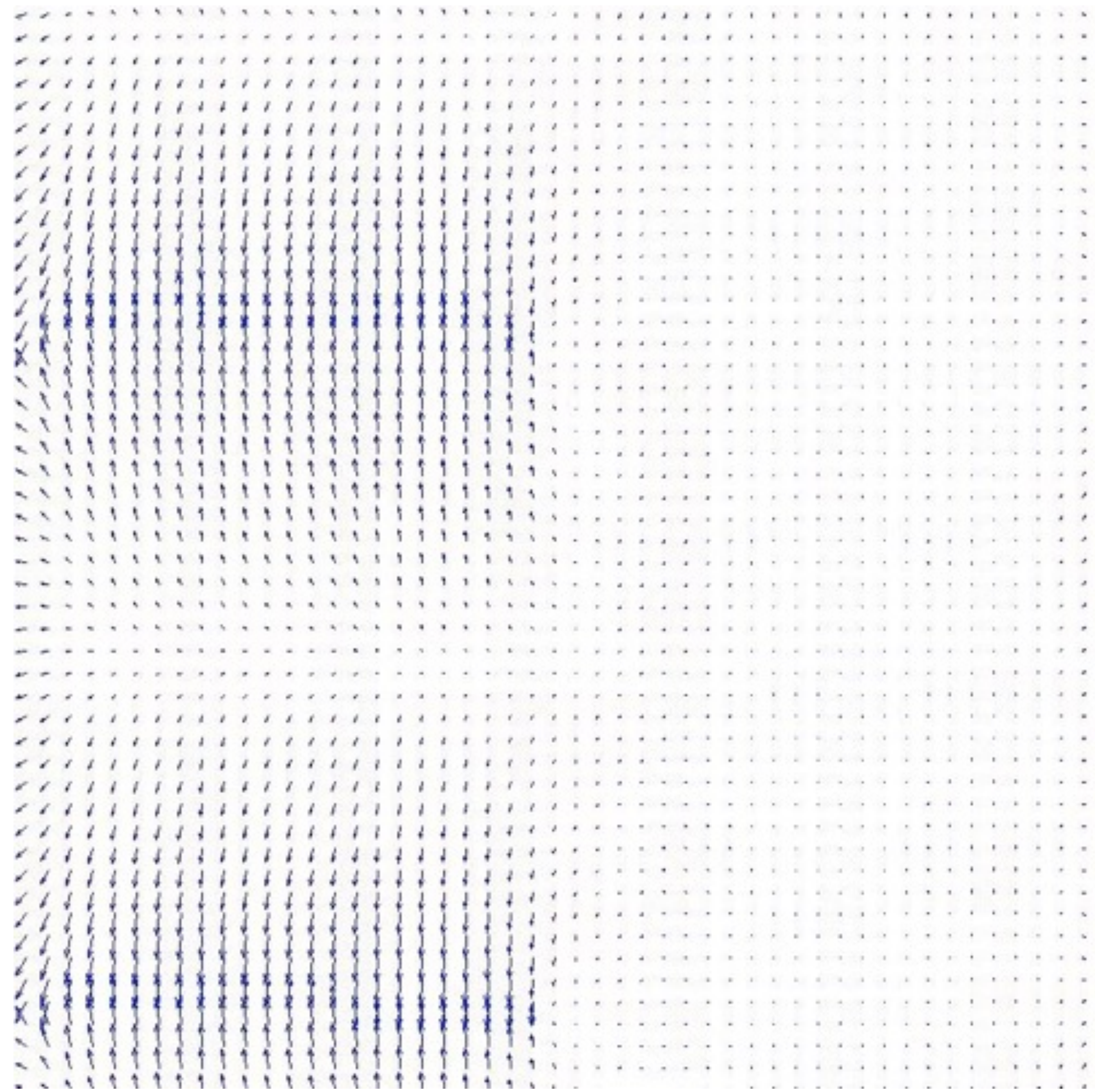
object



phase1

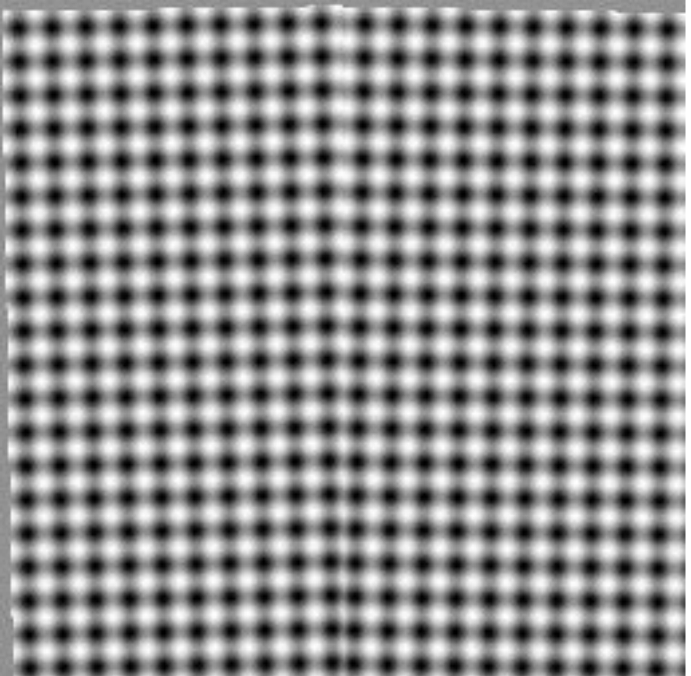


phase2

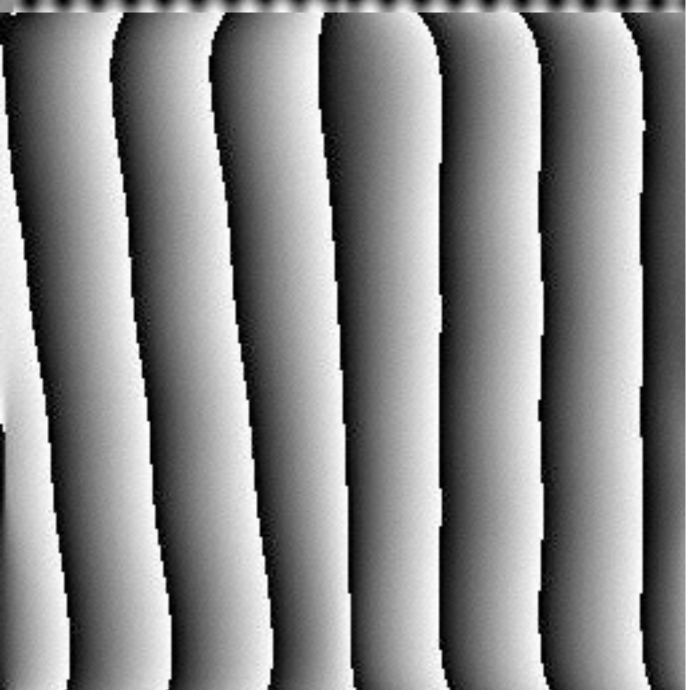


