Chapter 7

原子結構分析和應變

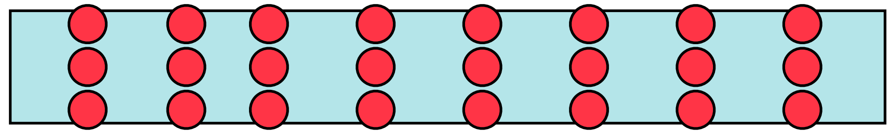
(Chapter 30, 31)

7.1 Weak Phase Object

NTHU

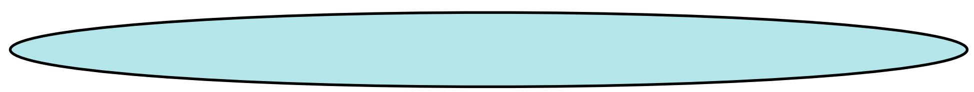
Assuming the object is a weak phase object

$$\psi_o = 1$$



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

Only the phase change involved
Amplitude does not change



$\Im(\psi_e) = \delta + i\Im[\varphi(x,y)]$ B.F.P. $\Im(\psi_e) \bullet T(H)$

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

defocus | spherical aberration | spatial coherency | chromatic aberration

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

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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

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

This is so called phase contrast

Two Resolutions: How to Improve Resolution

TEM CENTER

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

幾何光學
分辨率

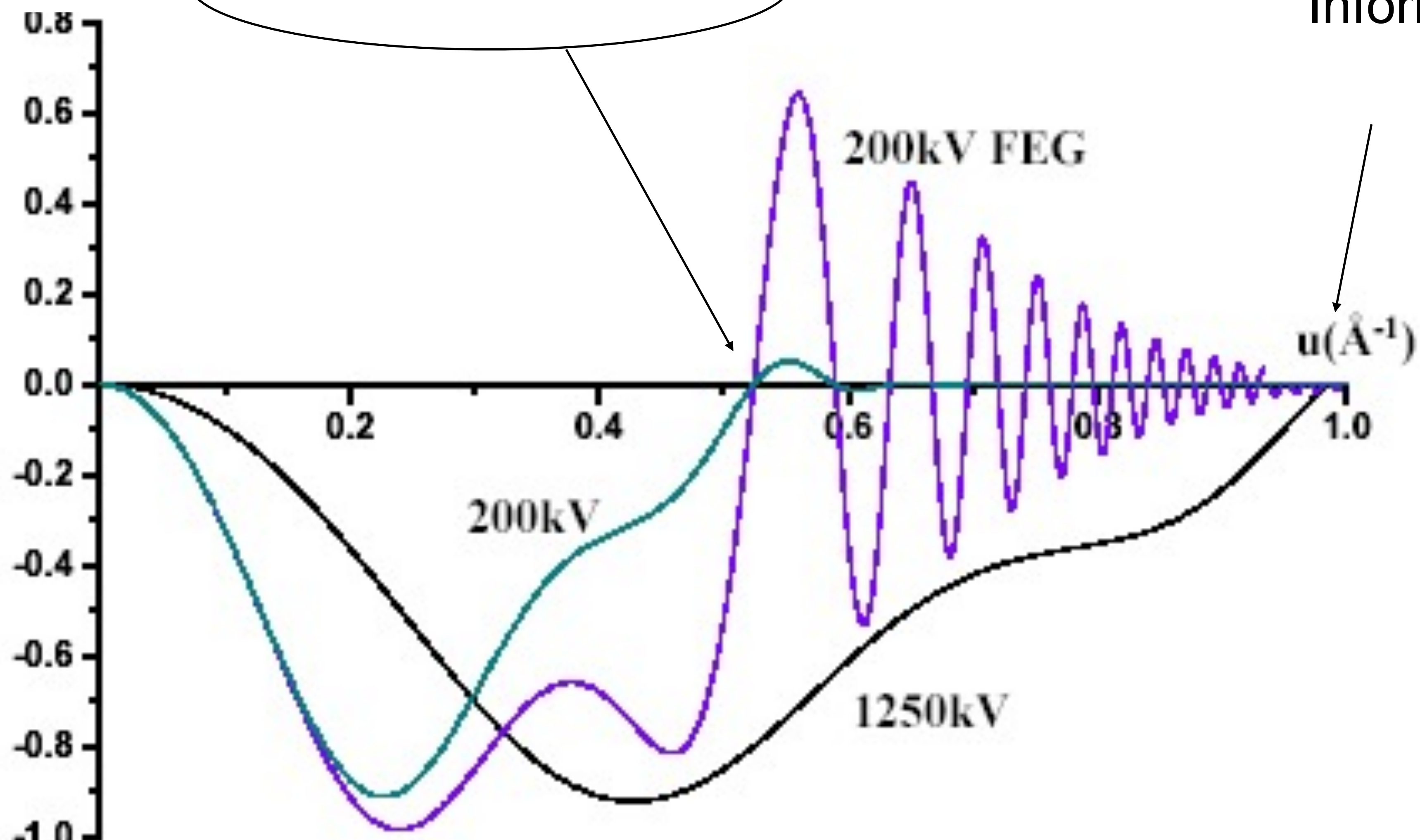
Scherzer Resolution
Point-point resolution
$d=0.66C_s^{1/4}\lambda^{3/4}$

$C_s\downarrow$ $\lambda\downarrow$ **(high voltage TEM Cs corrected TEM)**

Information limit

$C_c\downarrow$ $\alpha\downarrow$

Coherency $\uparrow$
(**FEG Gun**
Monochromator
Cc corrector
Cs corrector)



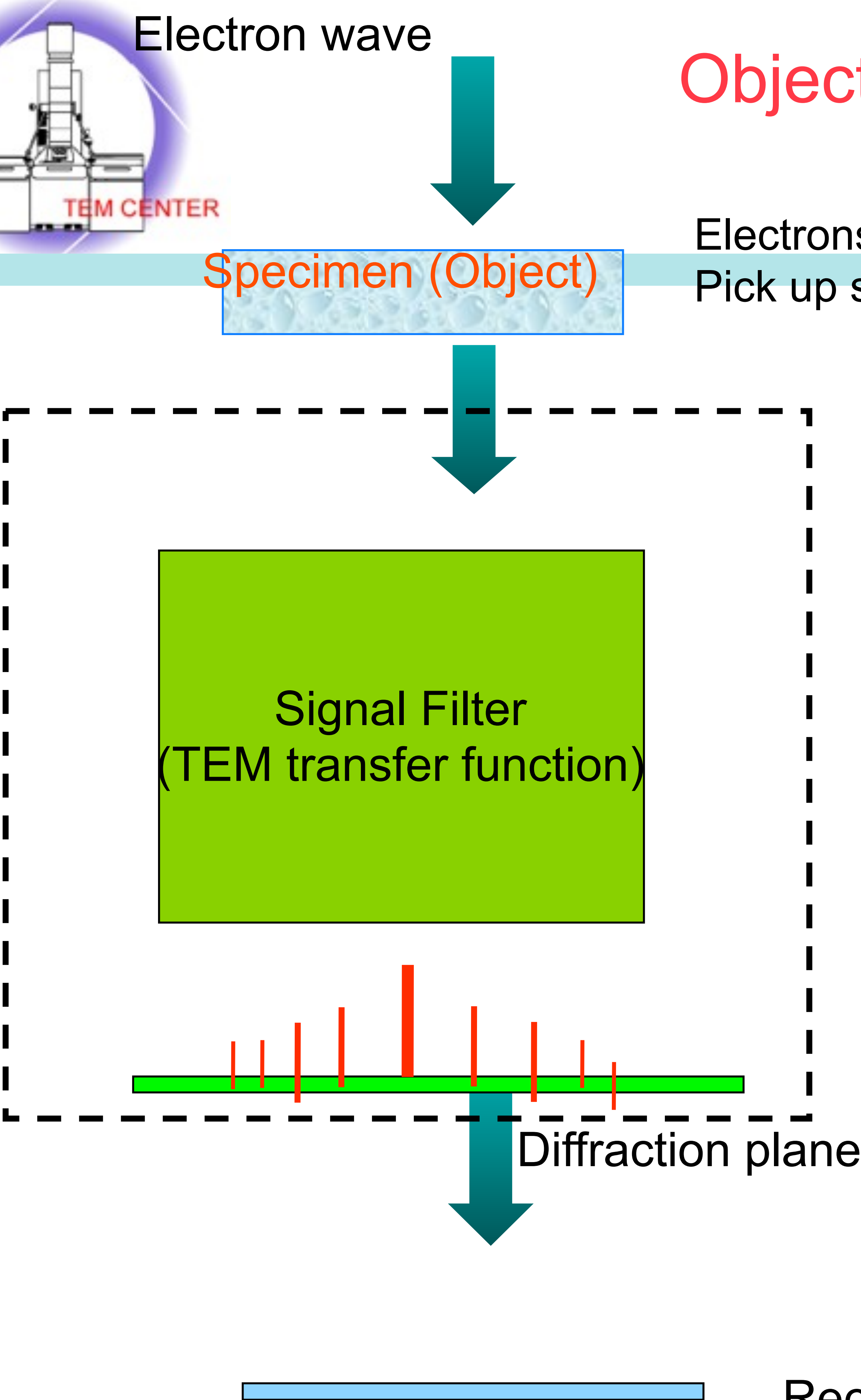
CTF curves of Scherzer focus $= -1.22(C_s\lambda)^{1/2}$

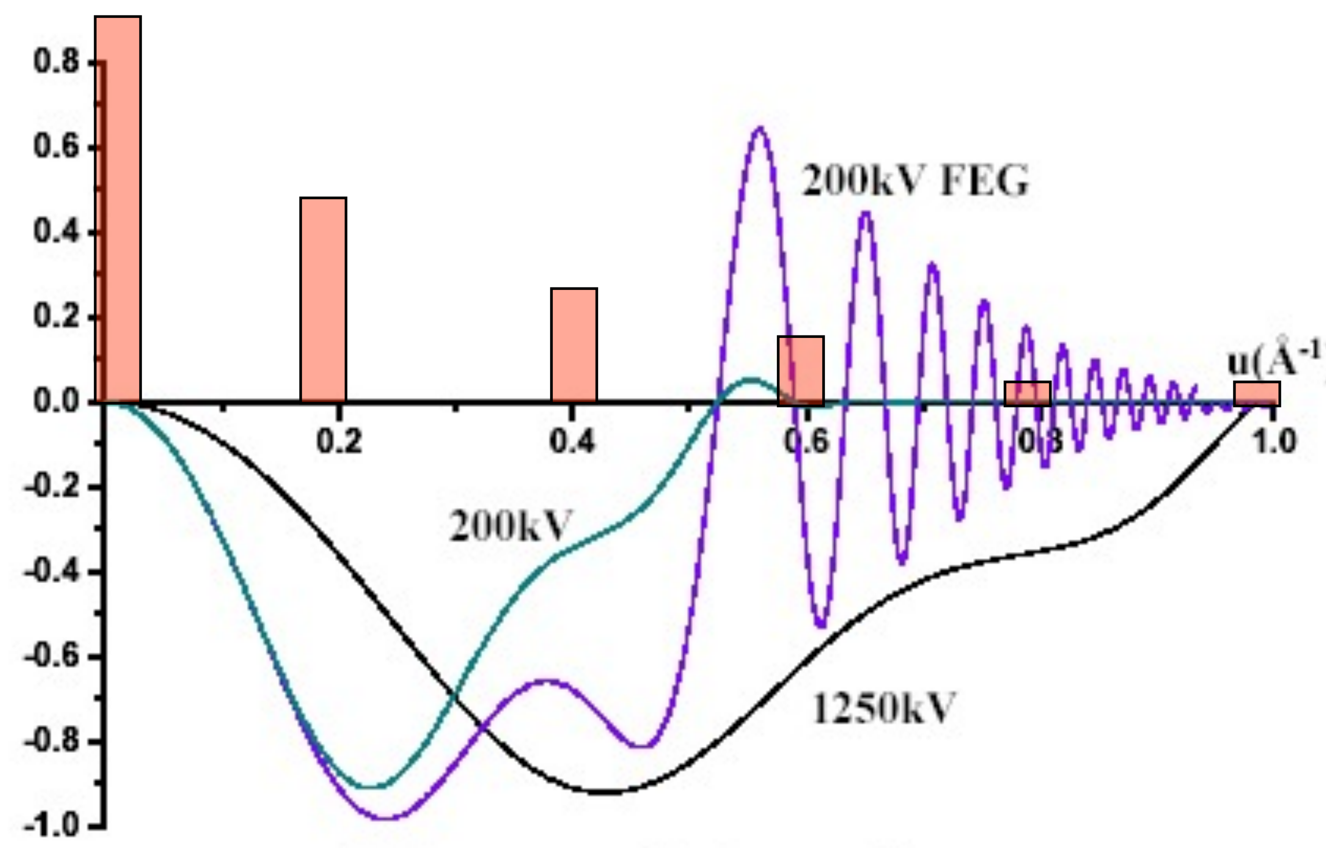
CTF有很寬之通帶

Objective lens acts as a signal filter

NTHU

Electrons interact with atoms
Pick up structure information

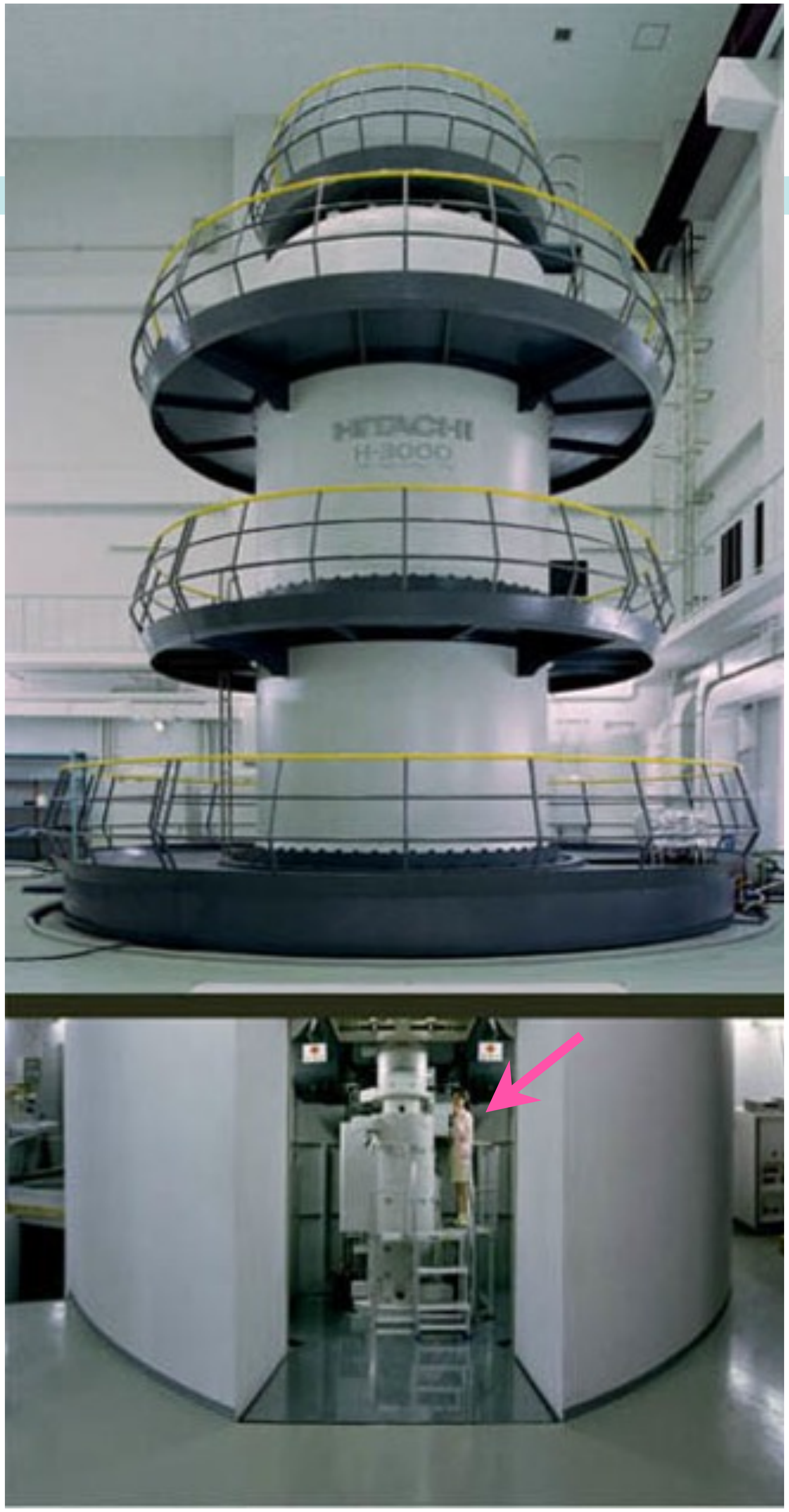




CTF curves of Scherzer focus

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.

