Extension of HRTEM resolution using semi-blind de-convolution and Gerchberg-Saxton algorithm: Application to interface

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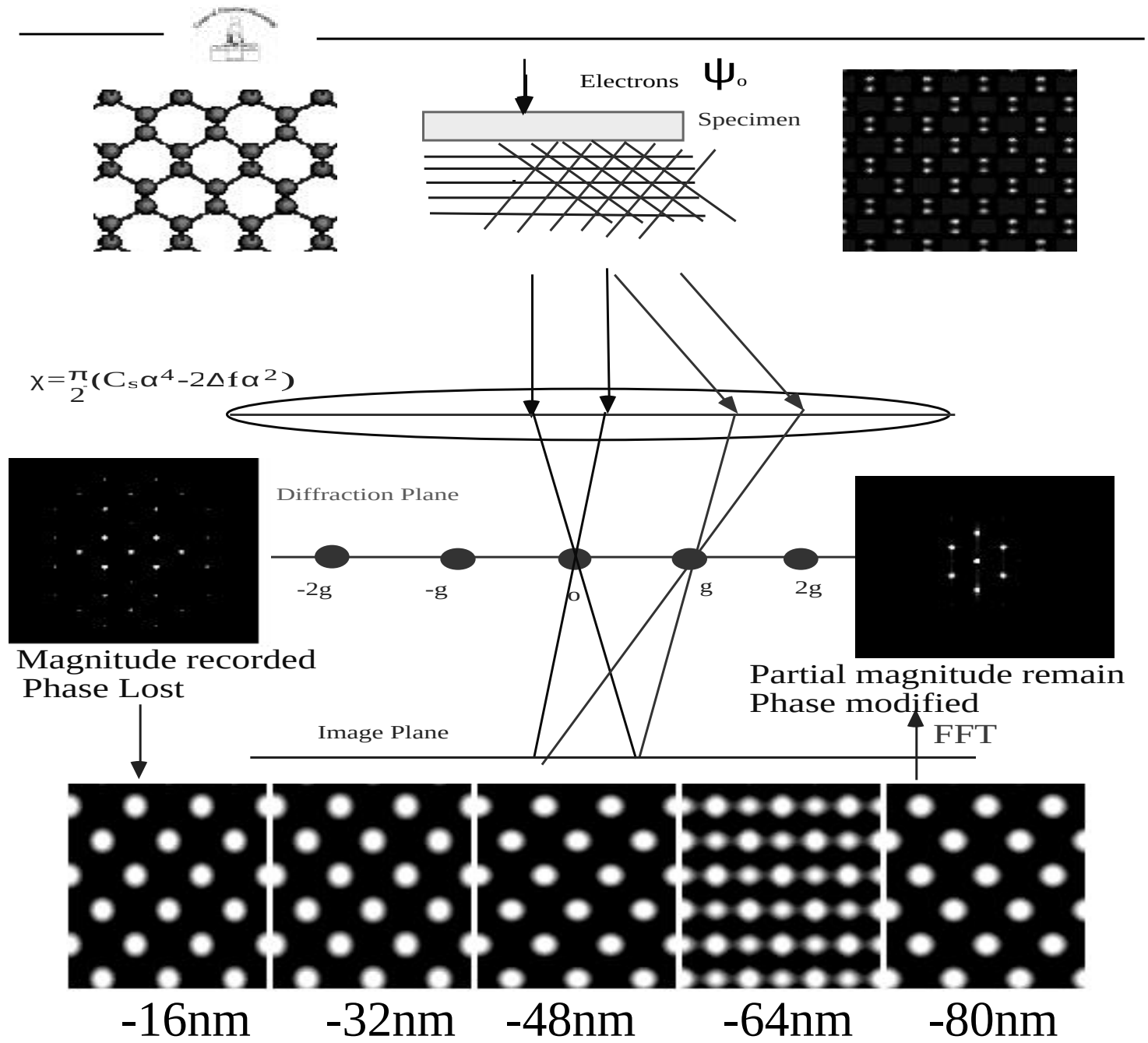
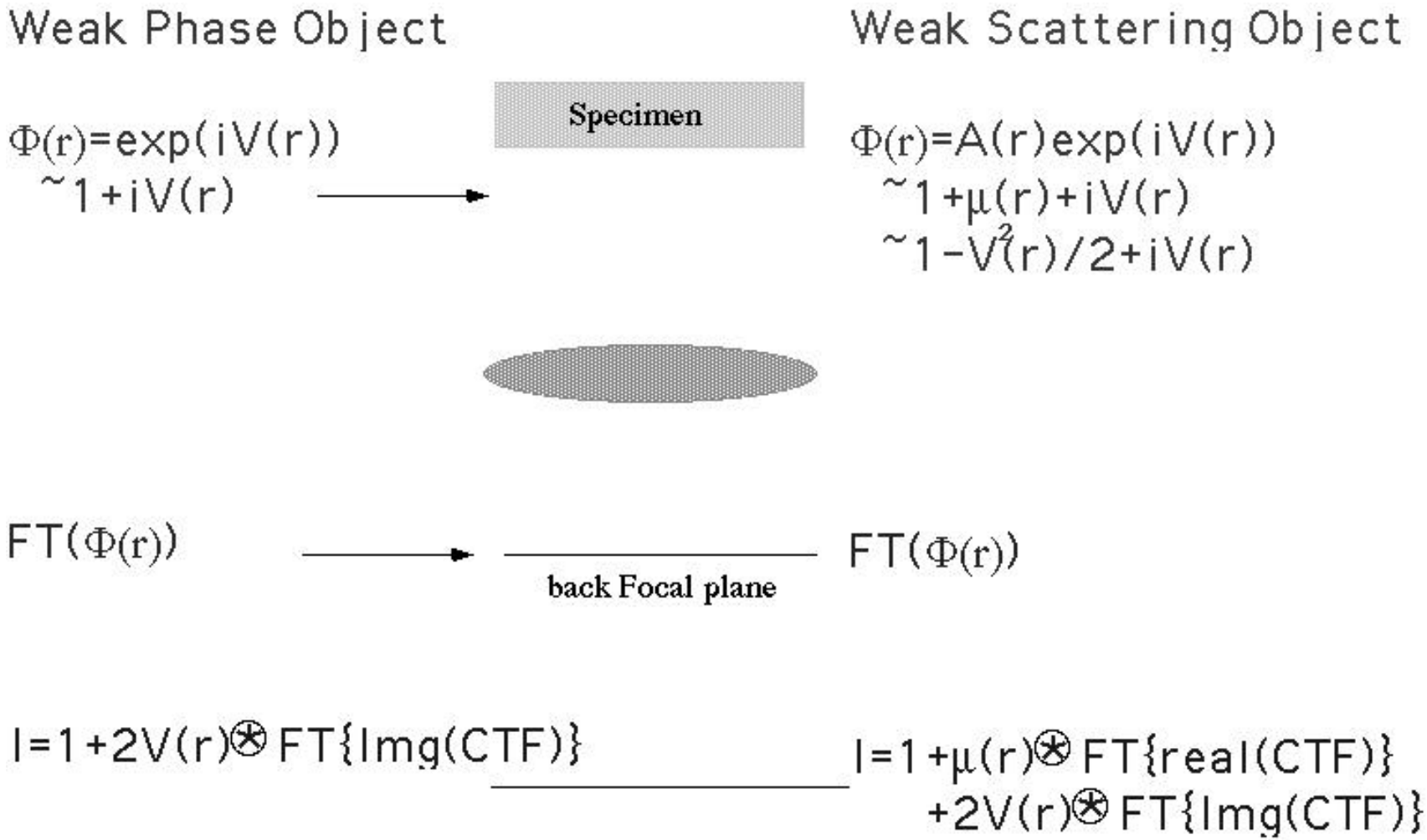
Workshop on New Approaches to the Phase problem