Displacement map

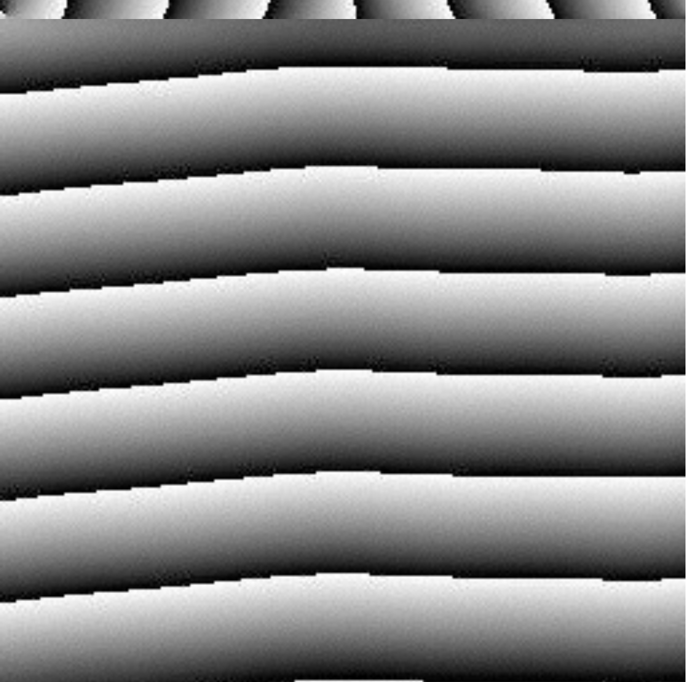
Rotation Case



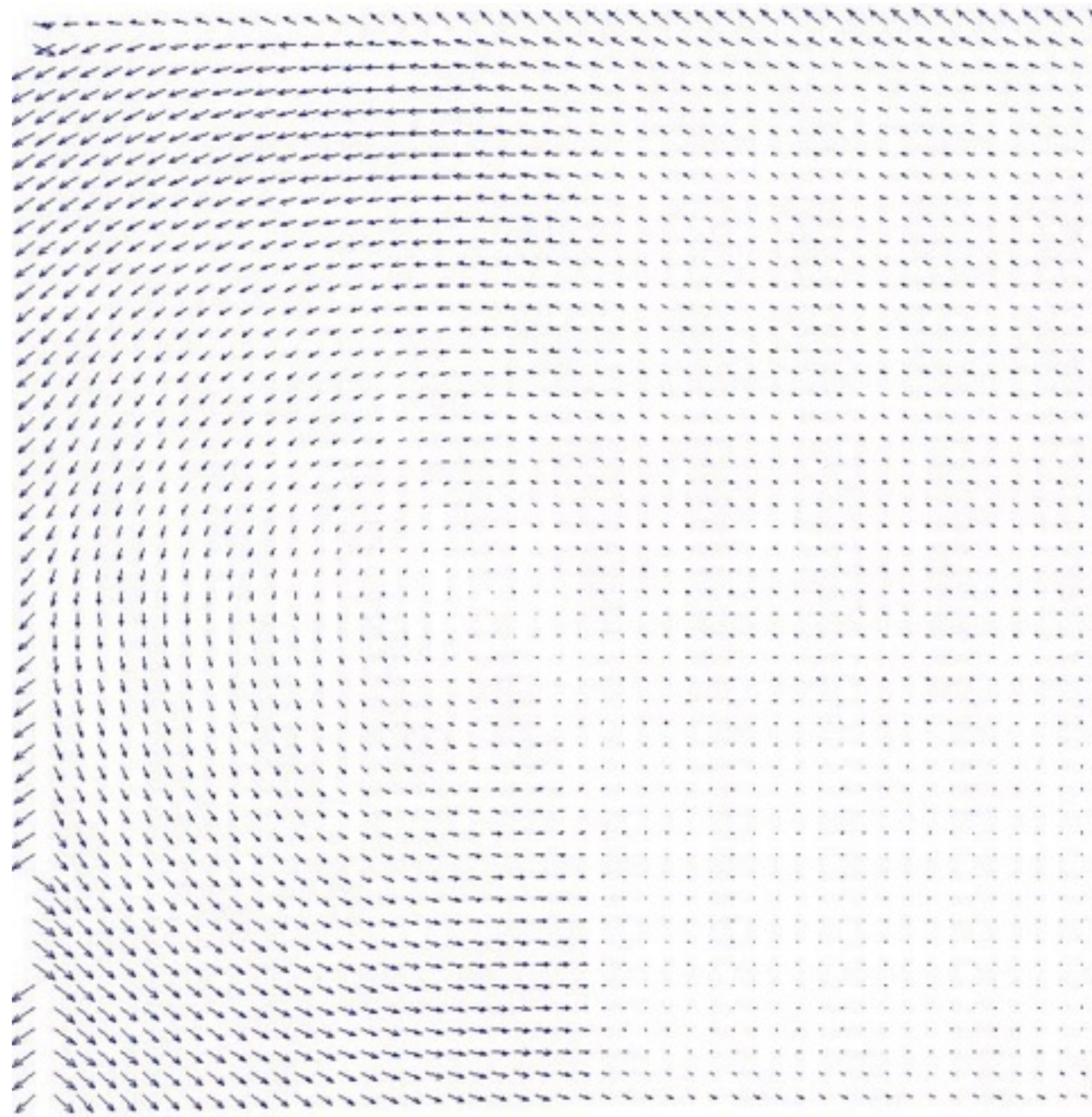
object



phase1



phase2