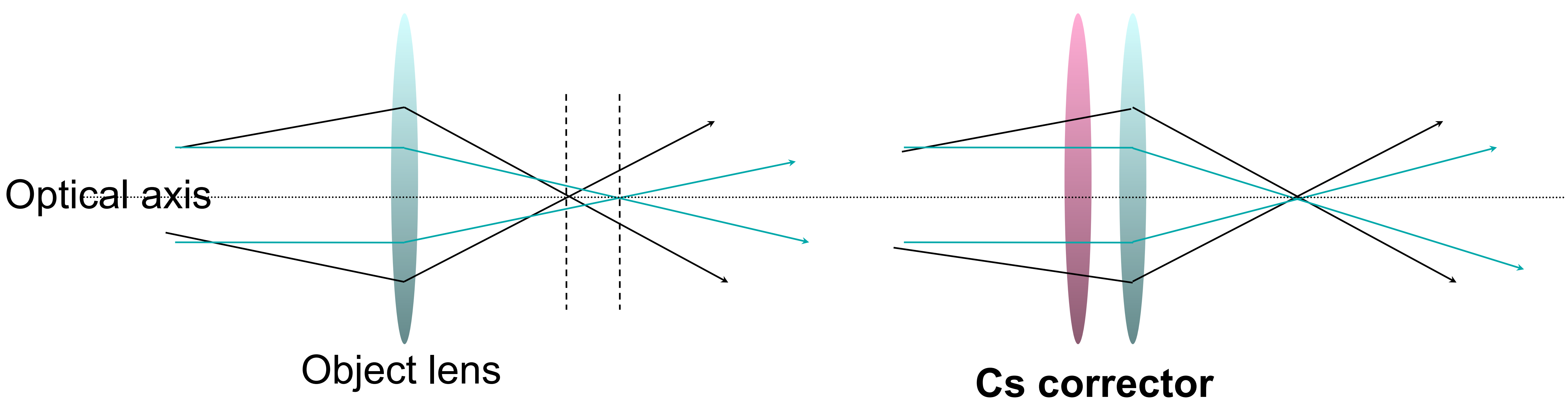
NTHU

- 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

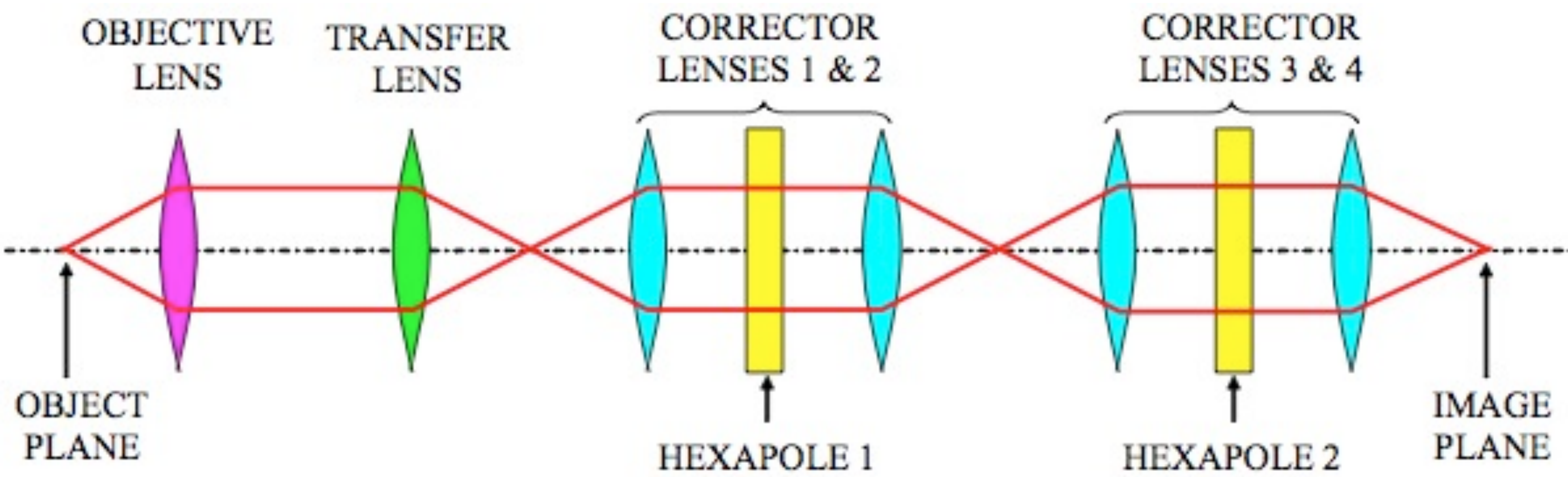
Spherical aberration Cs

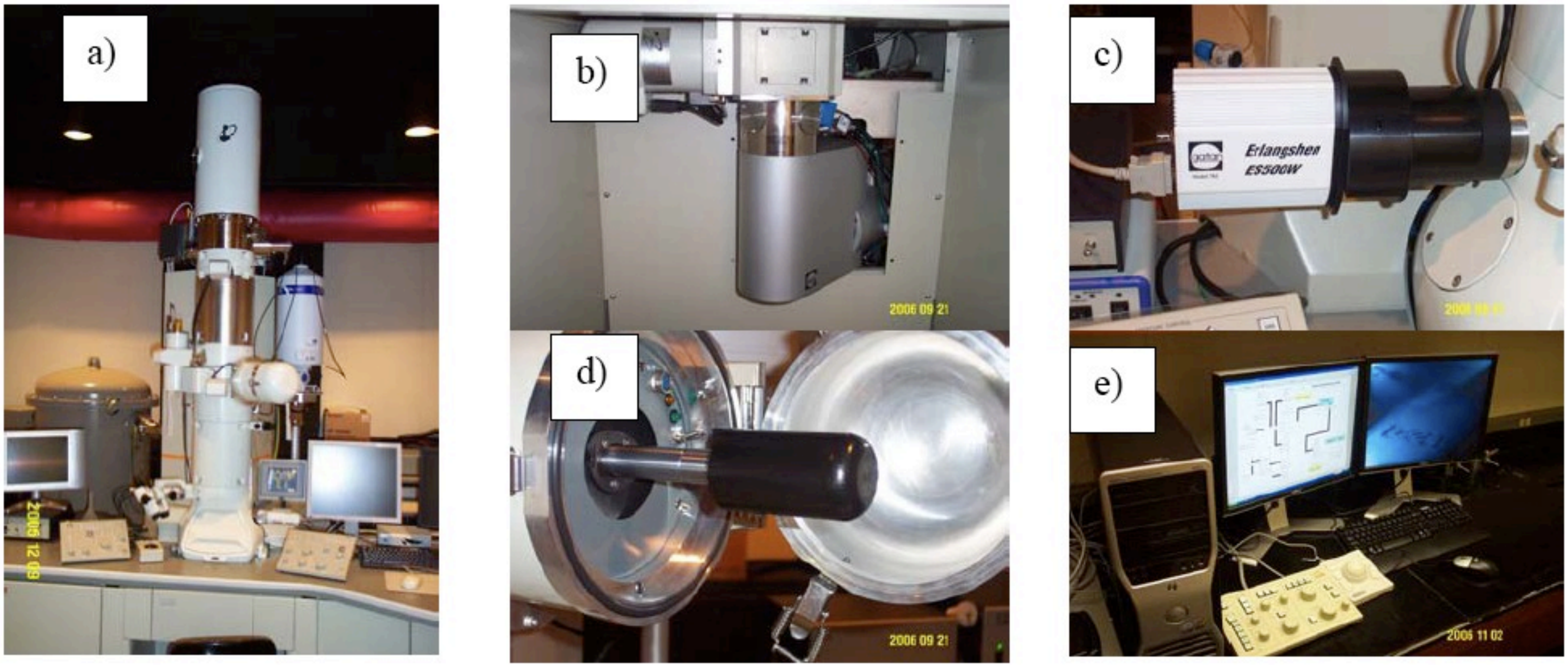


7.2 Hardware Correctors

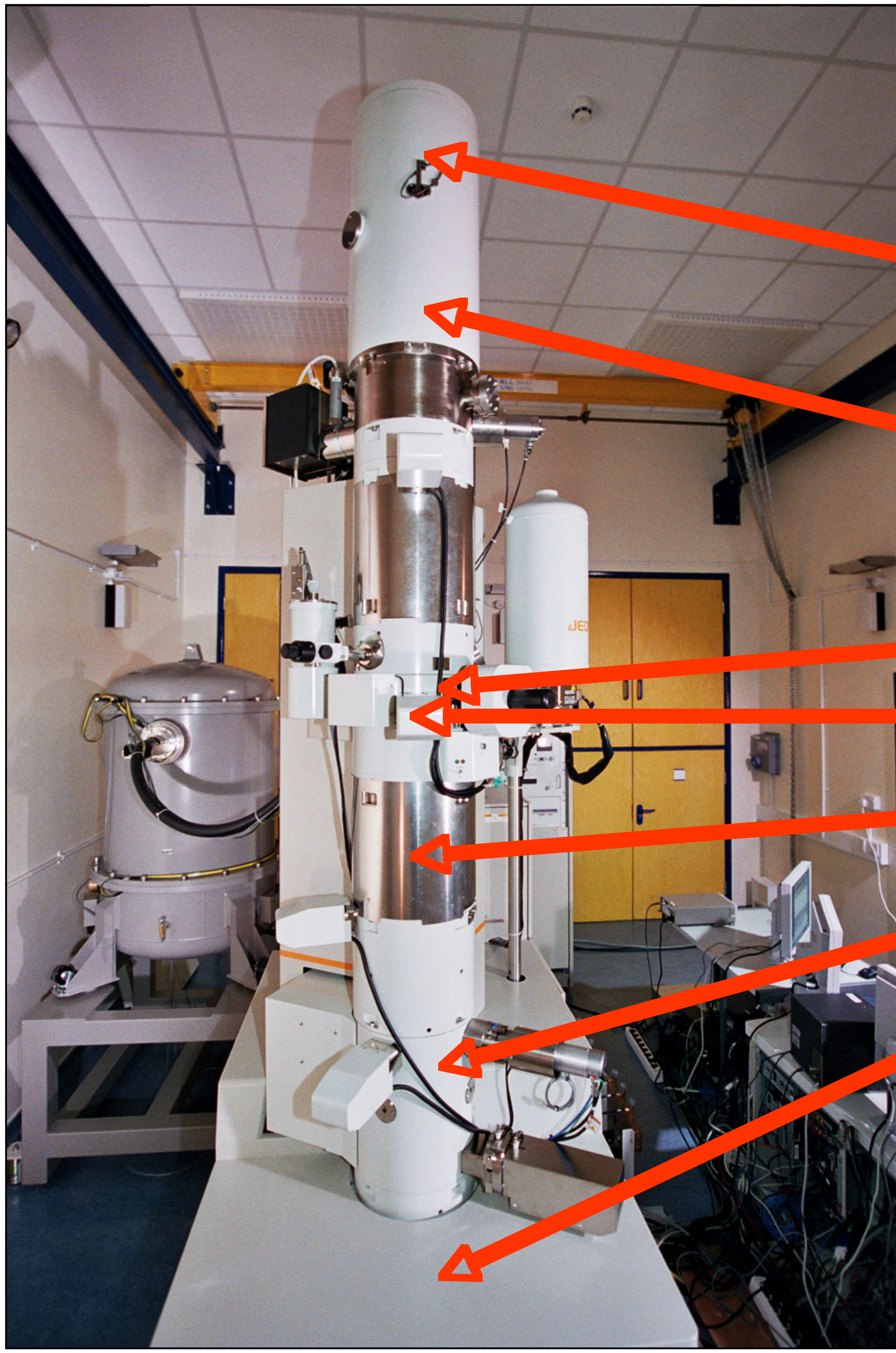
- Probe forming corrector
- Objective Lens Corrector

Aberration Corrector




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

HREM - initial JEOL 2200FS



FEG

200kV HT

X-Y piezo stage

URP polepiece

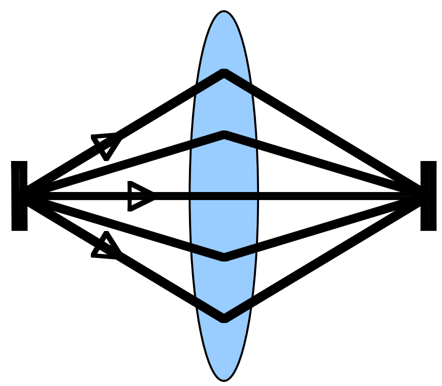
CEOS TEM corrector

Omega filter

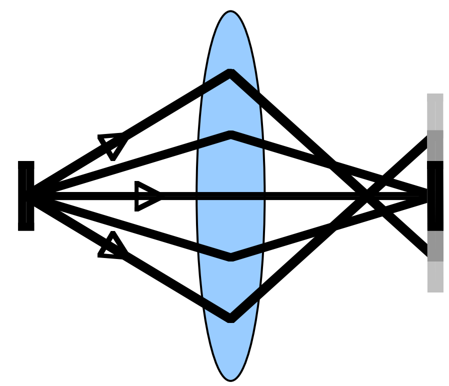
2k x 2k camera

purpose-built room

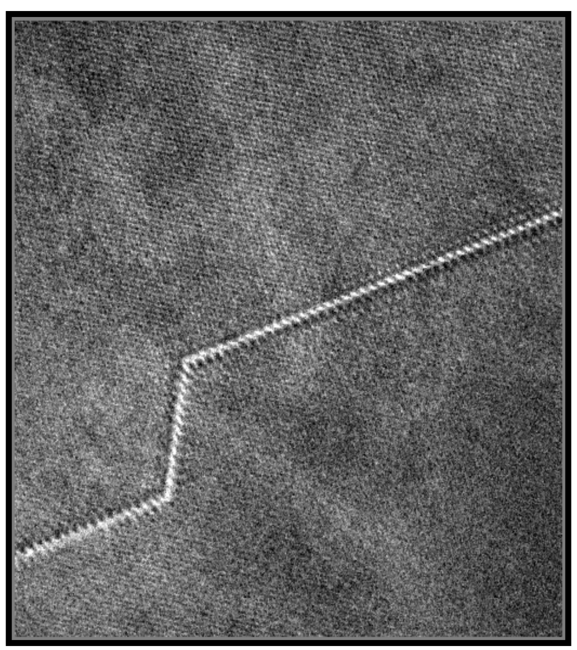
delocalisation



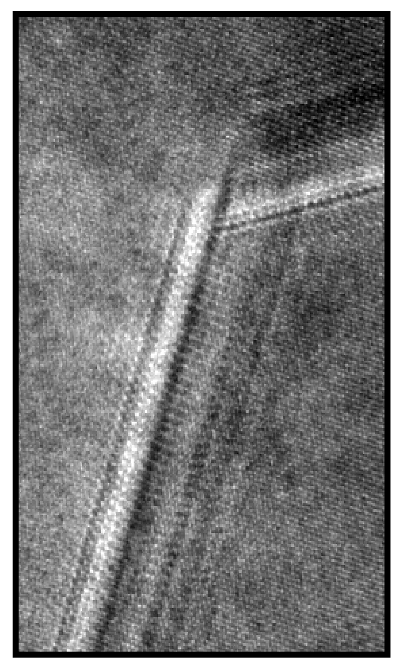
(a)



(b)