Δf -16nm -32nm -48nm -64nm -80nm



W. O. Saxton, “Computer Techniques for Image processing in Electron Microscopy”, Chap. 1 i

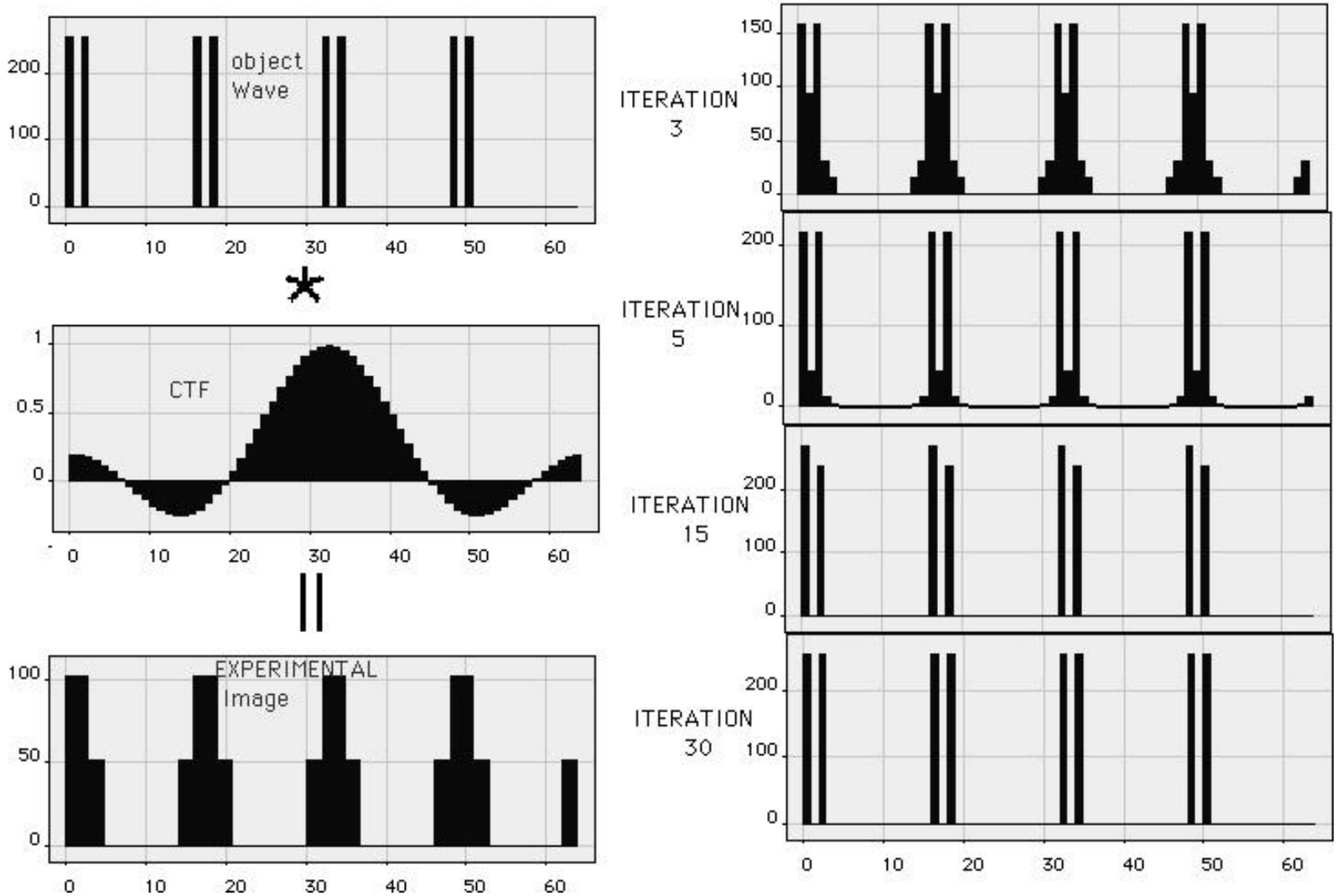
Maximum Entropy Deconvolution Method

blurring Image

MEM Image

I(blurring)=O(blurring function)*I(good image)

EXAMPLE of MAXENT Deconvolution



Lagrangian function for Weak Scattering Case

Minimization of L with conjugate gradient method

$$L=\underbrace{-\sum\mu(r)\ln(\mu(r)/D_\mu(r))-\sum V(r)\ln(V(r)/D_V(r))}_{\text{Entropy terms}}-\lambda_1(\sum\mu(r)-\text{flux1})-\lambda_2(\sum V(r)-\text{flux2})$$

$$-\lambda_3\sum(1+\mu(r)*\text{real}(CTF)+V(r)*\text{img}(CTF)-I^{exp})$$

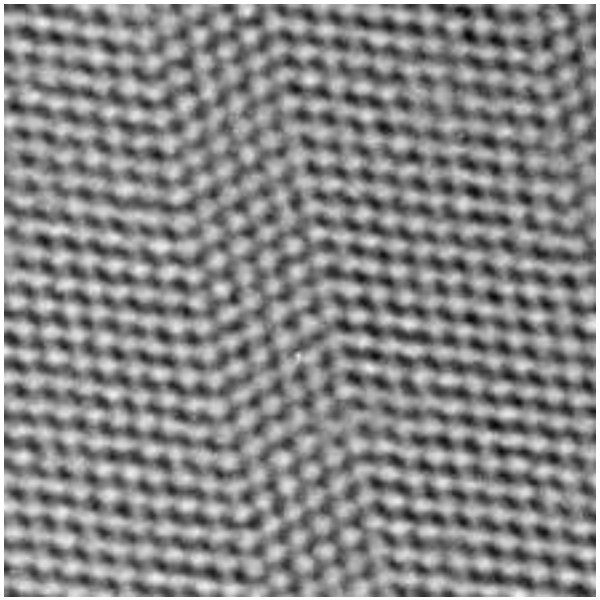
λ_1, λ_2, and $-\lambda_3$ are Lagrangian multipliers