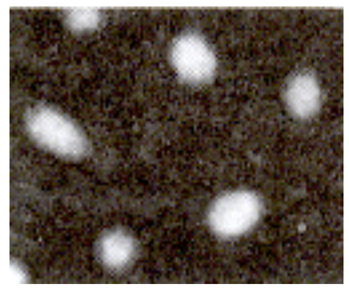


Displacement map

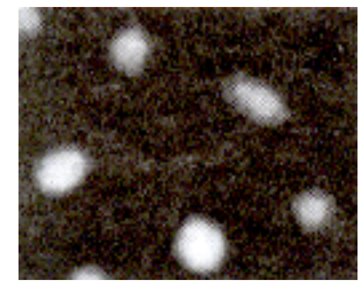
Alternative Strain Map

Template matching- cross correlation

Template



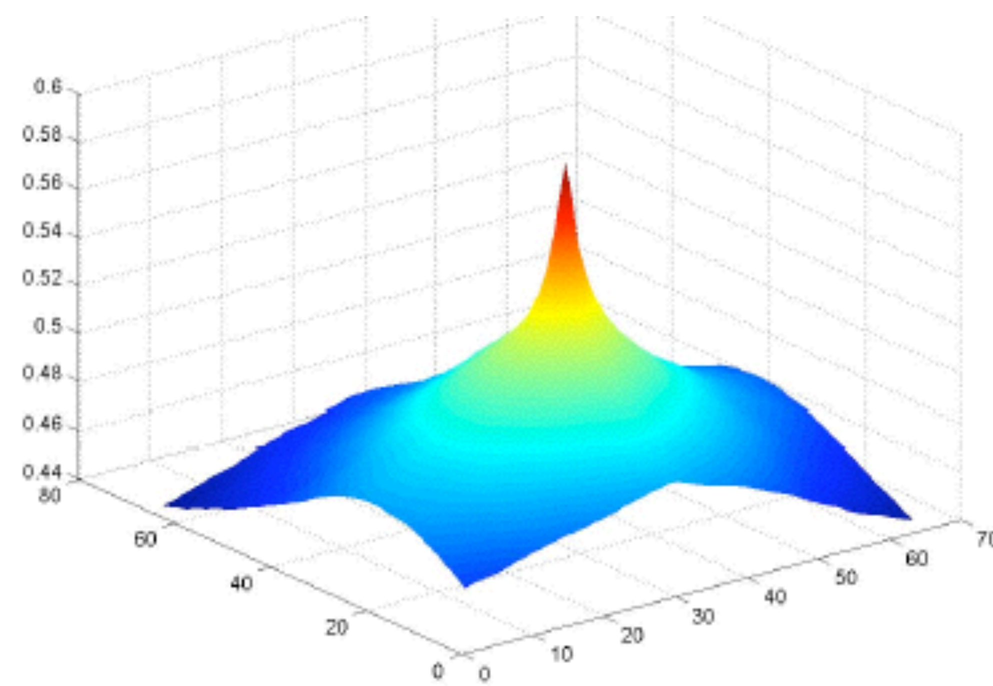
I1



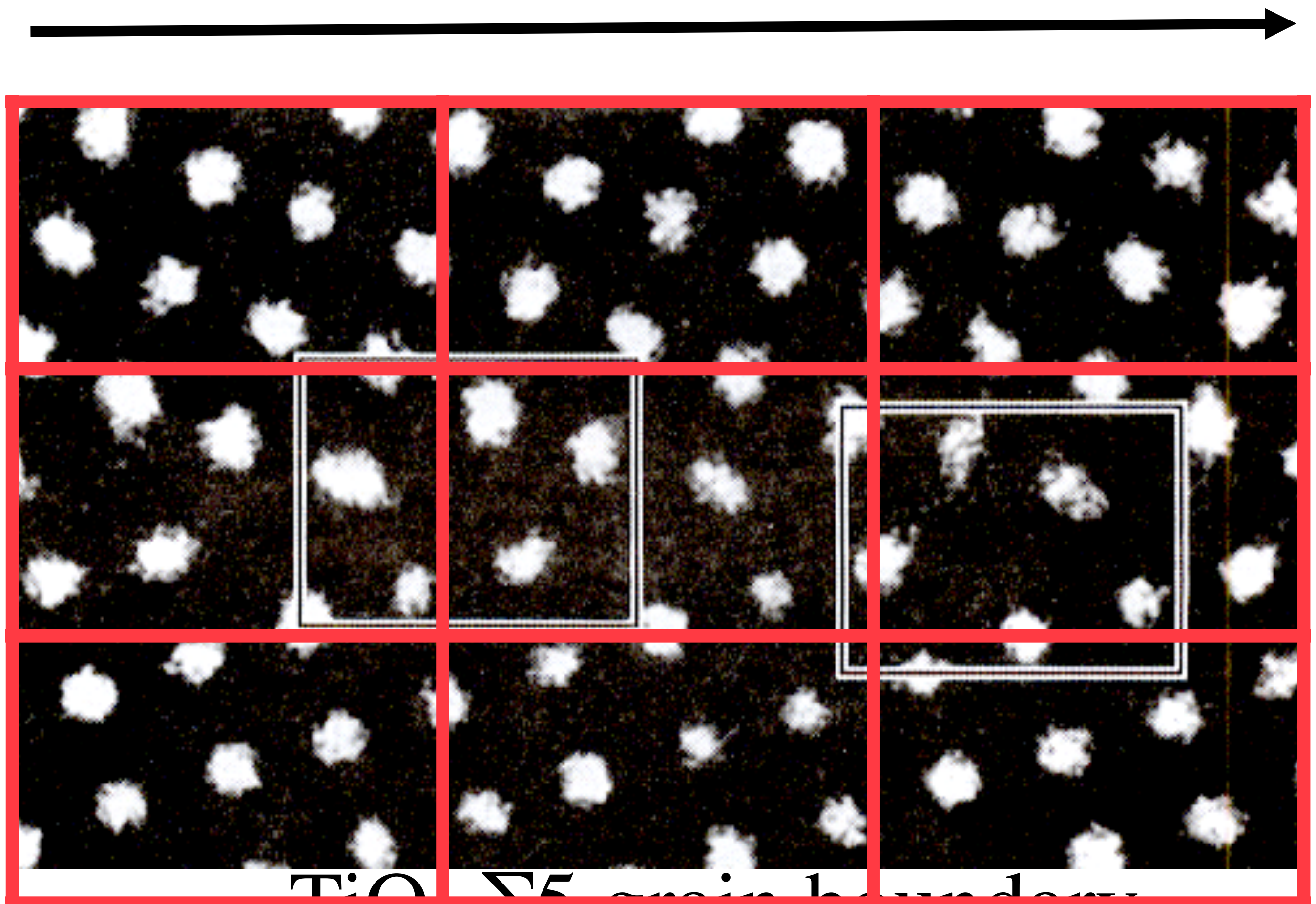
object

I2

$$ccf = \frac{\Im(I_1)\Im(I_2^*)}{|I_1||I_2|}$$