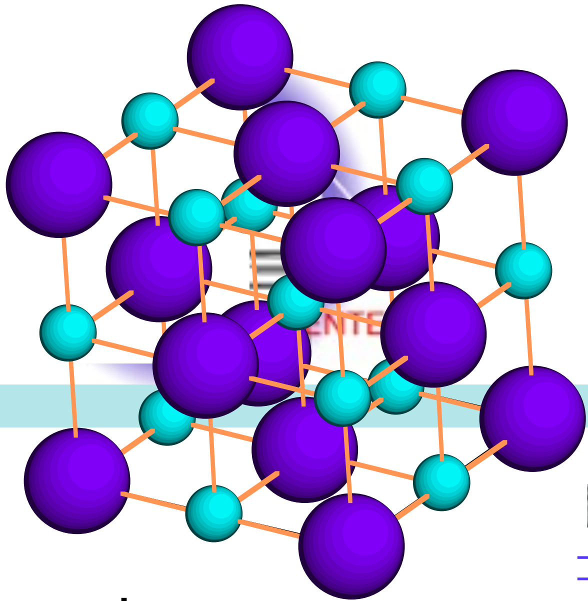
zero Cs

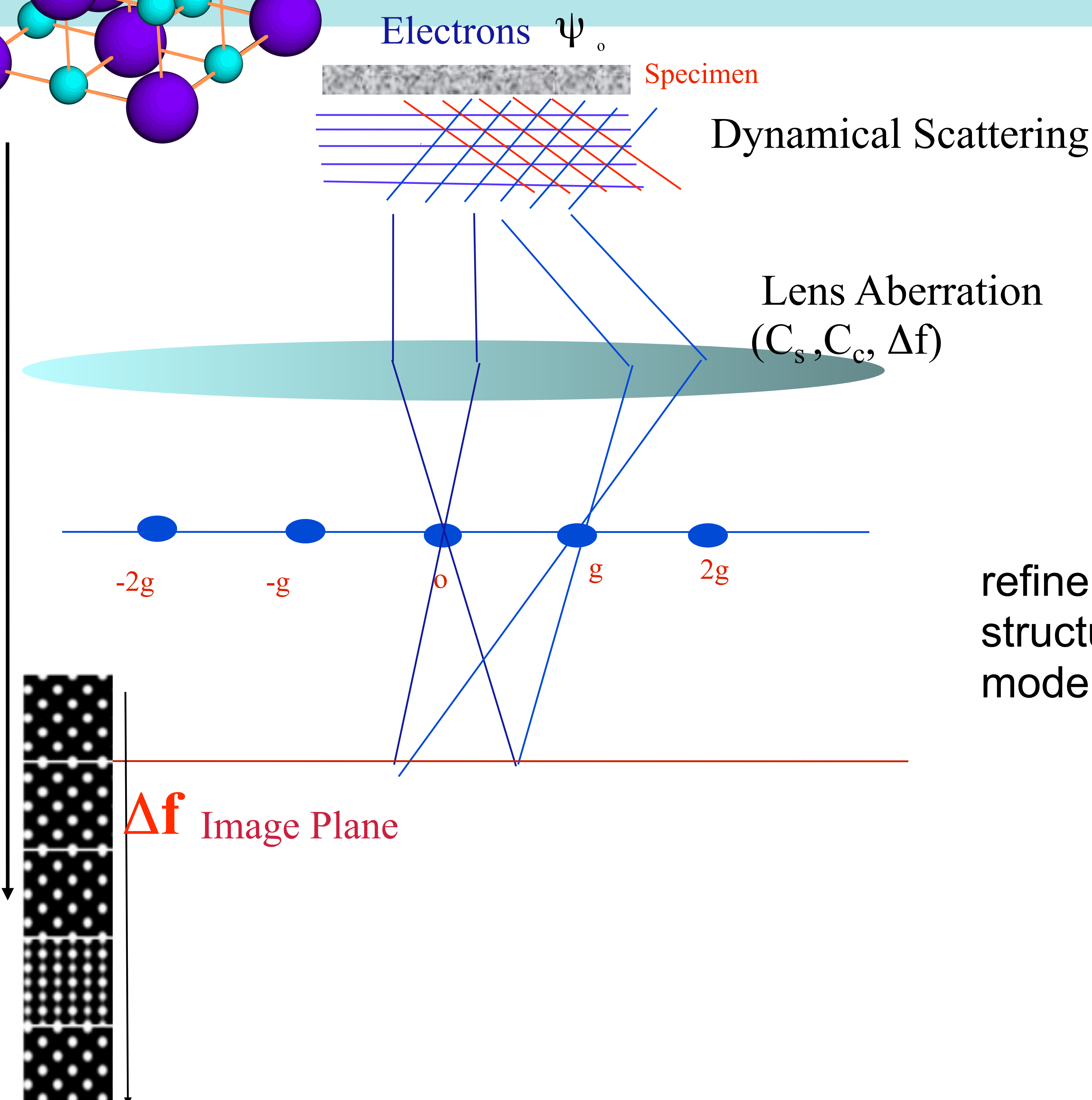


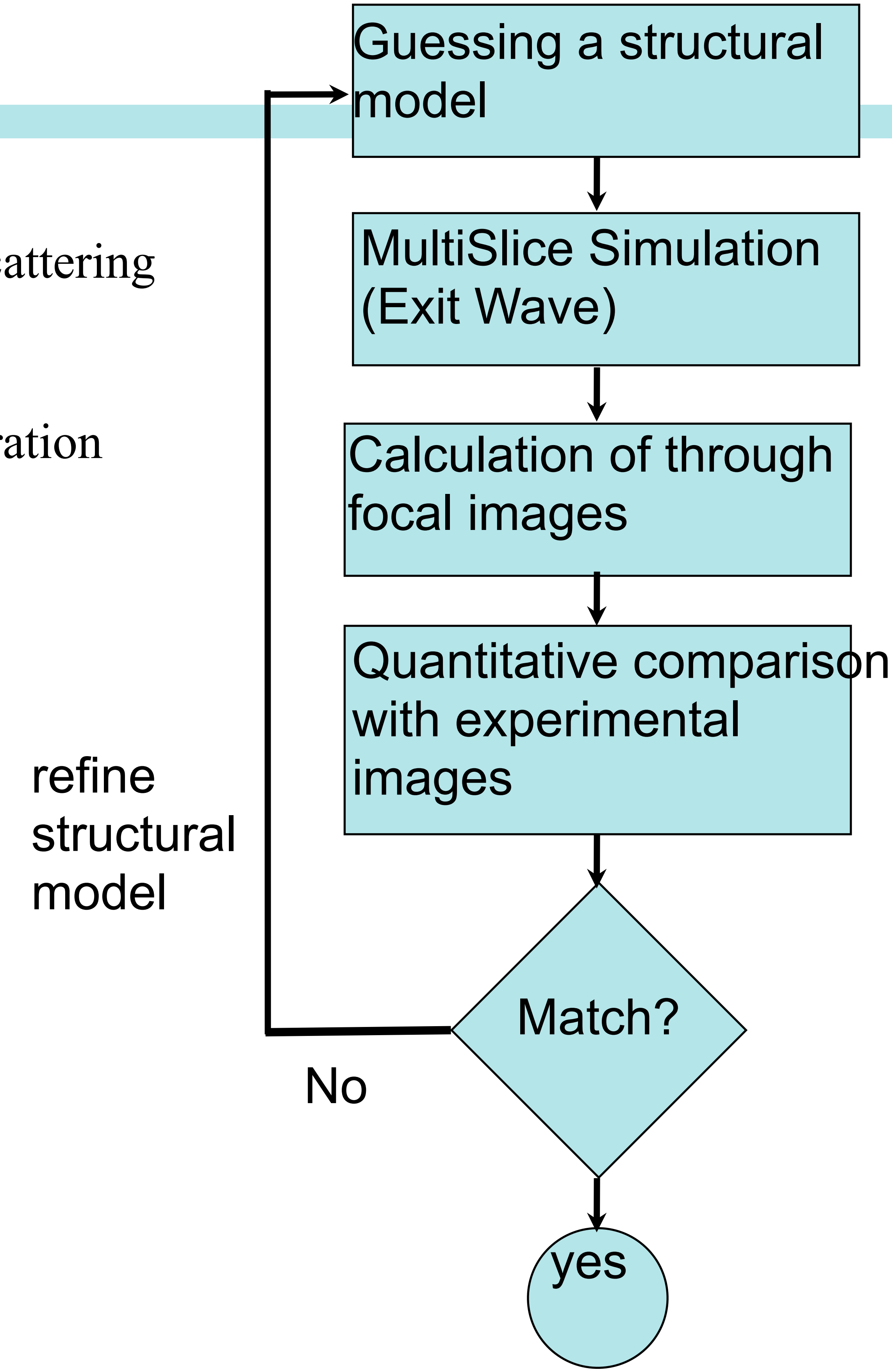
with Cs

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

Determination of Atomic Structure







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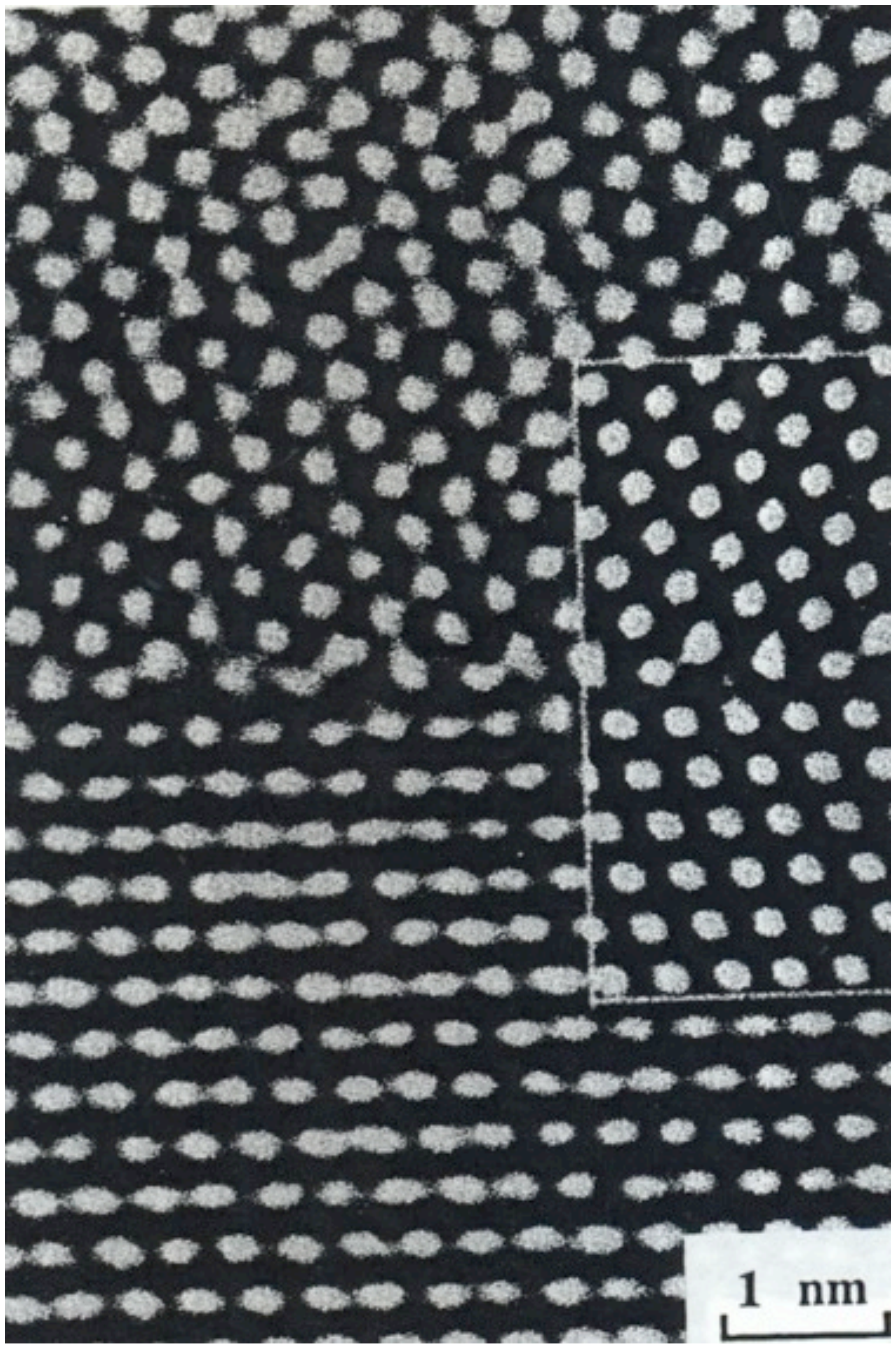
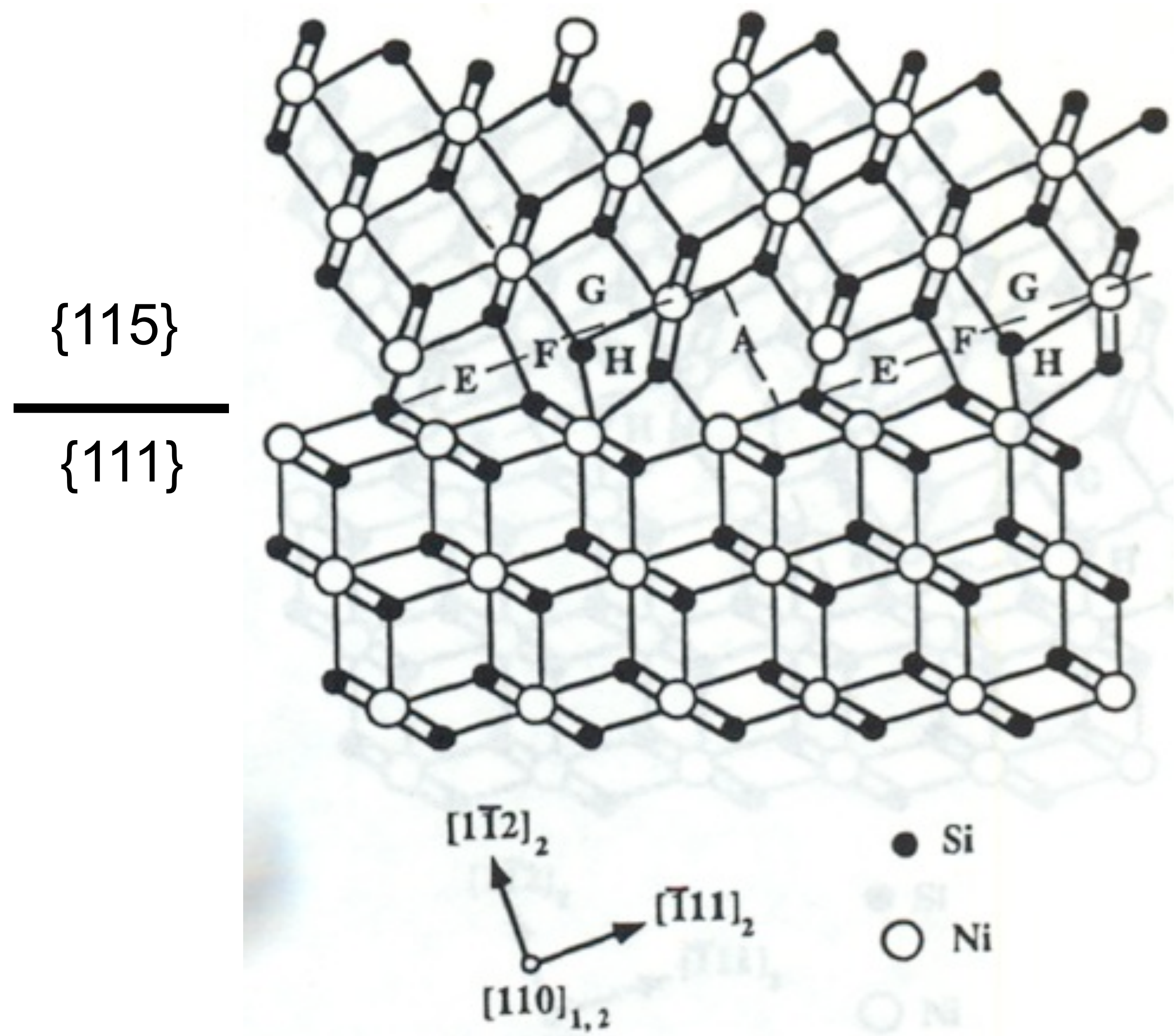
Example: $NiSi_2$ {115}/{111} Twin Boundary