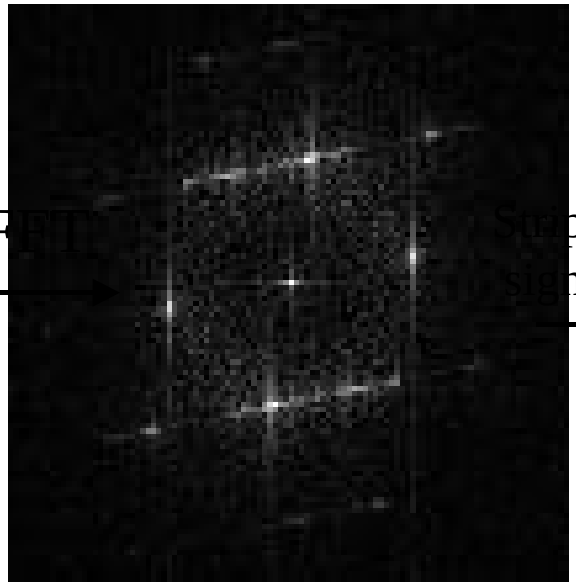
$D(r)=D_\mu(r)+i\,D_V(r)$:Initial Estimate

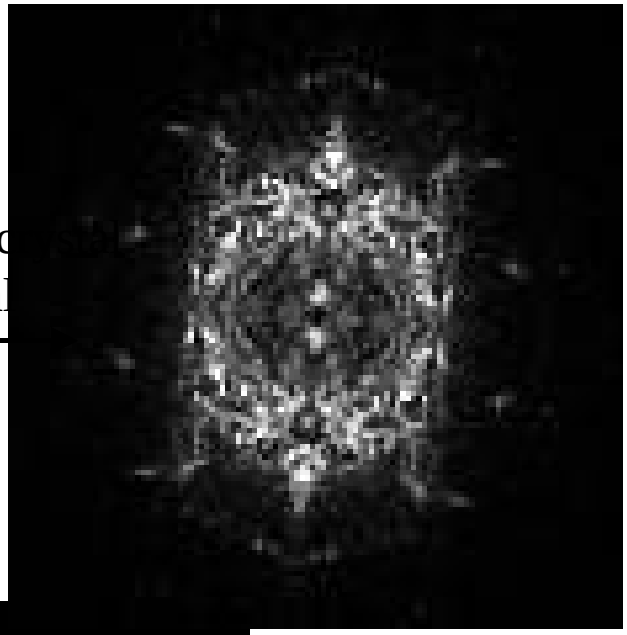
$$D_V(r)\cong FT^{-1}\{\underbrace{[\frac{IMG(CTF)^*}{|IMG(CTF)|^2+K}]}_{\text{Wiener Filter}}*FT(I^{exp}(r))\}$$