The value of ccf give an indication of similarity of two images

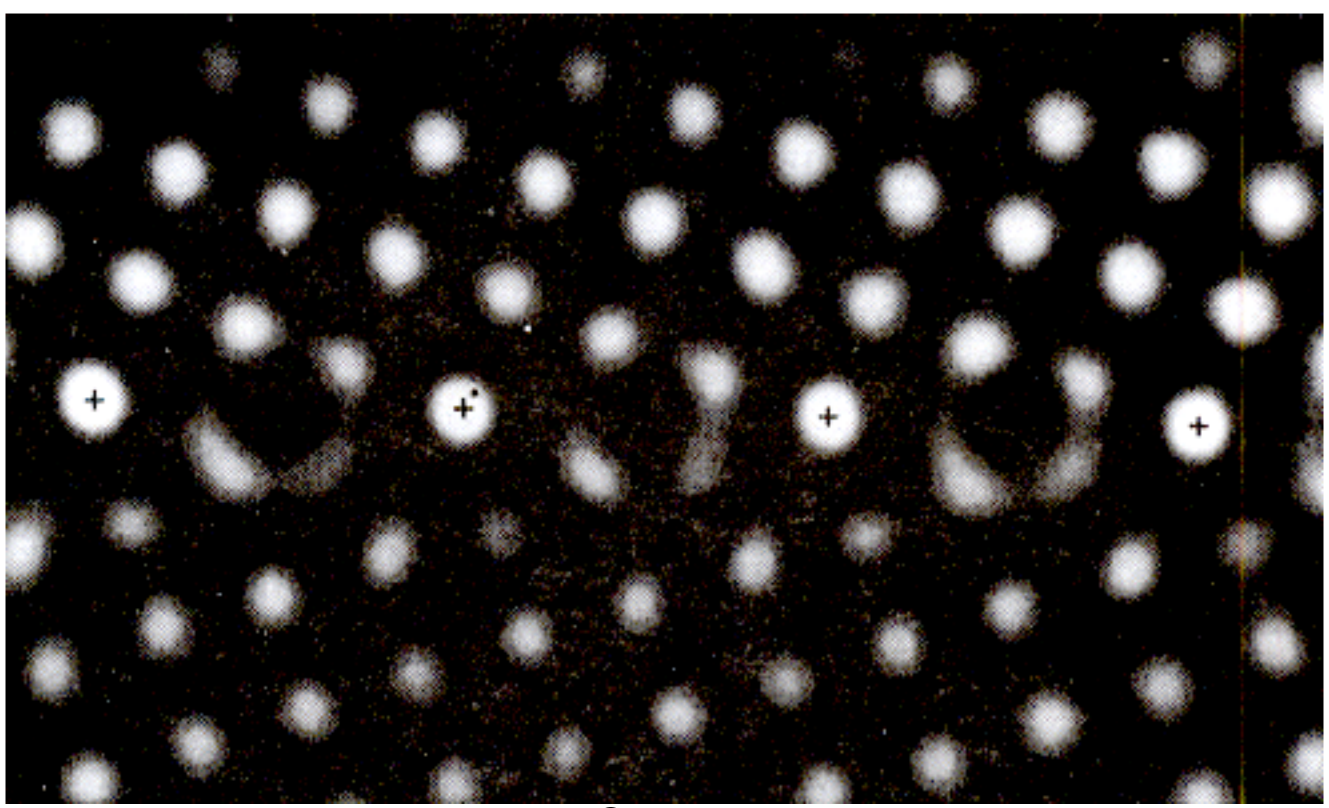


TiO_2 Σ5 grain boundary