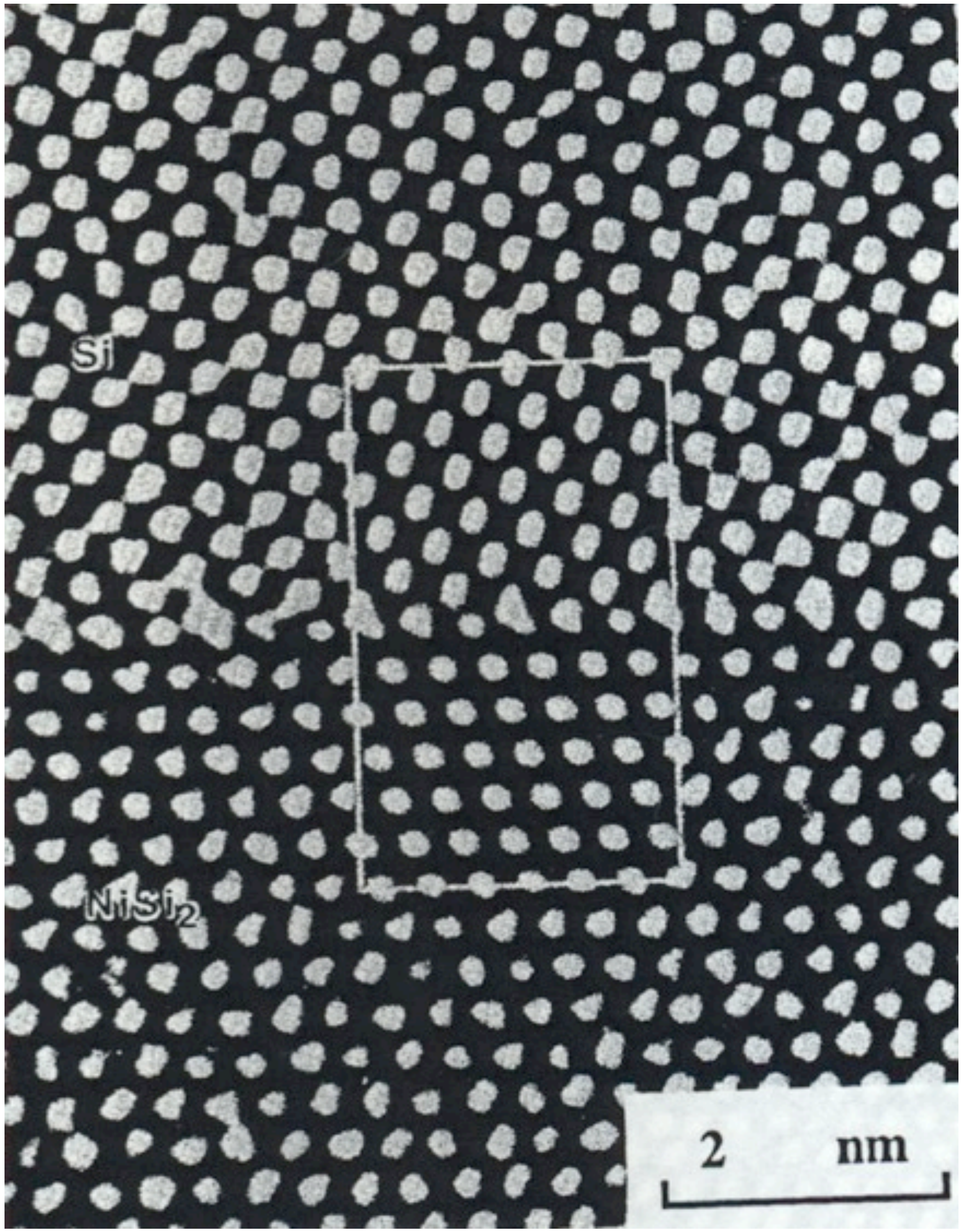
NTHU

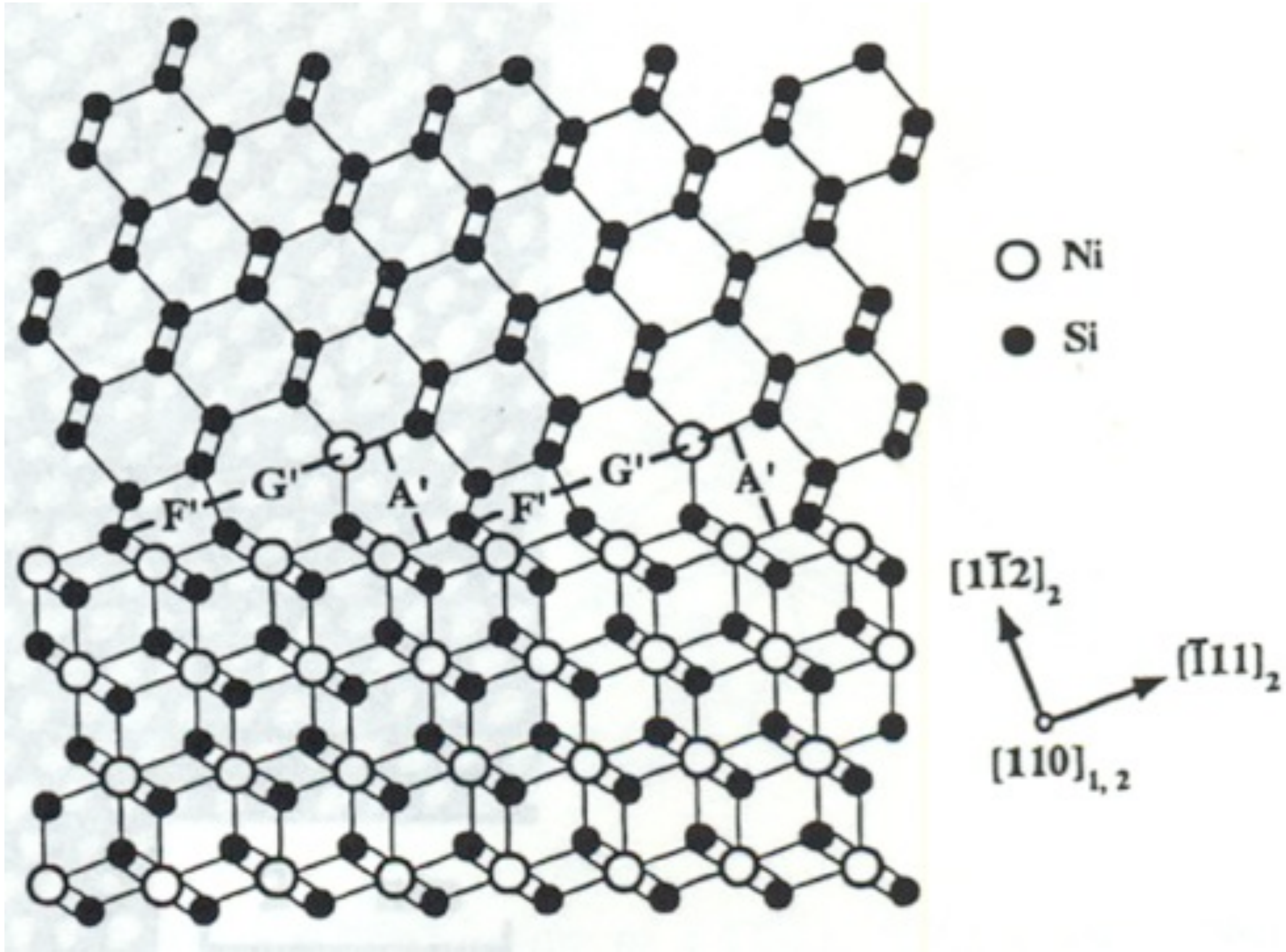




Example: Si{115}/ $NiSi_2$ {111} Twin Boundary

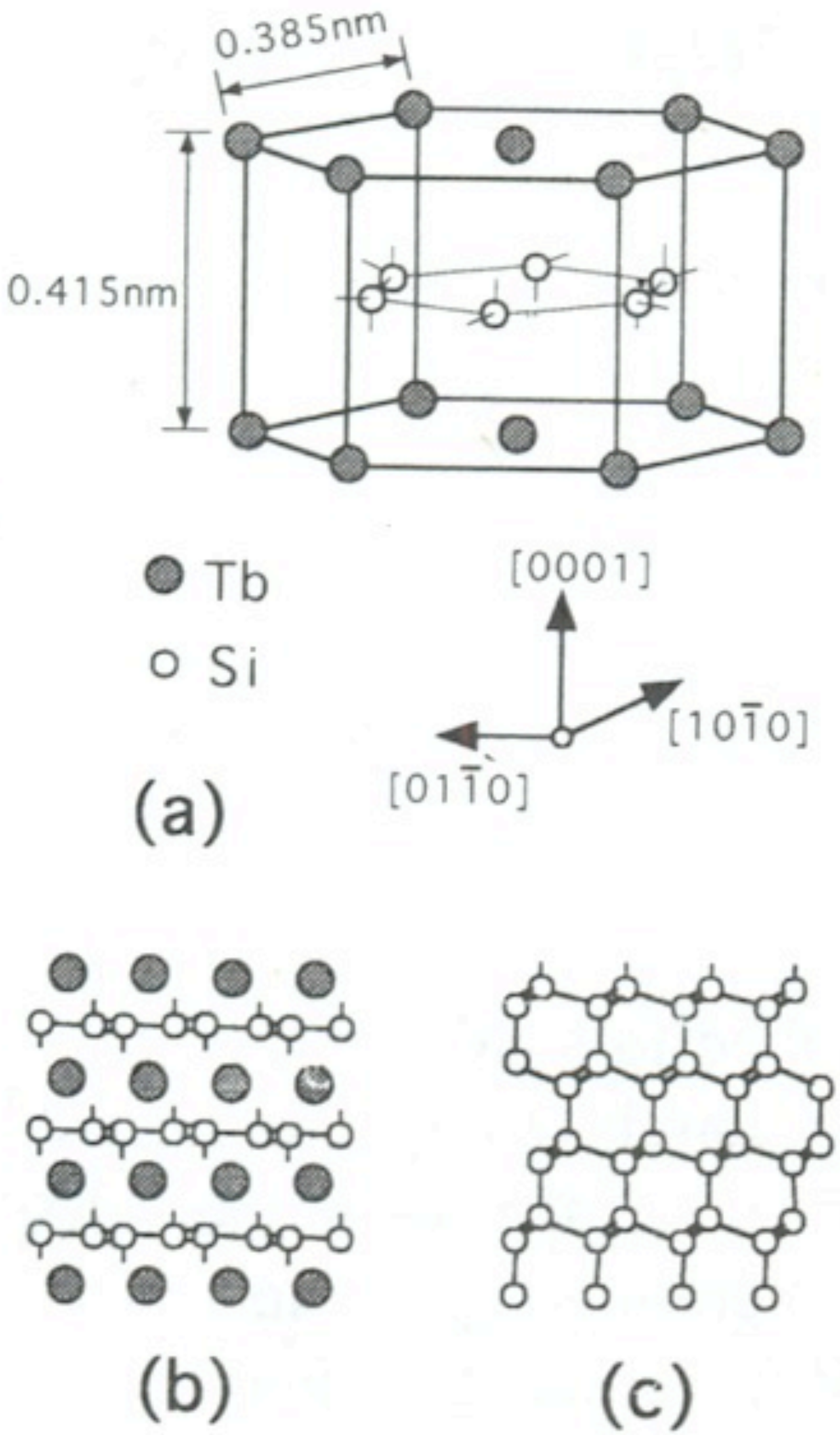
NTHU

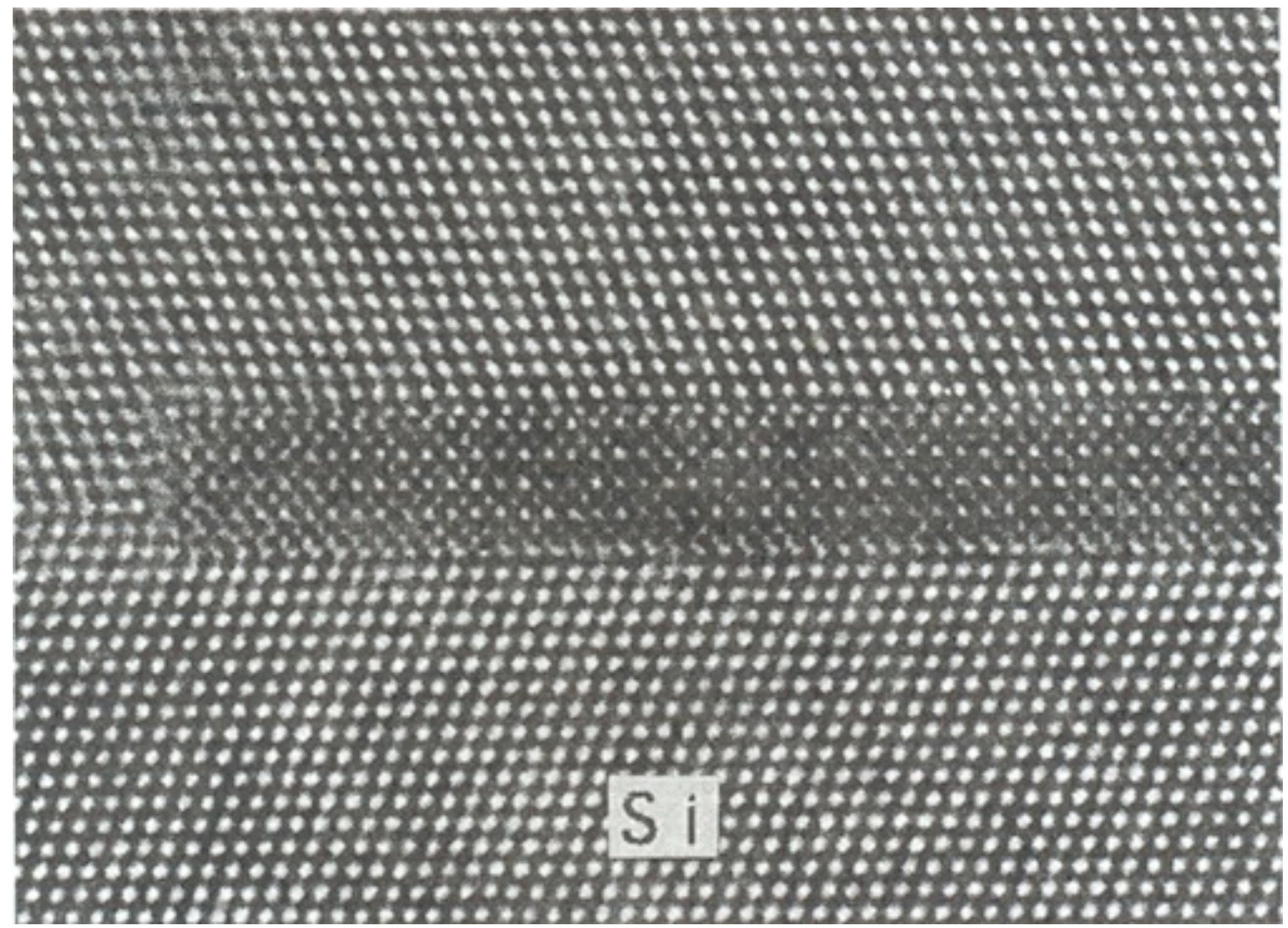




Example: $TbSi_2$/ Si Interface

NTHU





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7.3 Displacement Map

NTHU

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

Martin J. Hÿtch

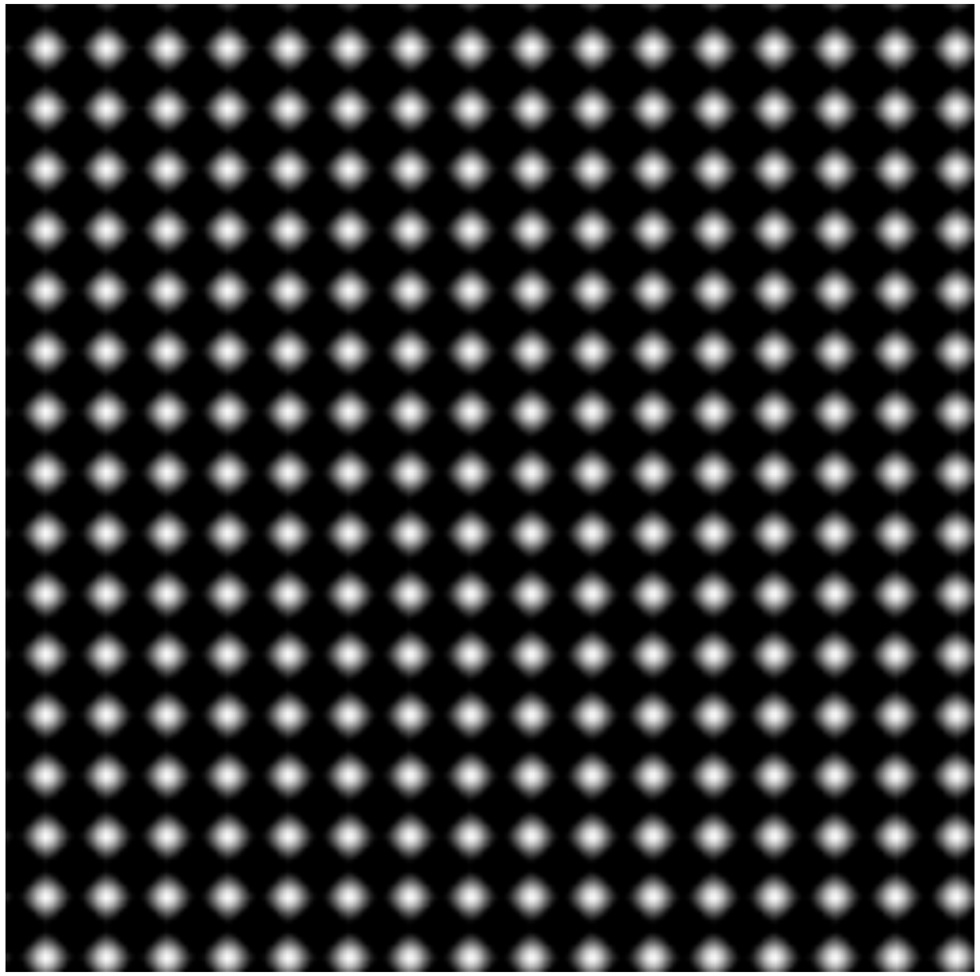
Microsc. Microanal. Microstruct. 8 (1997) 41–57

Quantitative measurement of displacement and strain fields from HREM micrographs

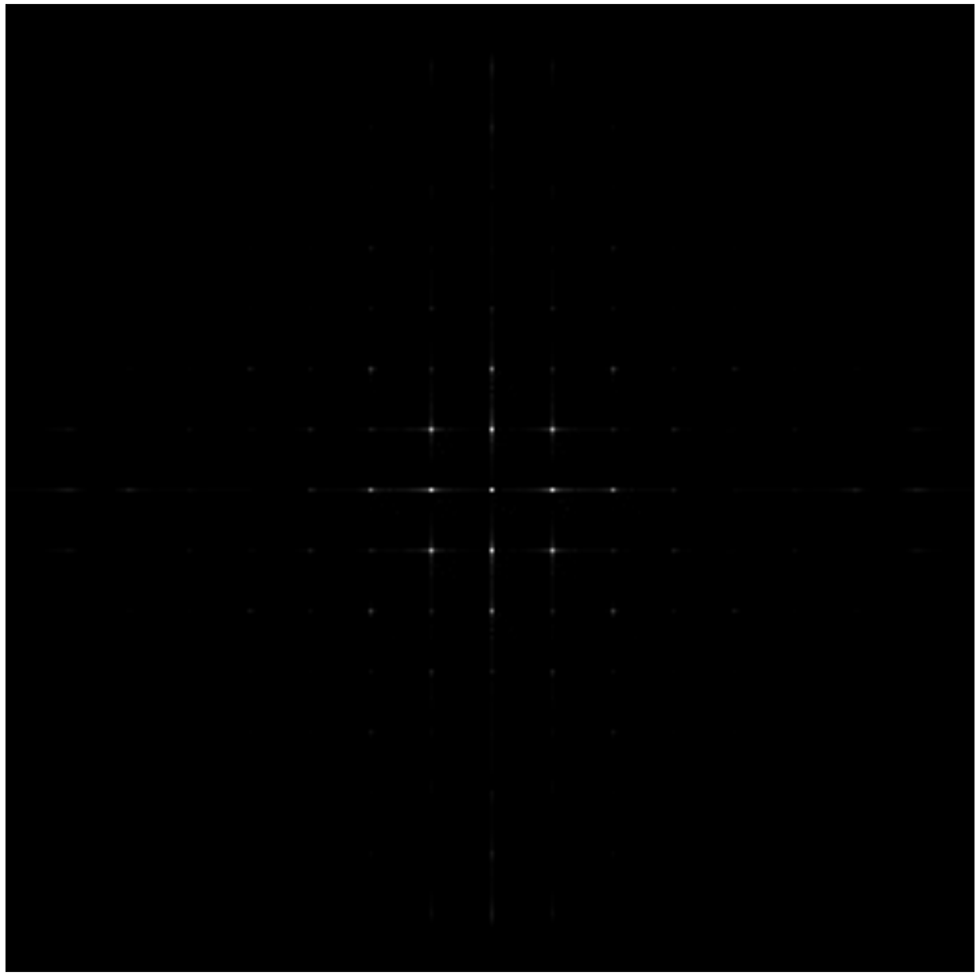
Ultramicroscopy 74 (1998) 131–146

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

7.3.1 Background on Geometric Phase

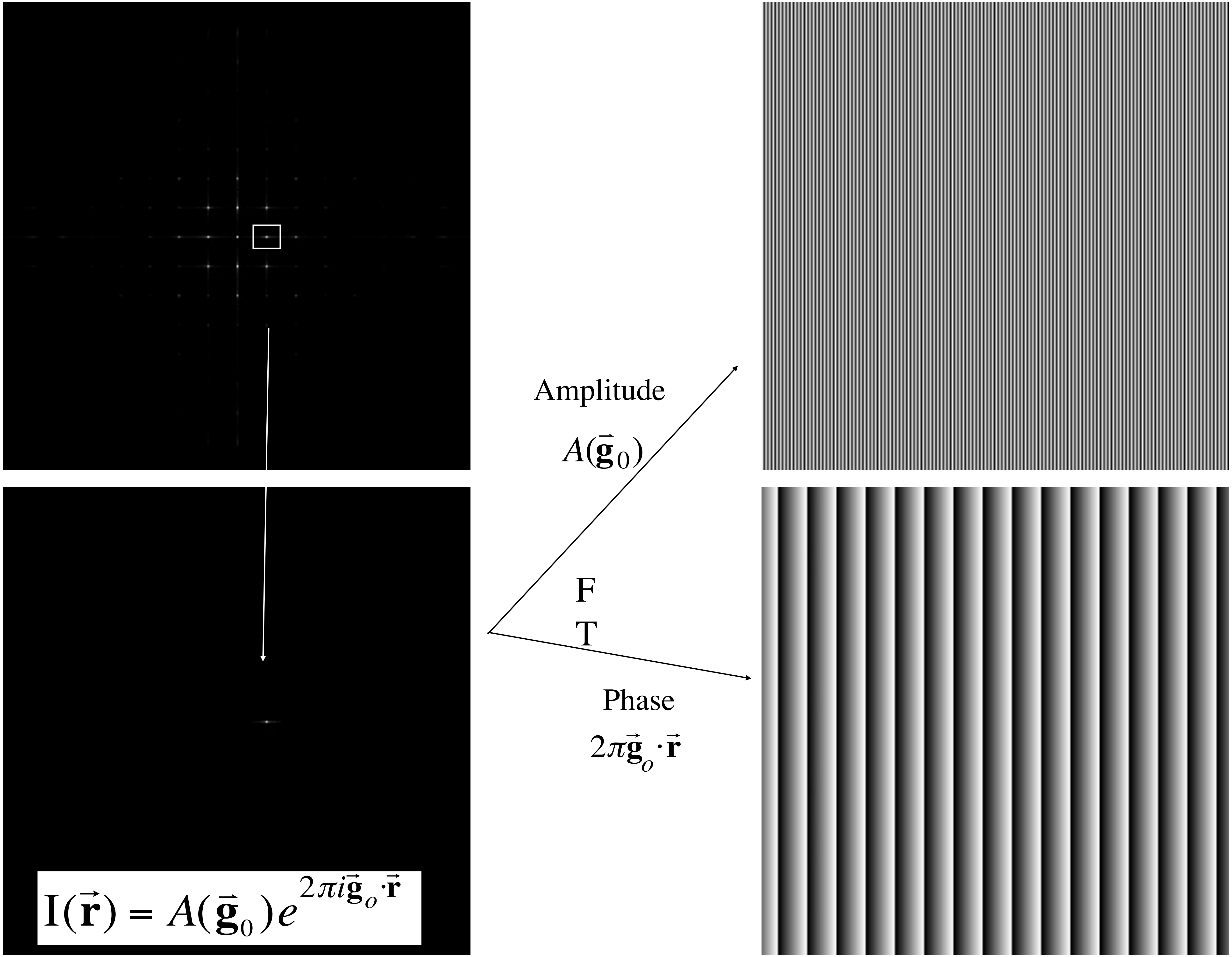


Fourier Transform

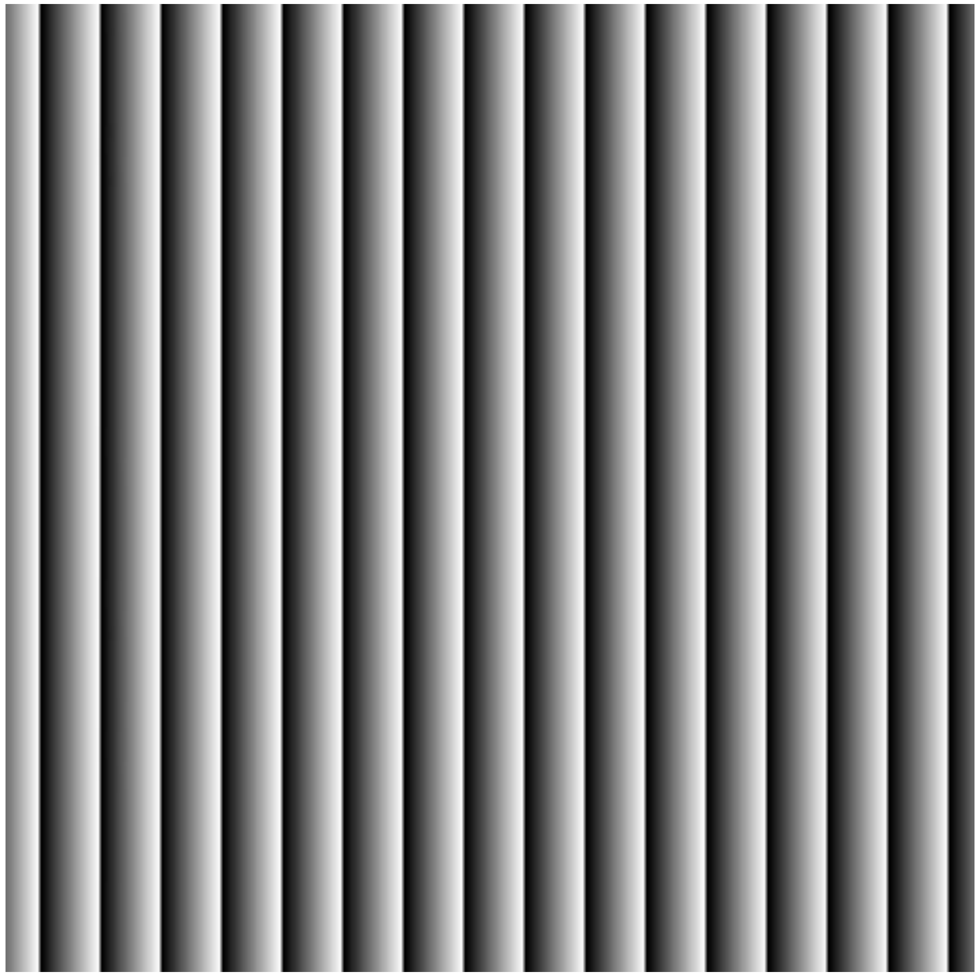


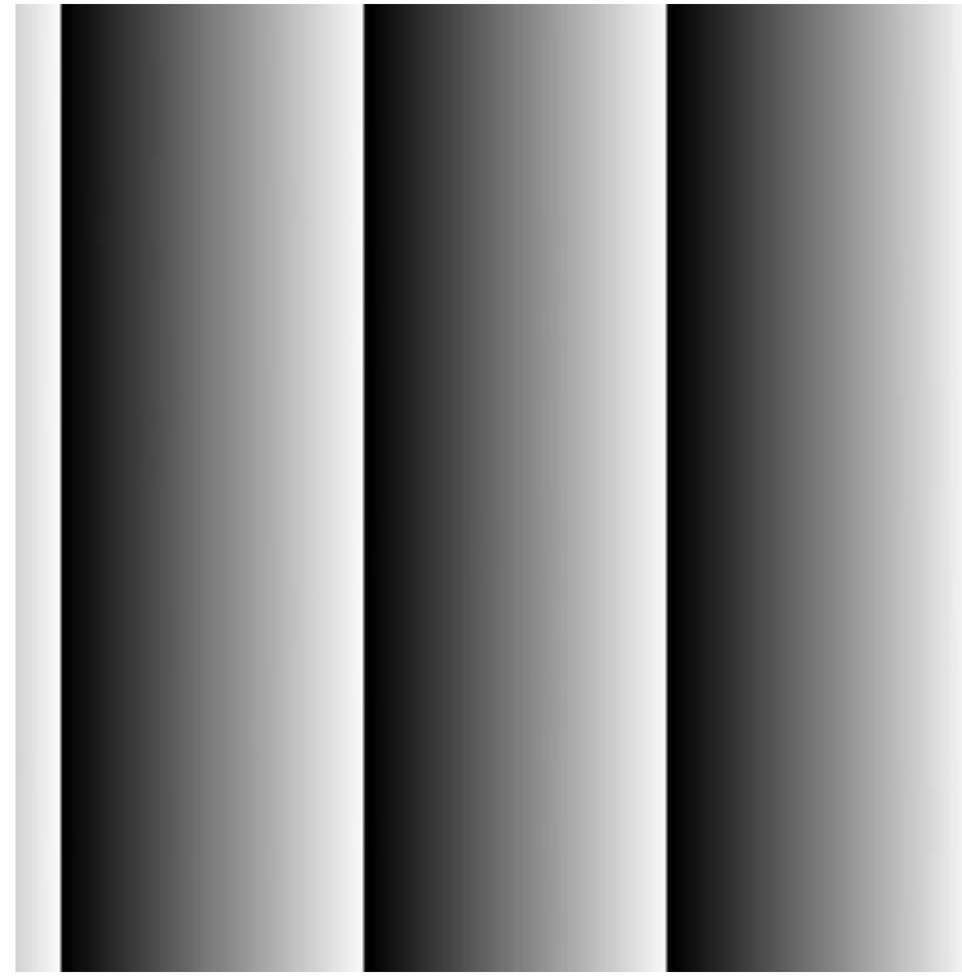
$$\mathrm{I}(\vec{\mathbf{r}}) = \sum_{\mathbf{g}} A(\vec{\mathbf{g}}) e^{2\pi i \vec{\mathbf{g}} \cdot \vec{\mathbf{r}}}$$

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

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

• Displacement Field description

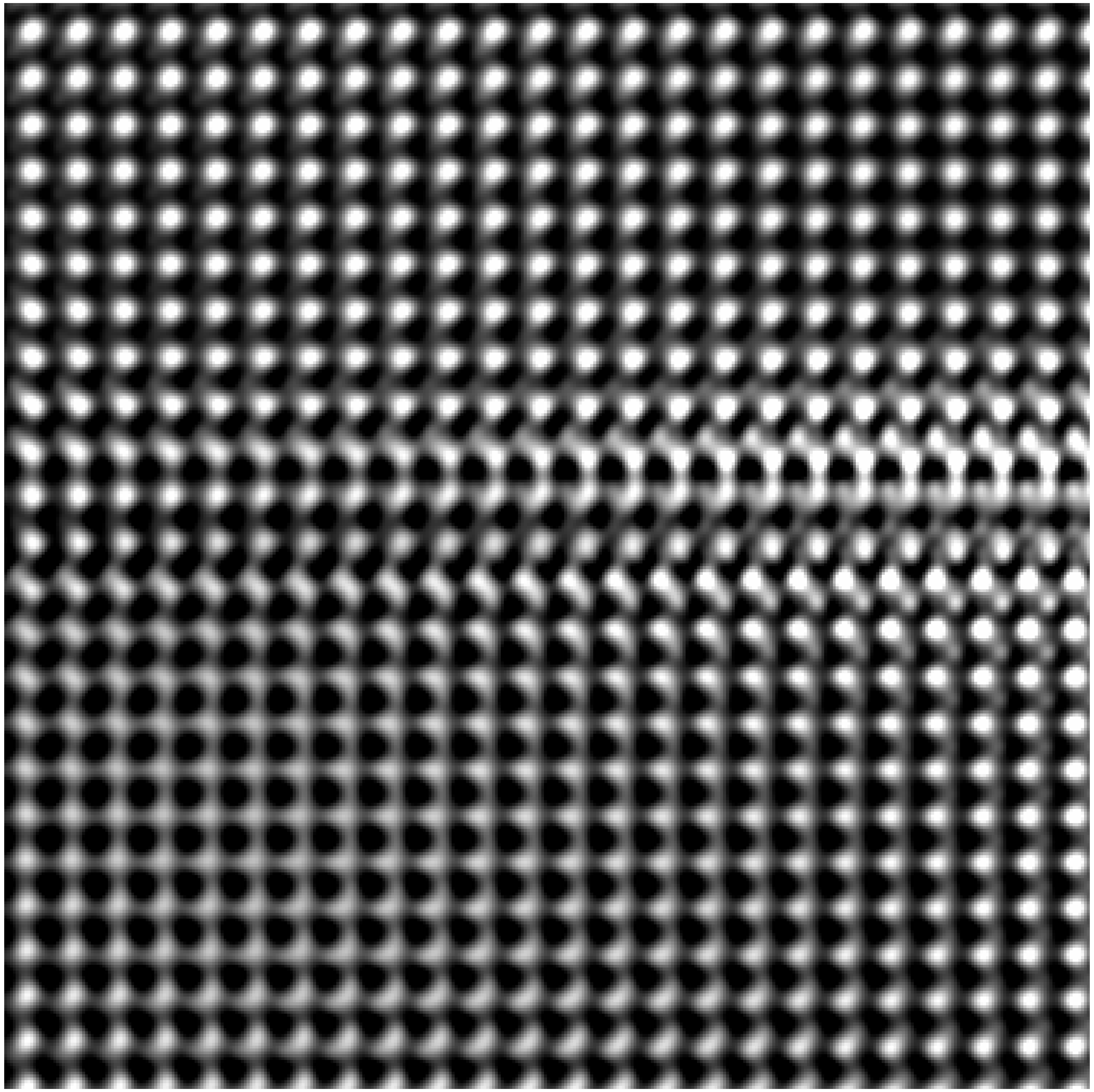
$$\vec{\mathbf{g}}(\vec{\mathbf{r}})\cdot\vec{\mathbf{r}} = \frac{1}{u_0 + \delta(\vec{\mathbf{r}})}\hat{\mathbf{g}}_0 \cdot \vec{\mathbf{r}} =$$

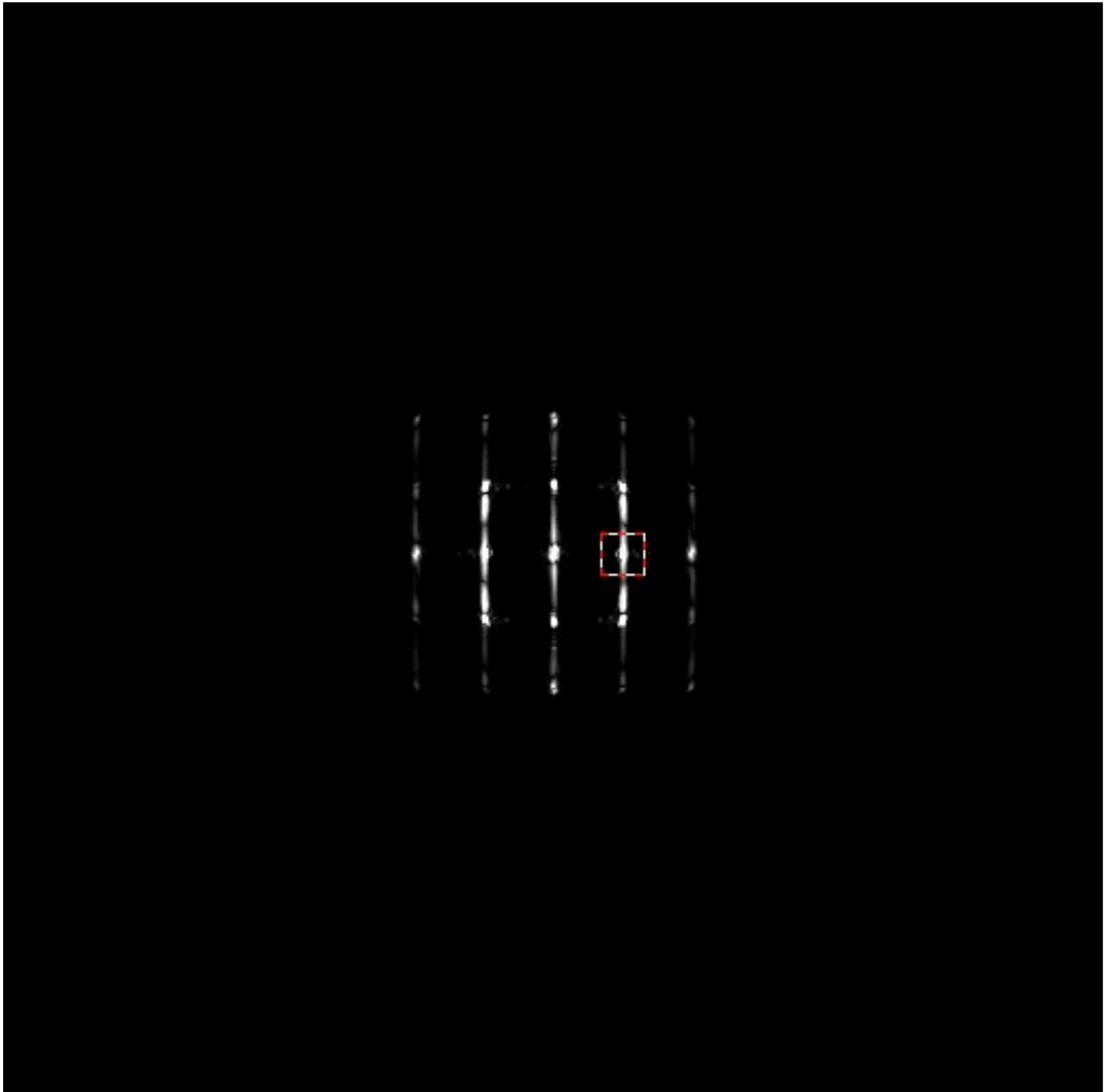
$$\frac{1}{u_0}\hat{\mathbf{g}}_0 \cdot \vec{\mathbf{r}} - \frac{1}{u_0}\hat{\mathbf{g}}_0 \cdot \frac{\delta(\vec{\mathbf{r}})}{u_0}\vec{\mathbf{r}} = \vec{\mathbf{g}}_0 \cdot \vec{\mathbf{r}} - \vec{\mathbf{g}}_0 \cdot \Delta\vec{\mathbf{u}}(\vec{\mathbf{r}})$$

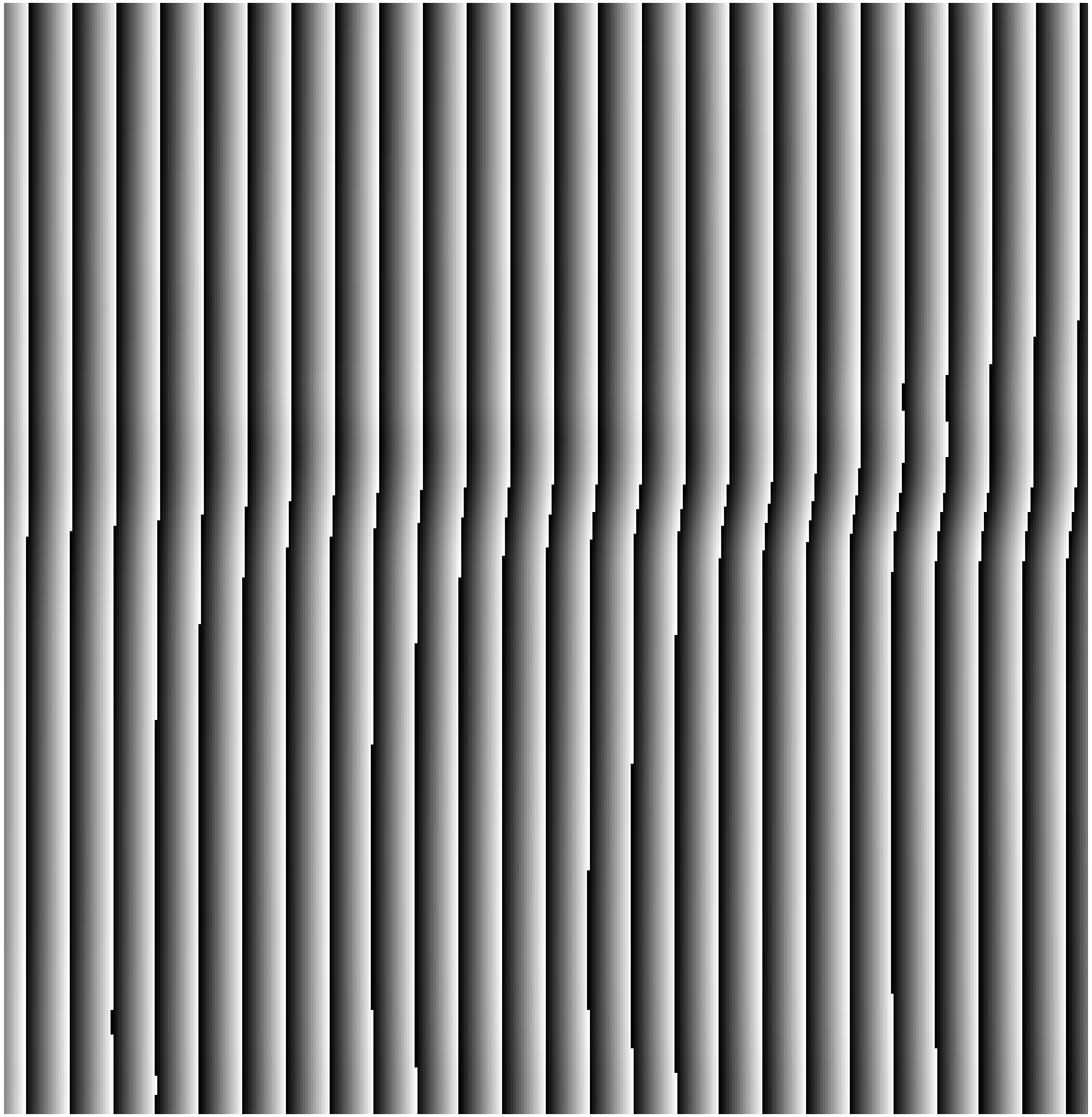
- Amplitude and Phase

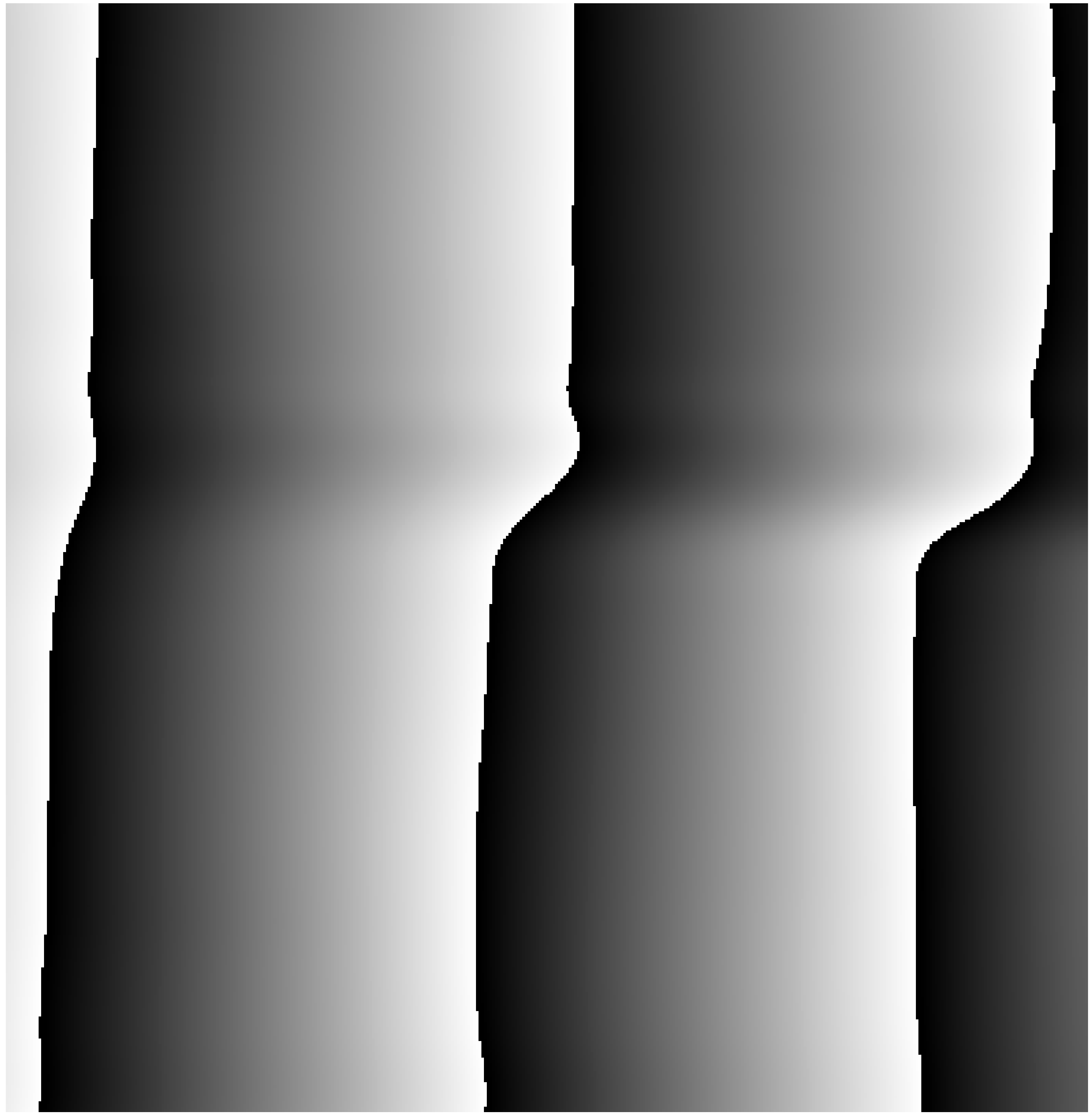
$$\mathrm{I}(\vec{\mathbf{r}}) = A(\vec{\mathbf{r}})e^{2\pi i \mathbf{g}(\mathbf{r})\cdot\mathbf{r}} = A(\vec{\mathbf{r}})e^{2\pi i(\mathbf{g}_0 + \Delta\mathbf{g}(\mathbf{r}))\cdot\mathbf{r}}$$

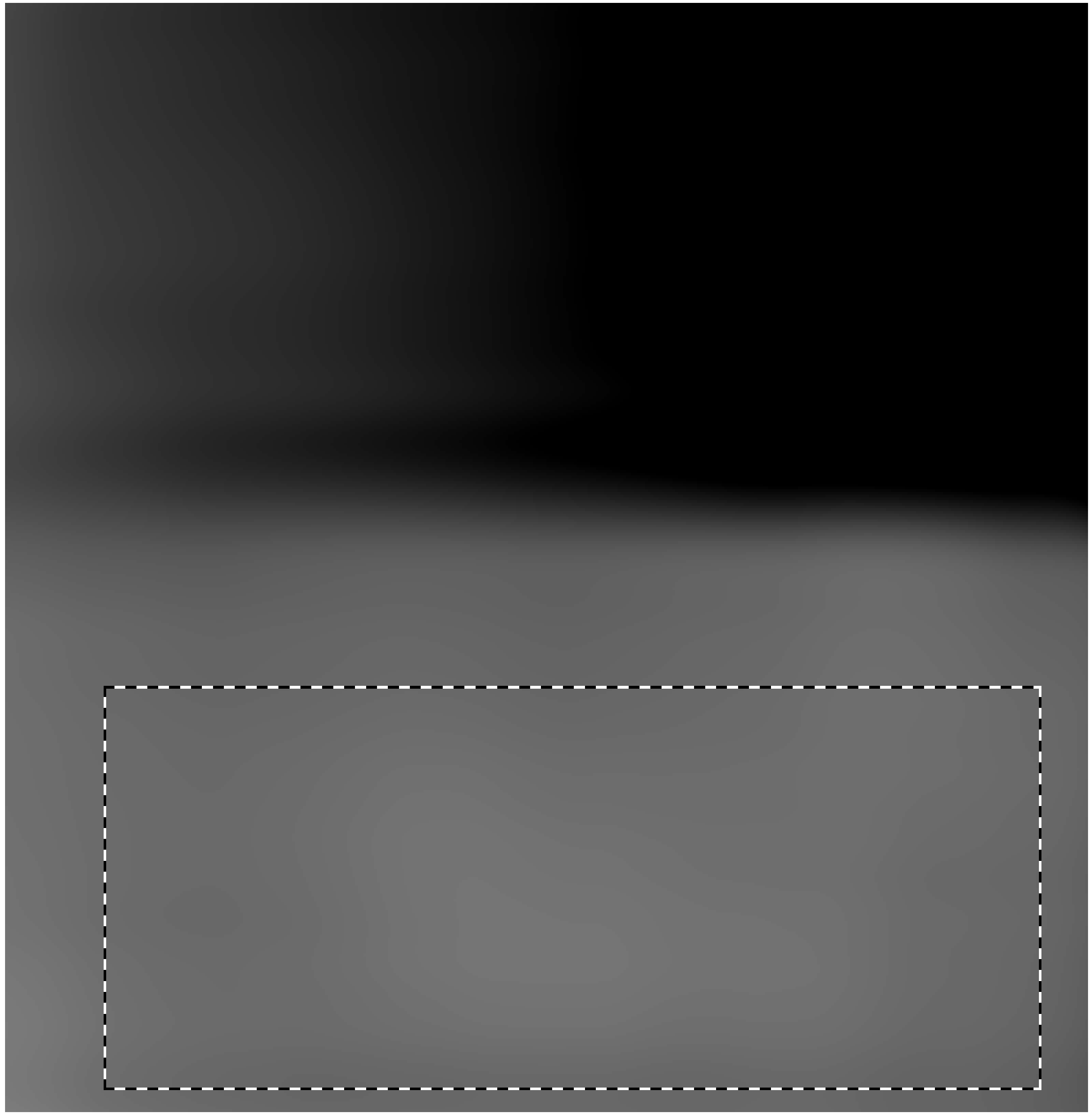
$$= A(\vec{\mathbf{r}})e^{2\pi i(\vec{\mathbf{g}}_0\cdot\vec{\mathbf{r}} + \vec{\mathbf{g}}_0\cdot\Delta\vec{\mathbf{u}}(\vec{\mathbf{r}}))} = A(\vec{\mathbf{r}})\exp(iP(\vec{\mathbf{r}}))$$