1. Scanning the template across the object image

2. Generating CCF map

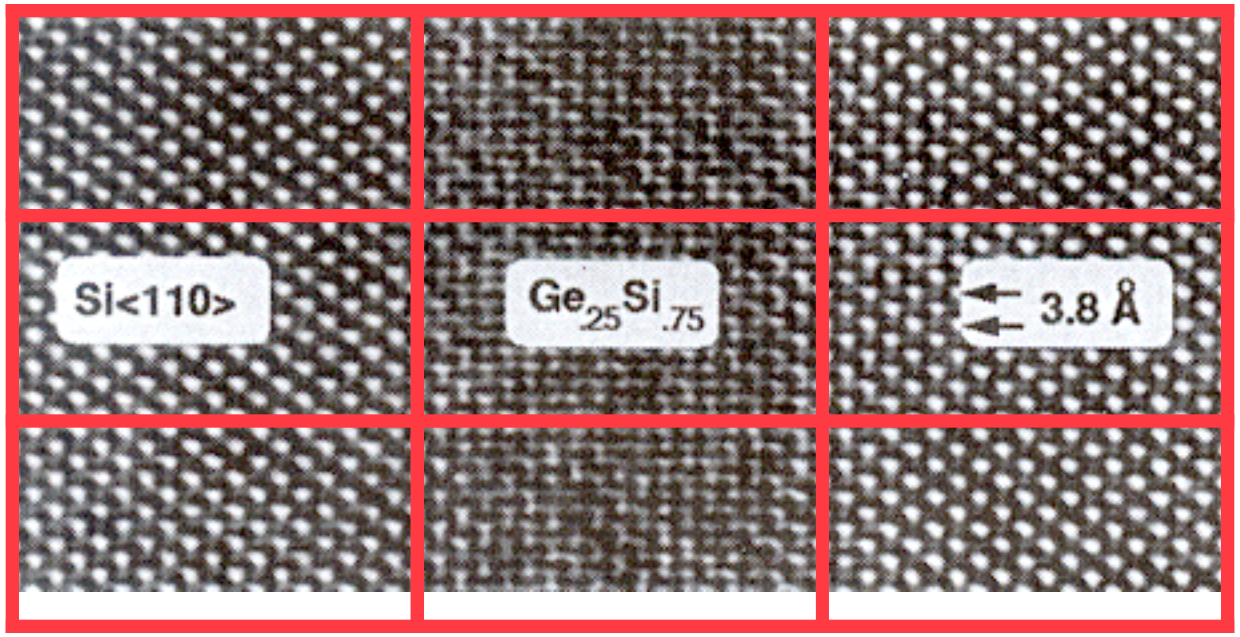
Pattern Recognition for structure identification