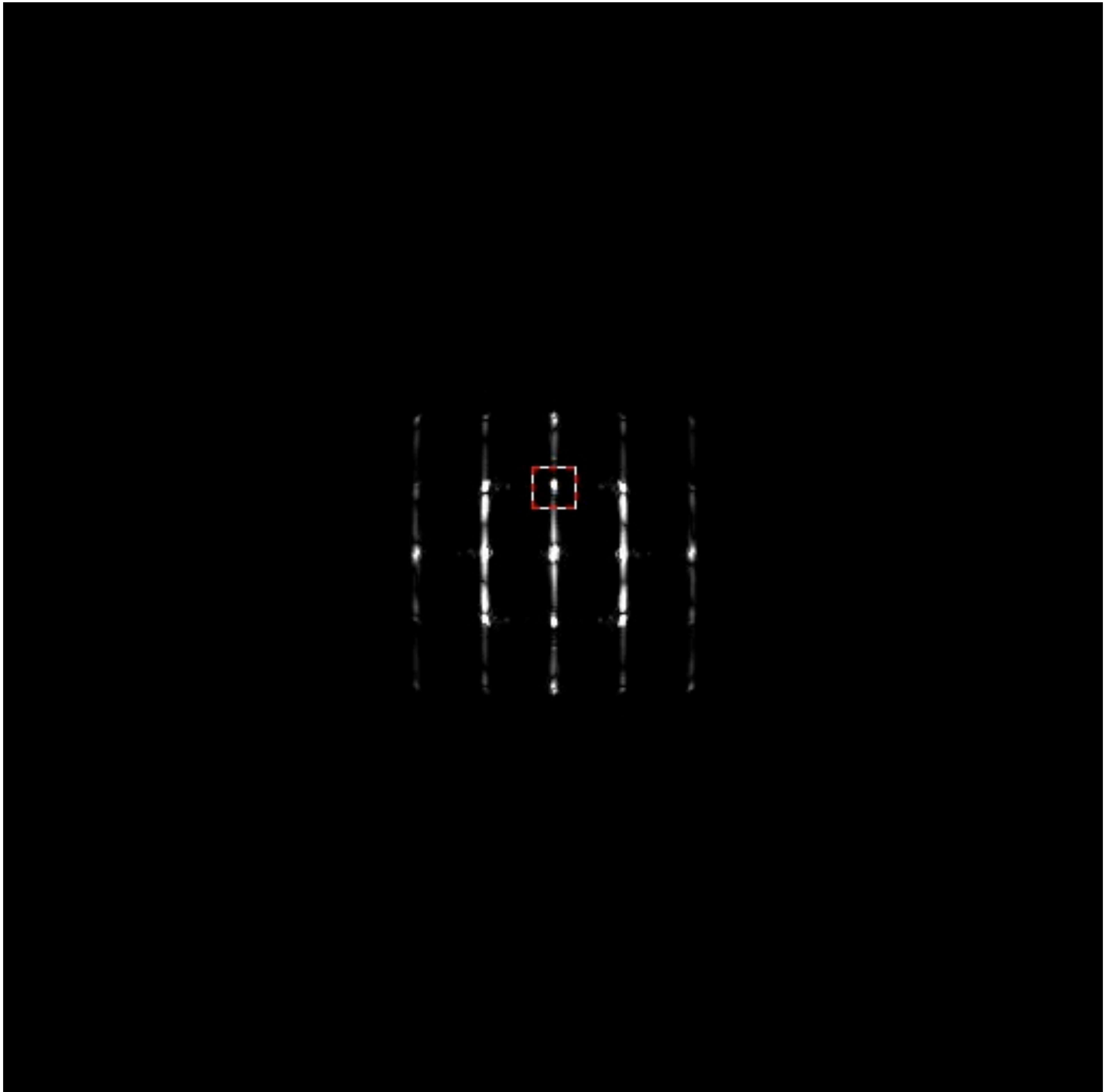


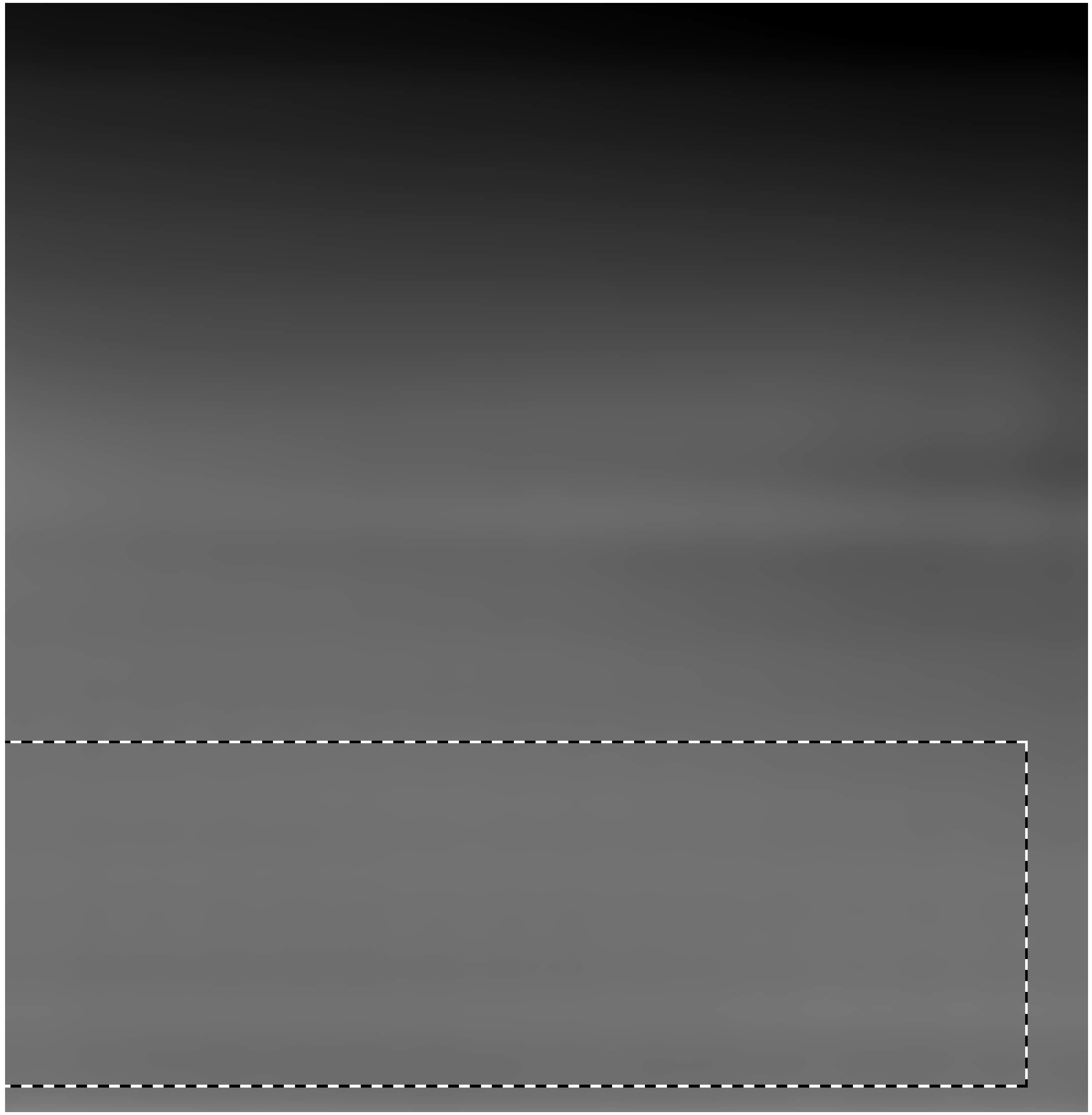












Displacement Field Calculation

- Requires 2 phase images from 2 different reflections

- Implicit definition of a reference lattice

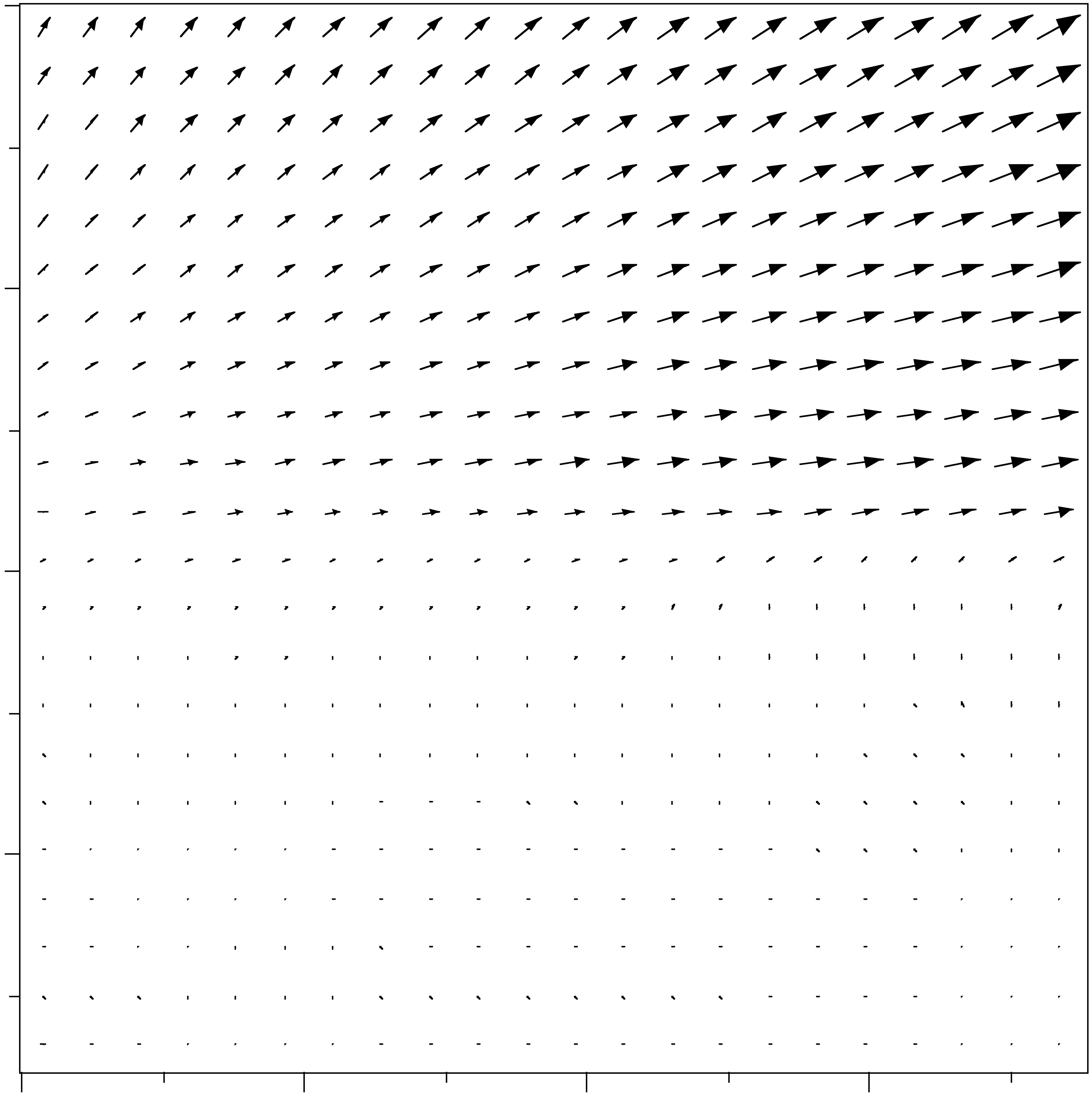
$$P_{g1}(\vec{r}) = 2\pi\ \vec{g}_1 . \vec{u}(\vec{r}) = 2\pi(g_{1x}.u_x(\vec{r}) + g_{1y}.u_y(\vec{r}))$$

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

- Solution for the displacements with respect to the reference lattice

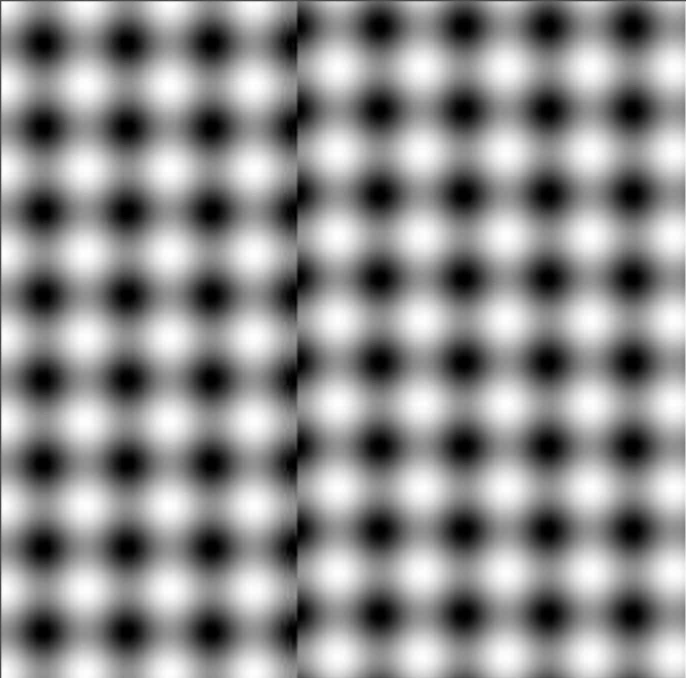
$$u_x(\vec{r}) = \frac{1}{2\pi}\left(\frac{P_{g1}(\vec{r}).g_{2y} - P_{g2}(\vec{r}).g_{1y}}{g_{1x}.g_{2y} - g_{1y}.g_{2x}}\right)$$

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

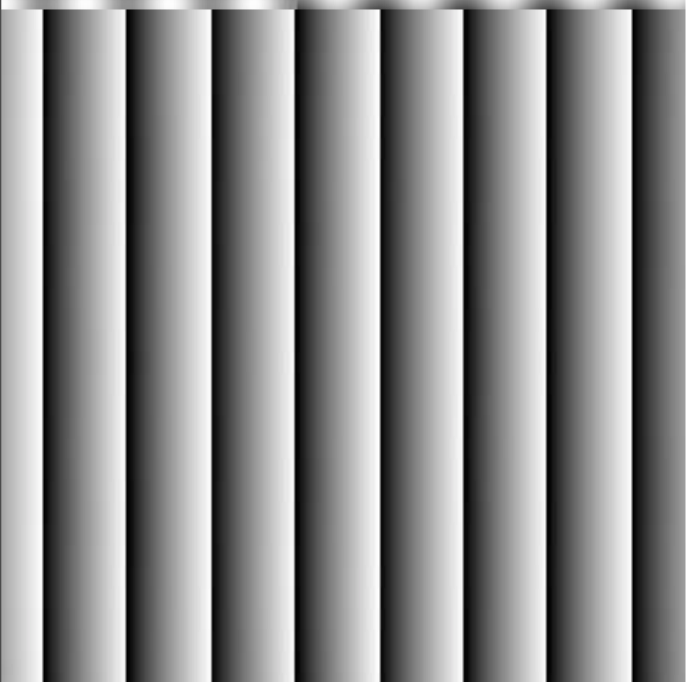


Tuesday, October 25,

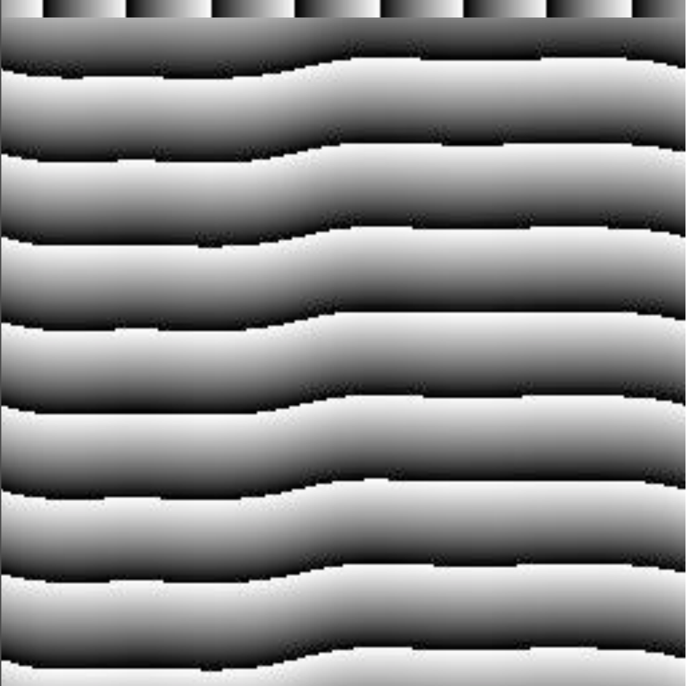
Shift Case



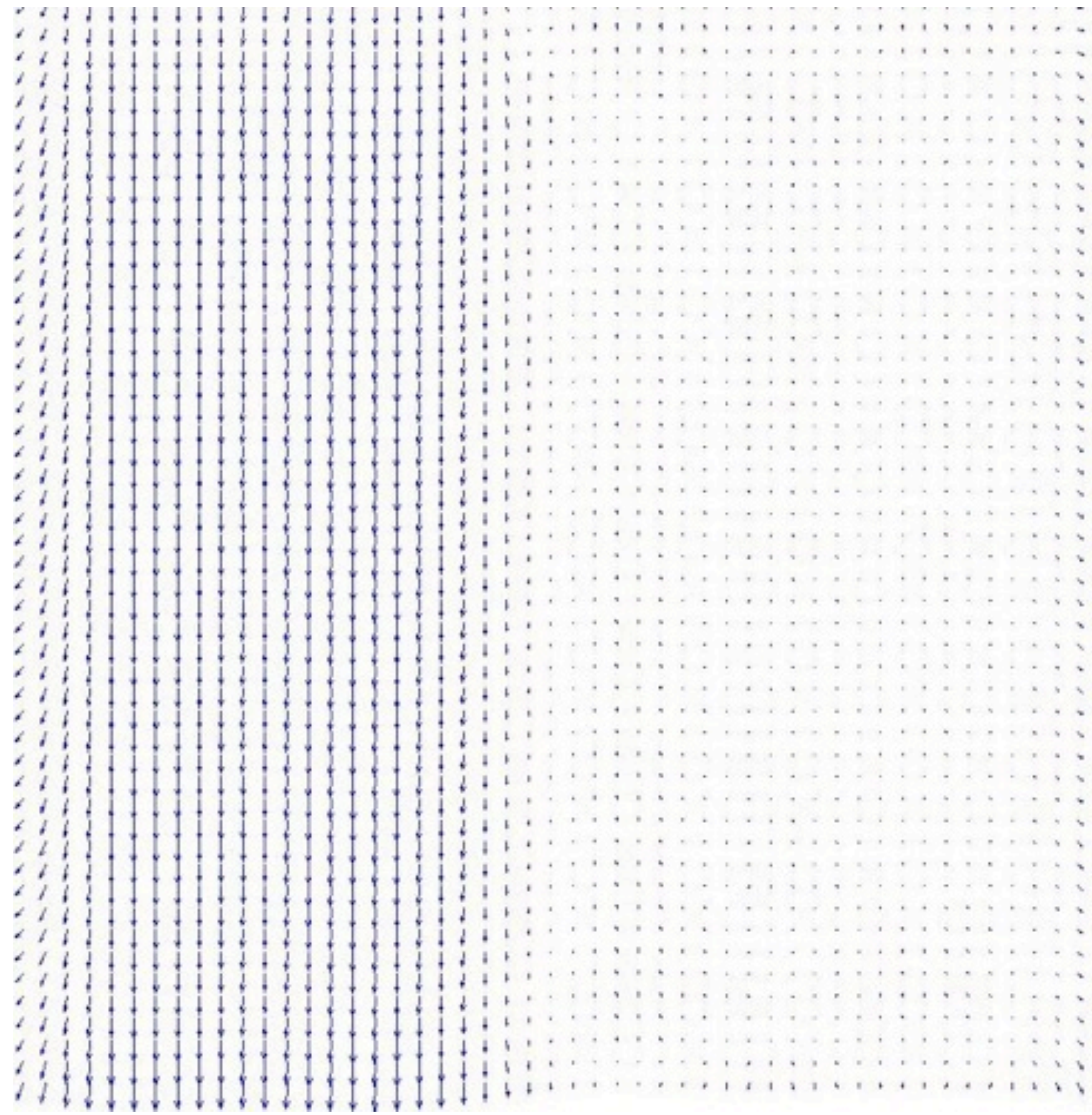
object



phase1

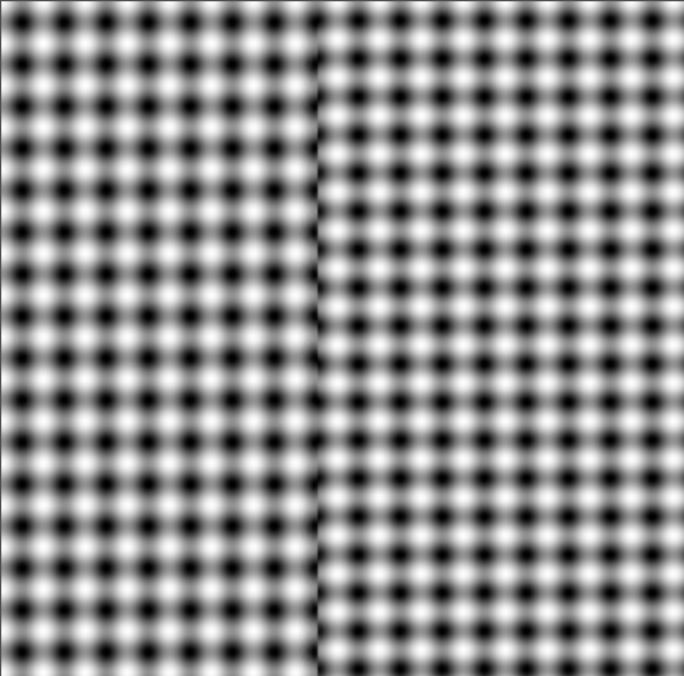


phase2

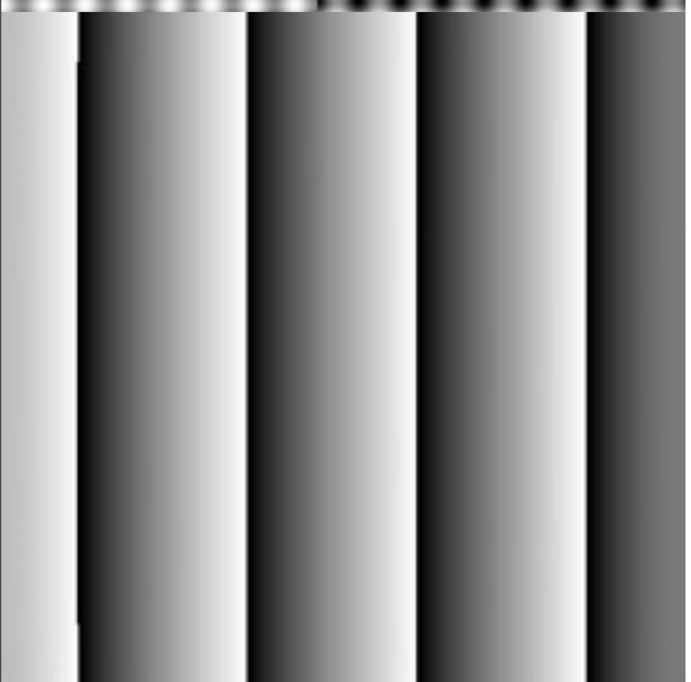


Displacement map

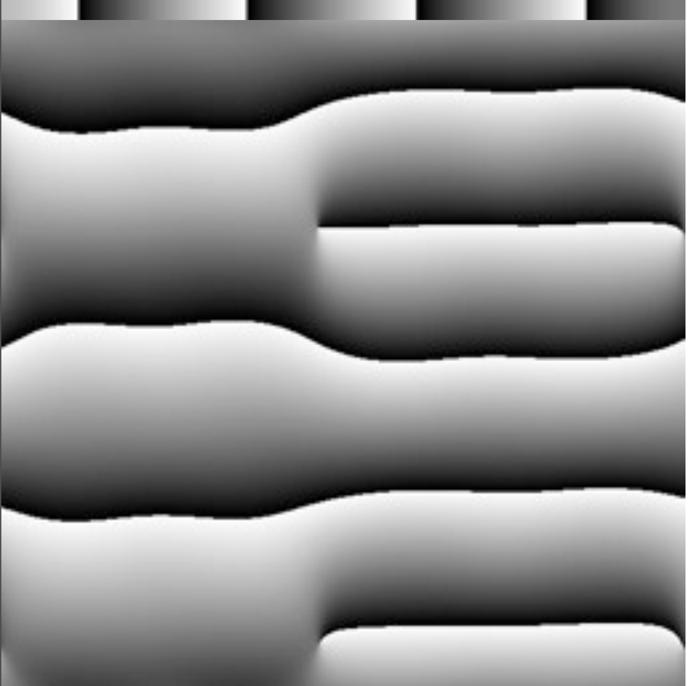
Dilatation Case



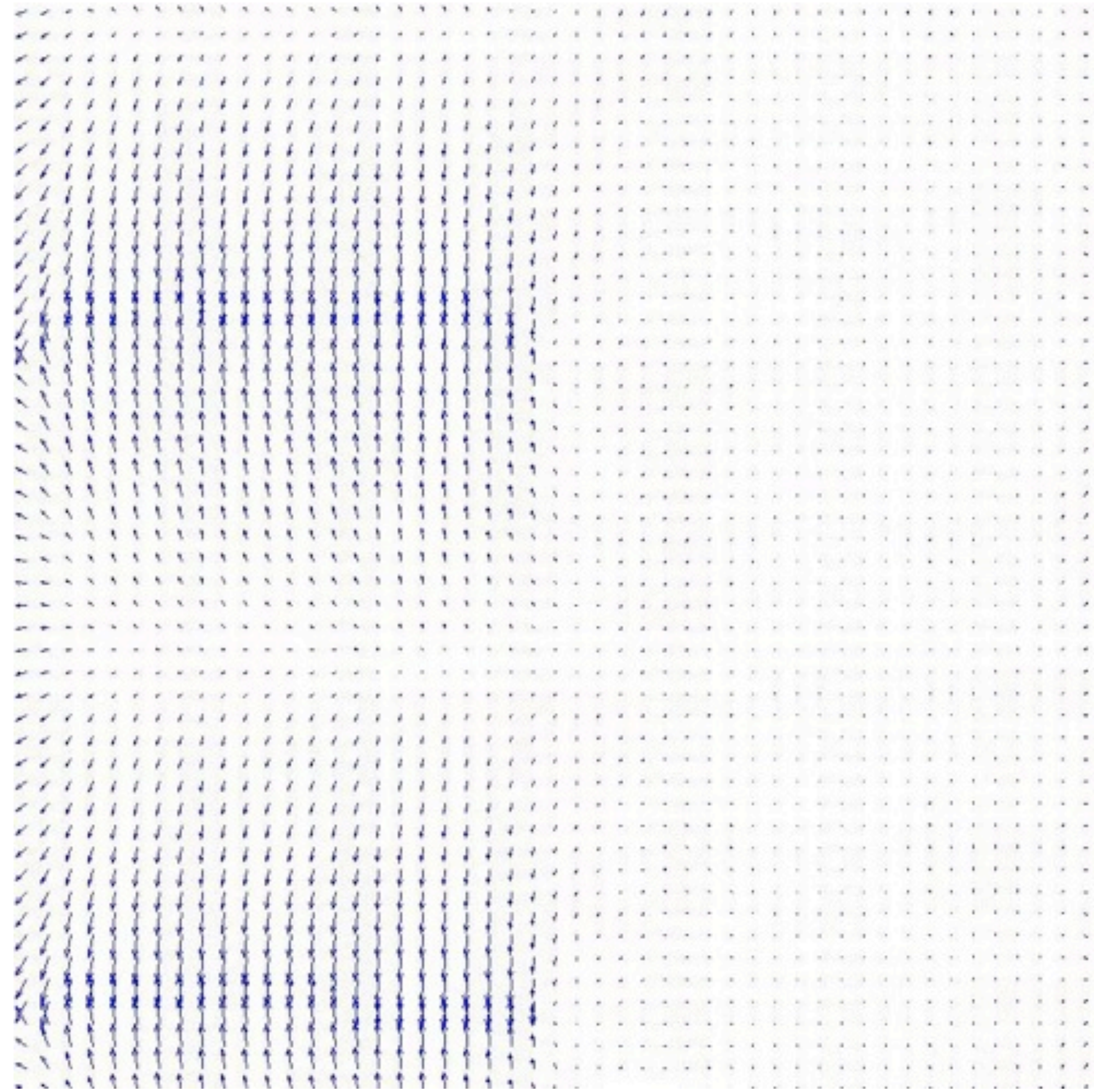
object



phase1

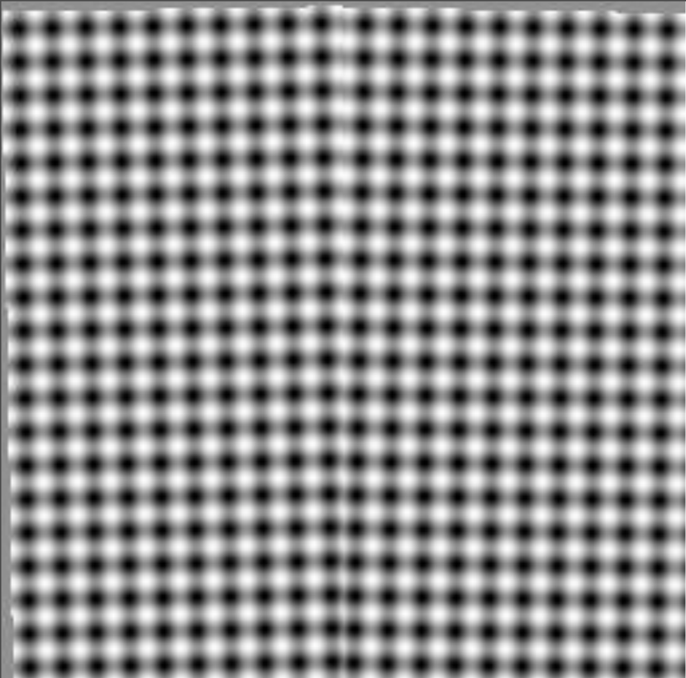


phase2

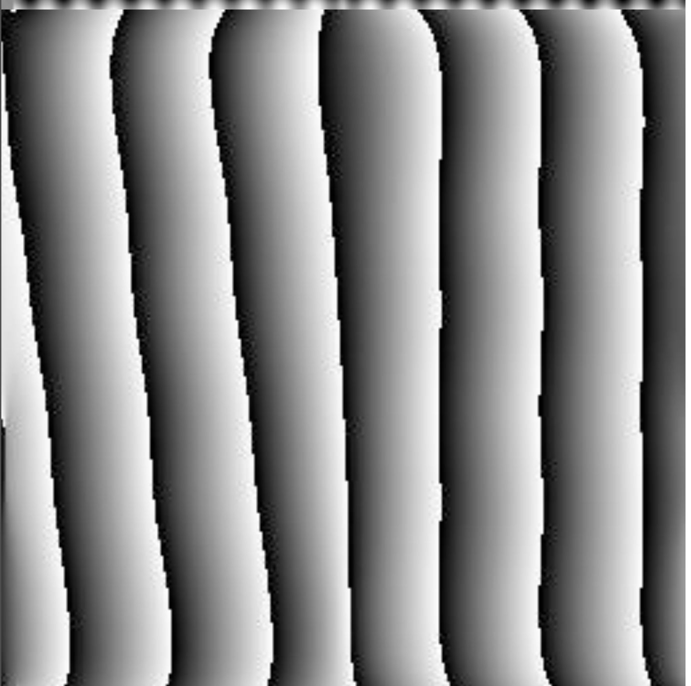


Displacement map

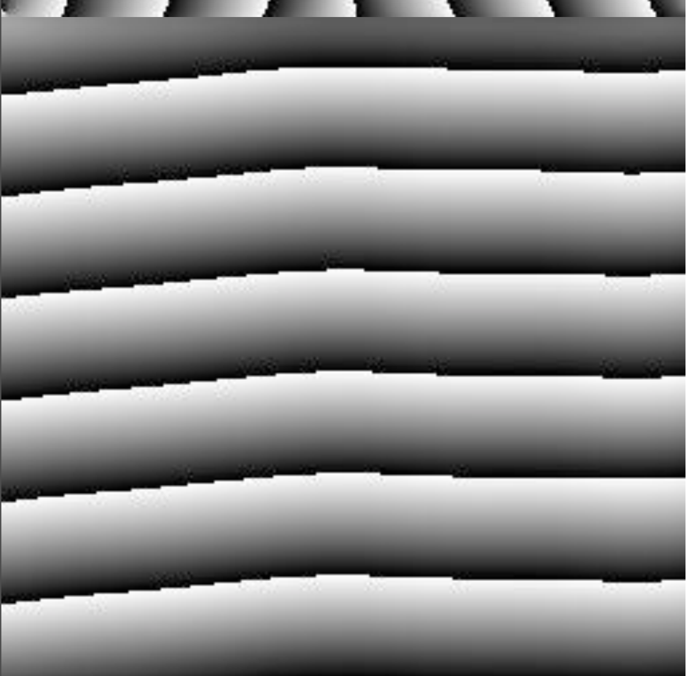
Rotation Case



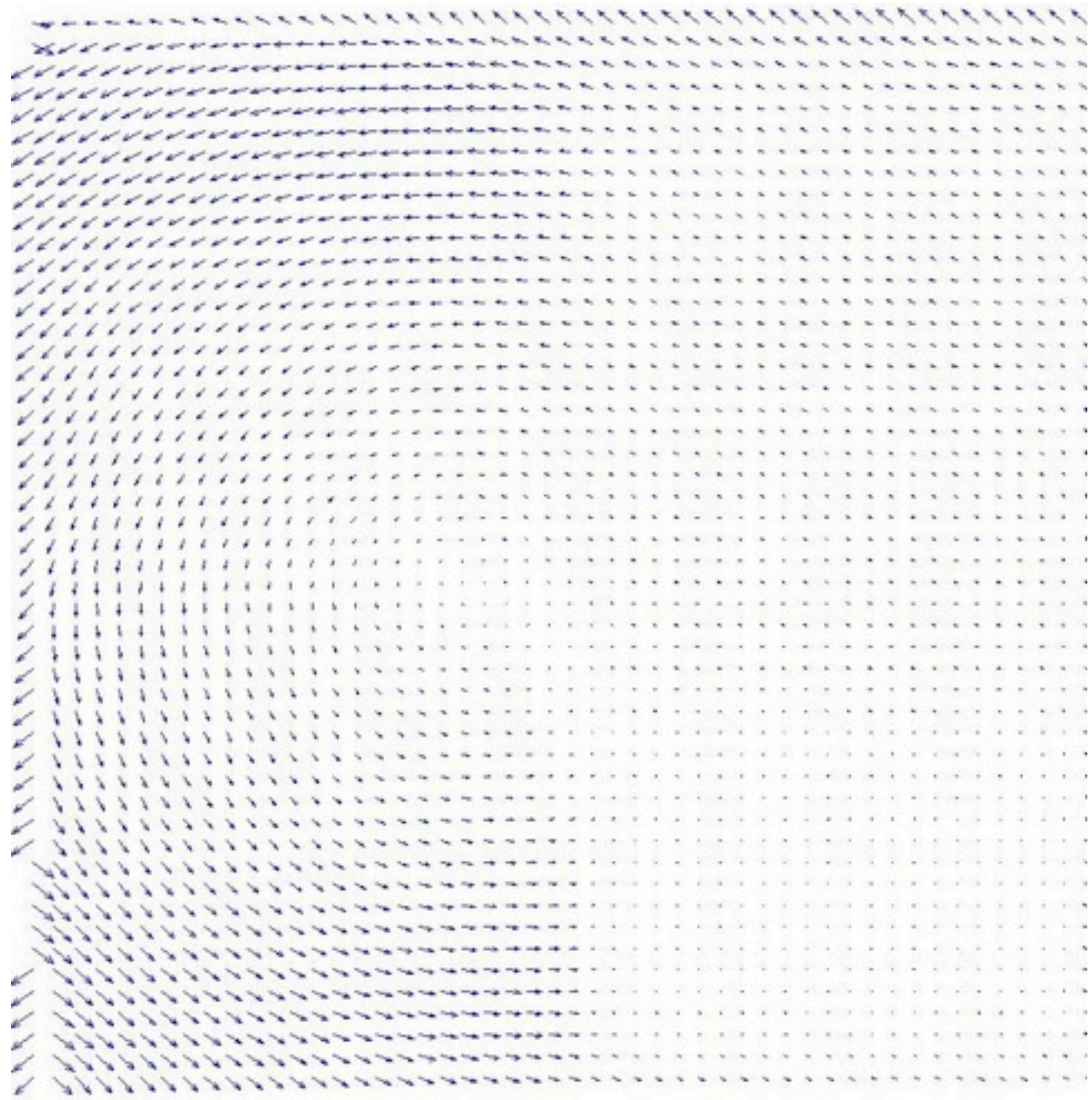
object



phase1



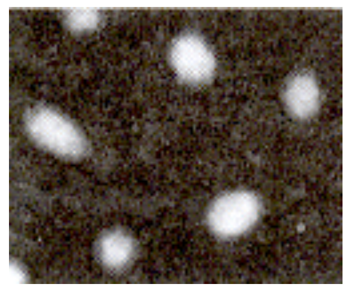
phase2

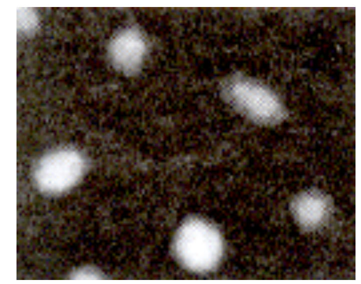