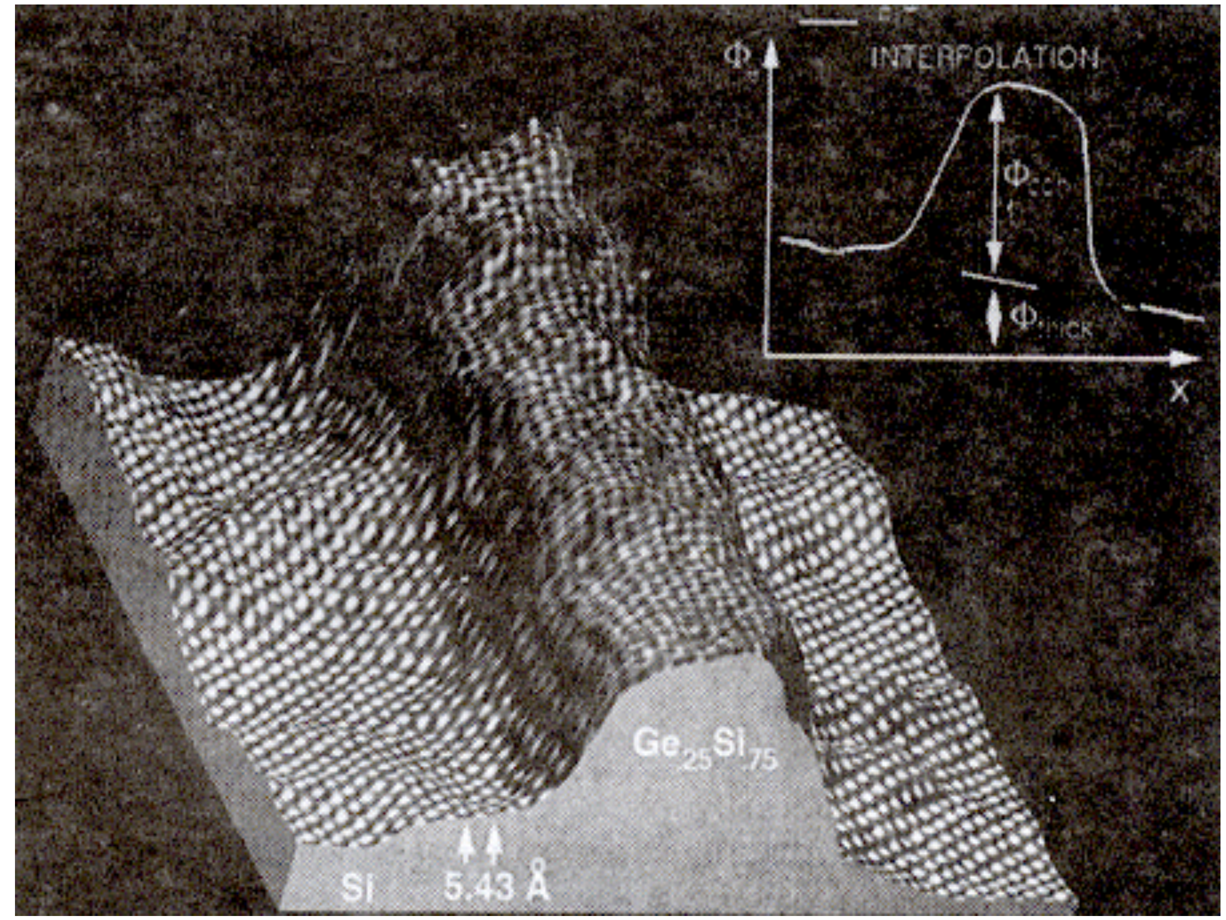


ccf map

Atom Resolution Compositional Map

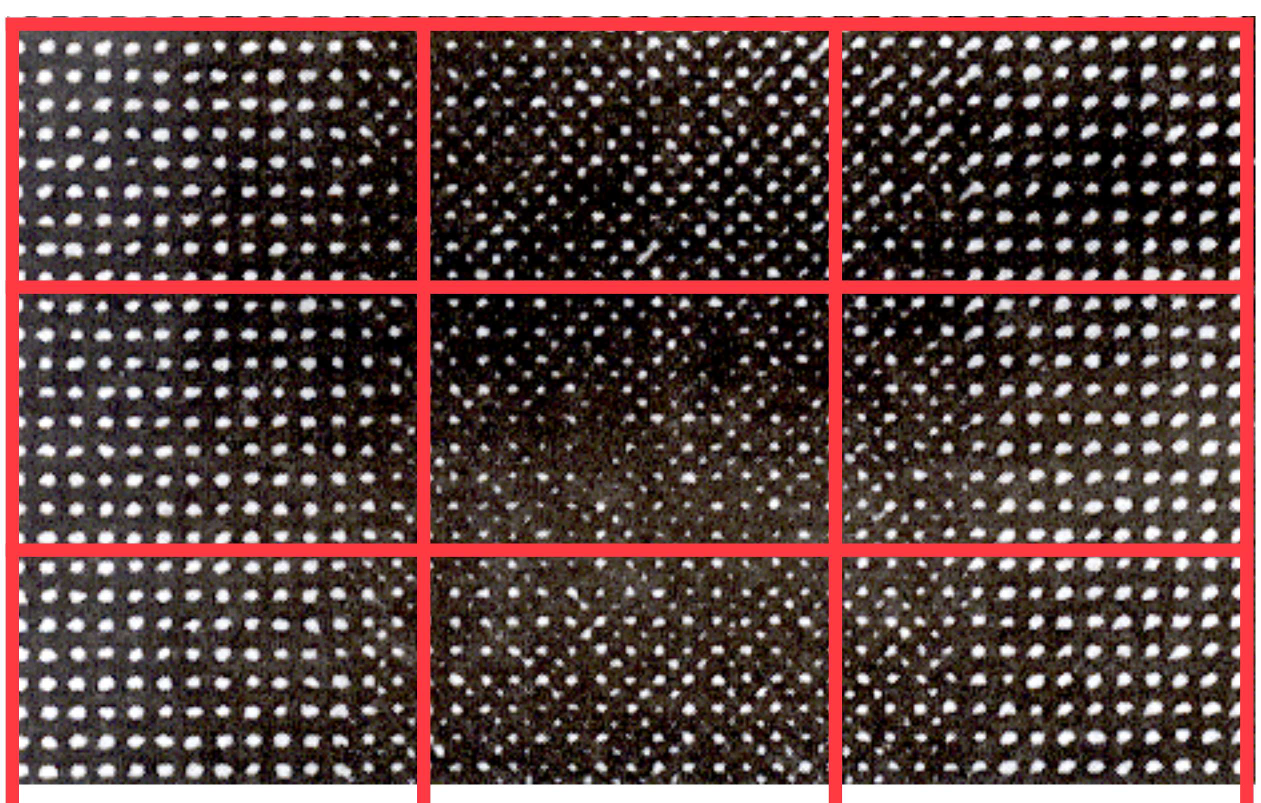