Displacement map

Alternative Strain Map

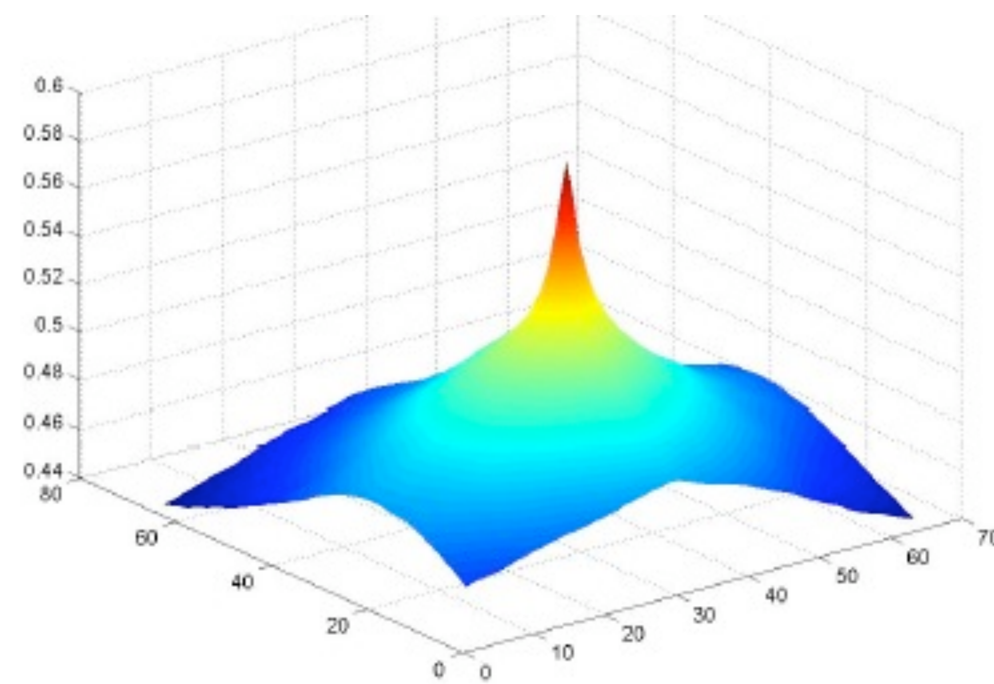
Template matching- cross correlation

Template  I1

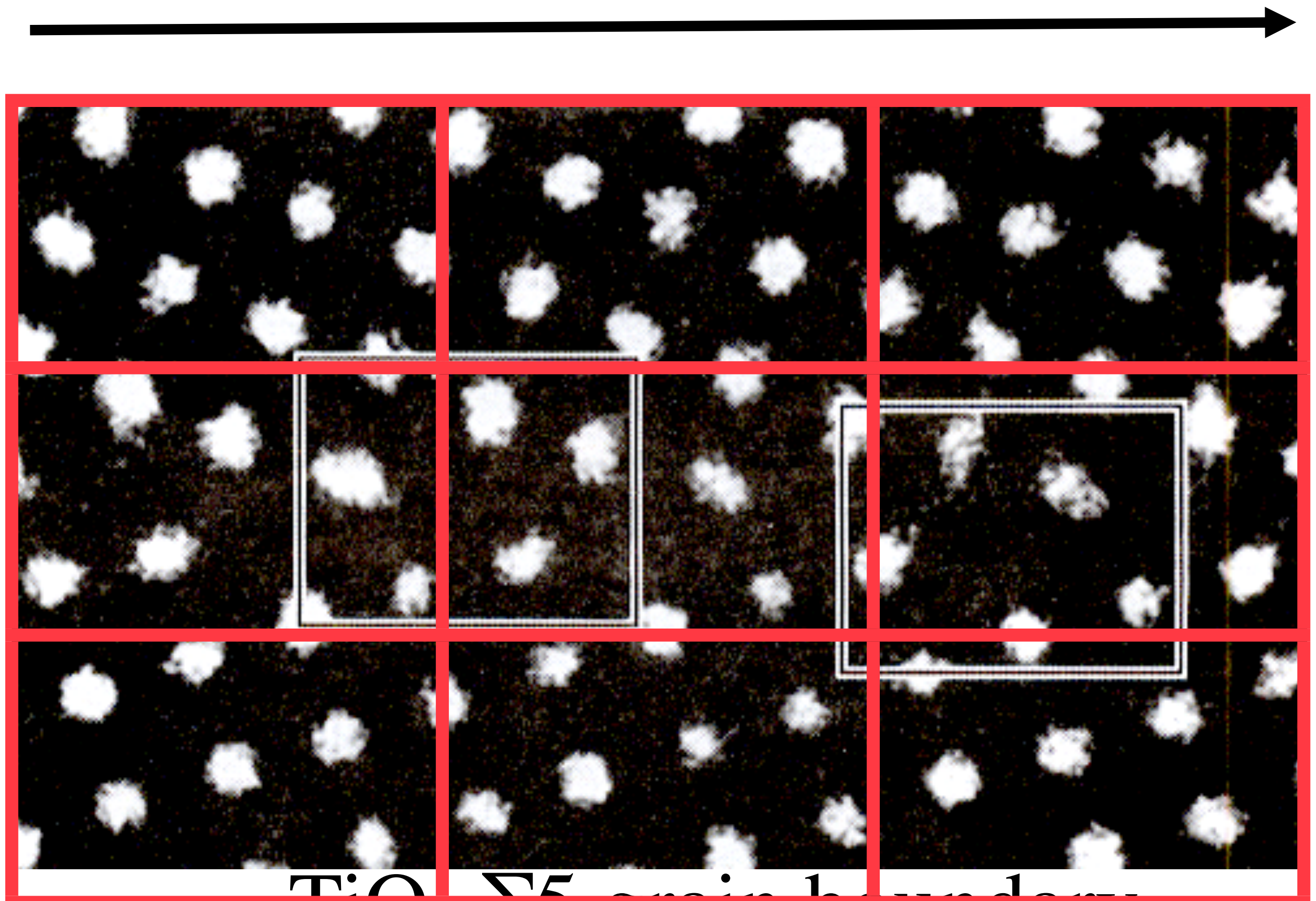
 object

I2

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



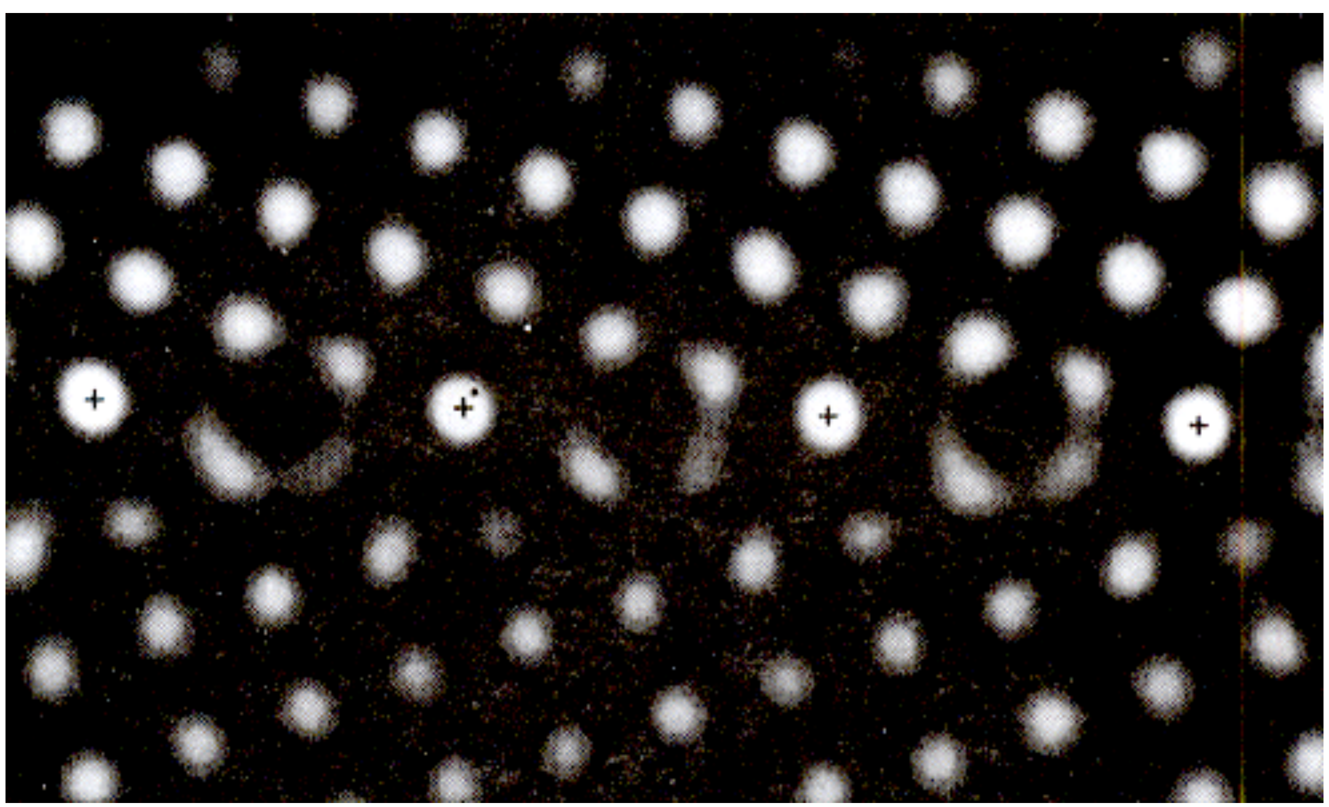
The value of ccf give an indication of similarity of two images



TiO_2 Σ5 grain boundary

1. Scanning the template across the object image

2. Generating CCF map

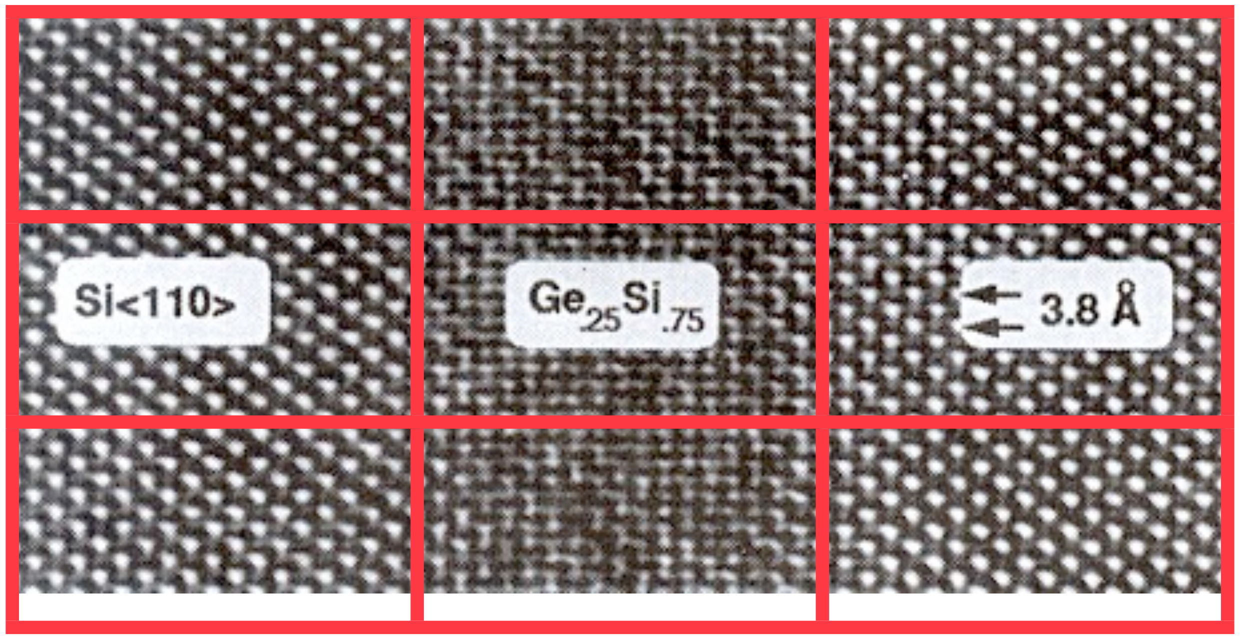


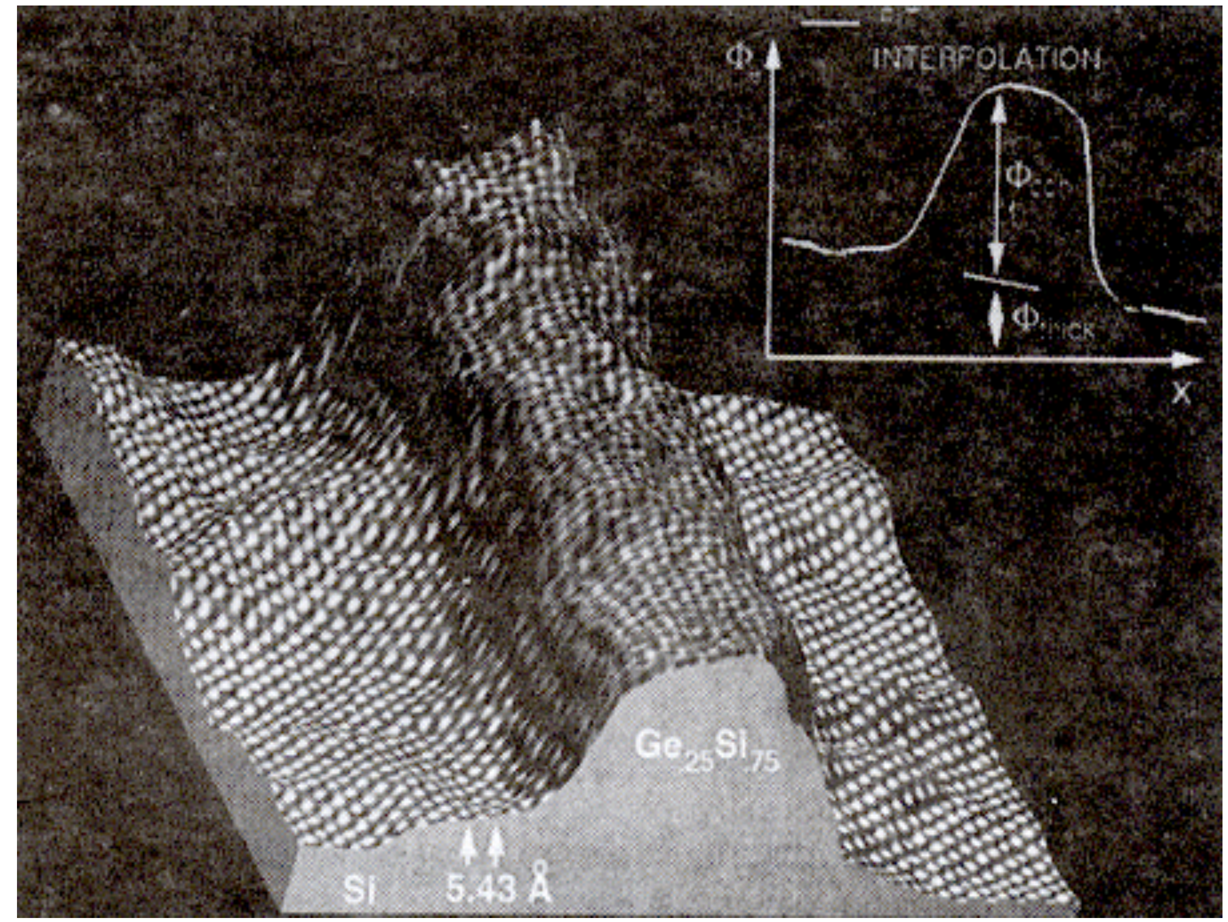
ccf map

Pattern Recognition for structure identification

Atom Resolution Compositional Map

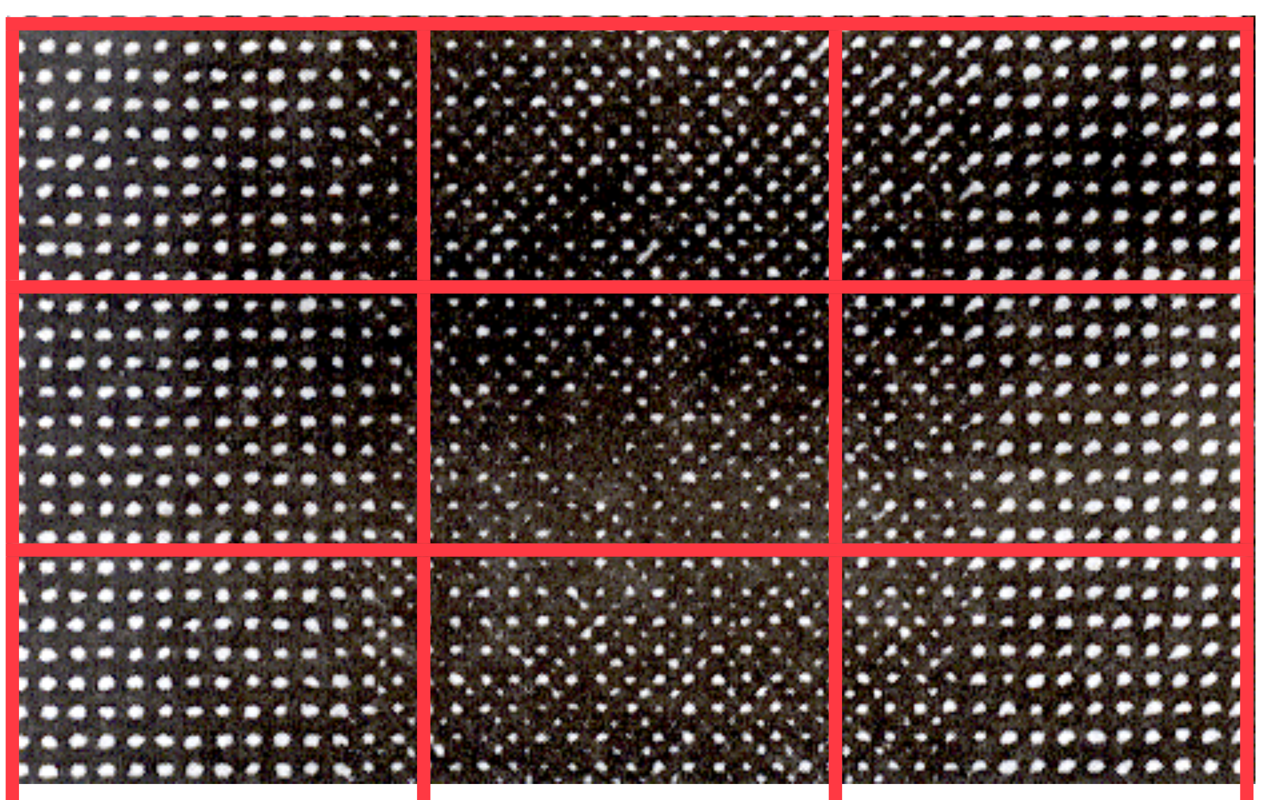
Si/GeSi quantum well

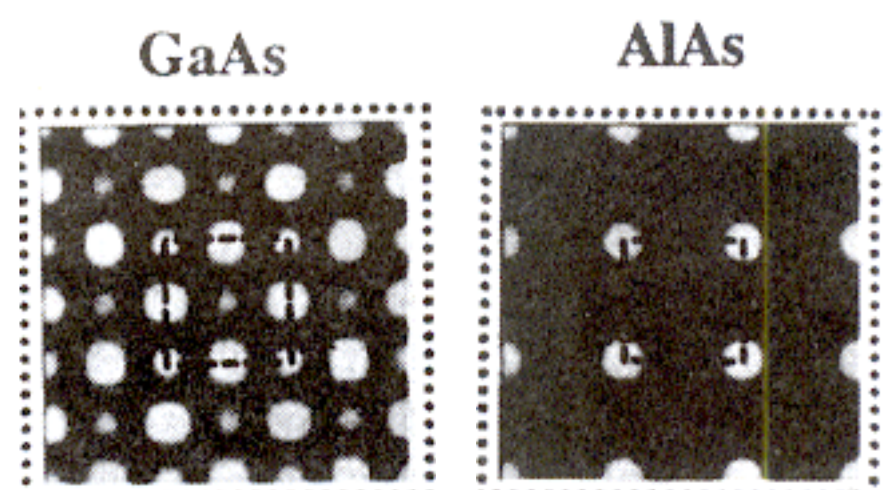




CCF map with HRTEM skin

(Al)GaAs GaAs (Al)GaAs





template