Si/GeSi quantum well



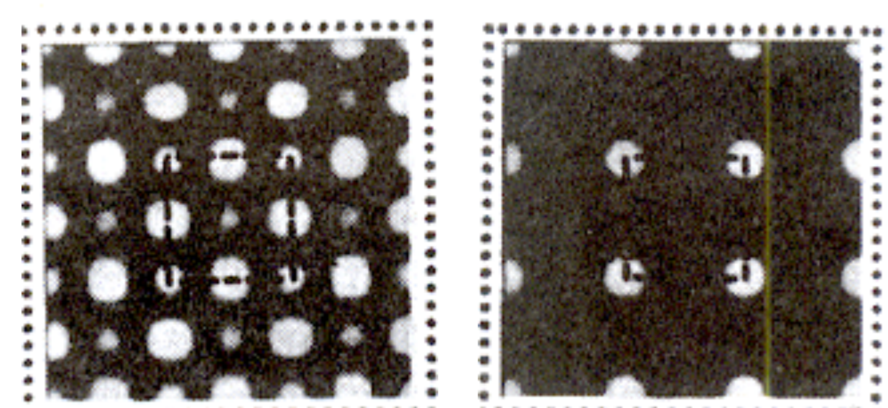


CCF map with HRTEM skin

(Al)GaAs GaAs (Al)GaAs



GaAs AlAs



template