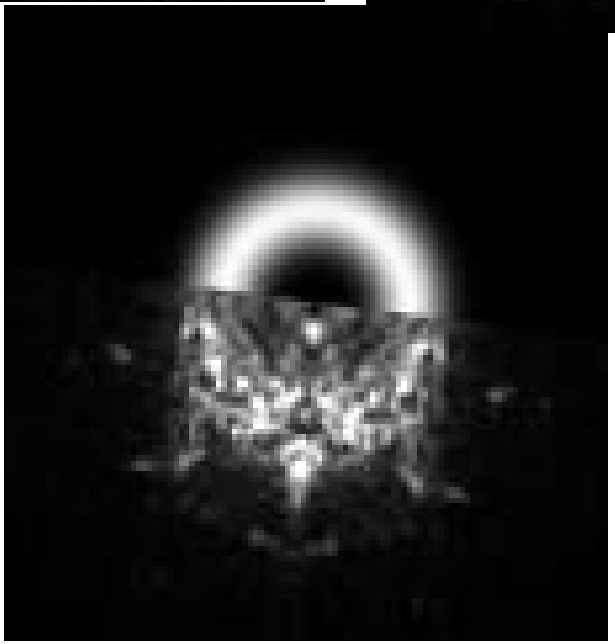
$$D_\mu(r)=1-(D_V^2(r)/2)$$

β−SiC twin boundary



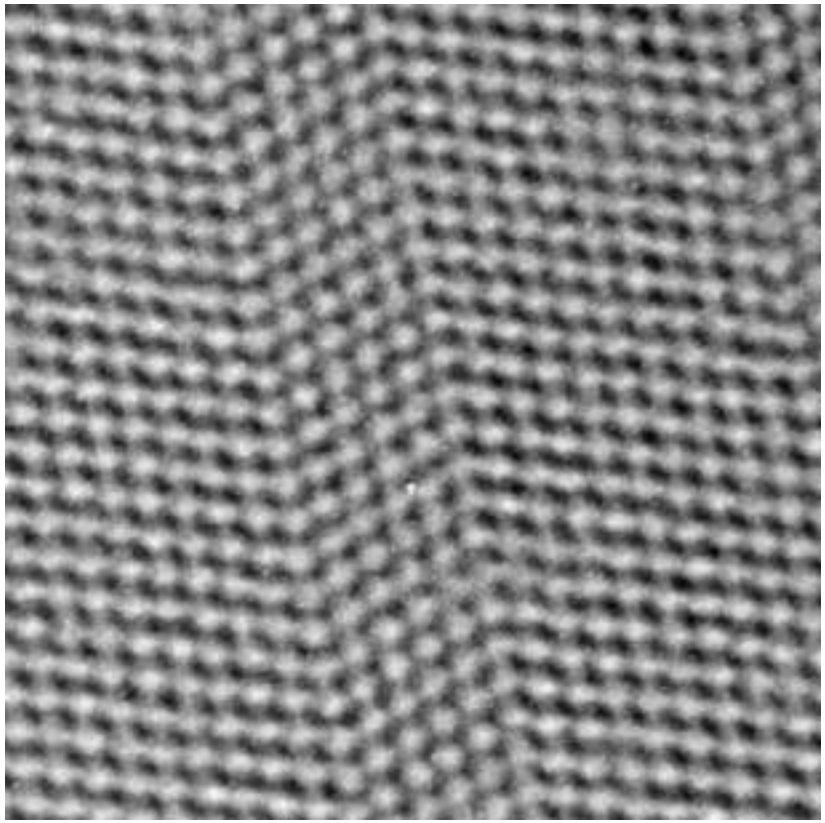




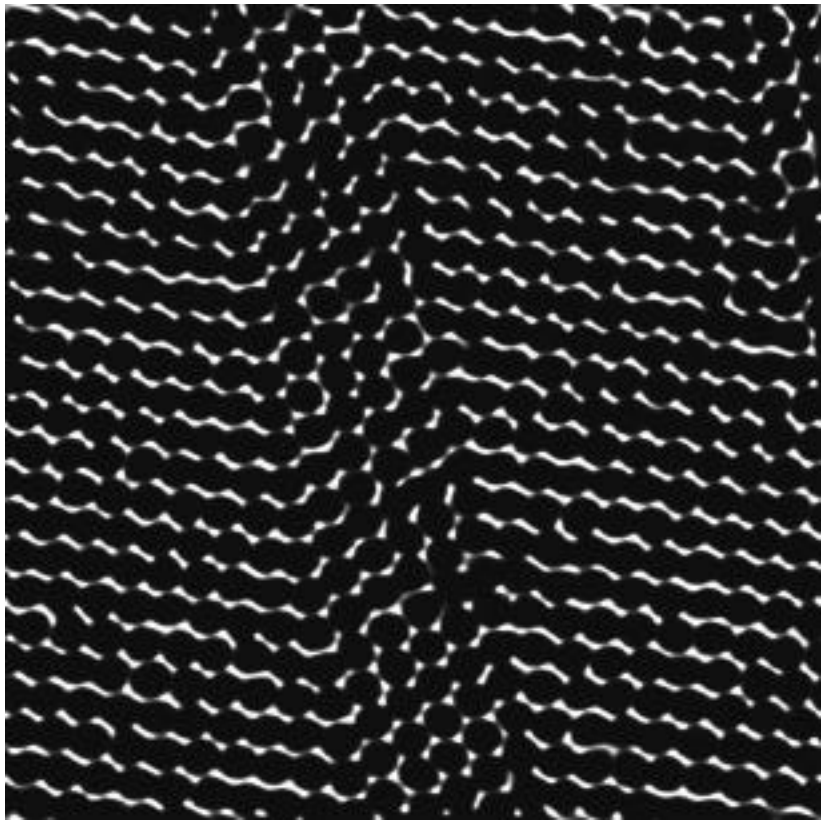


Cs=1.4mm
Δf=-42.5nm
Stigmatism
A=-1nm
θ=82.5°

β−SiC twin boundary

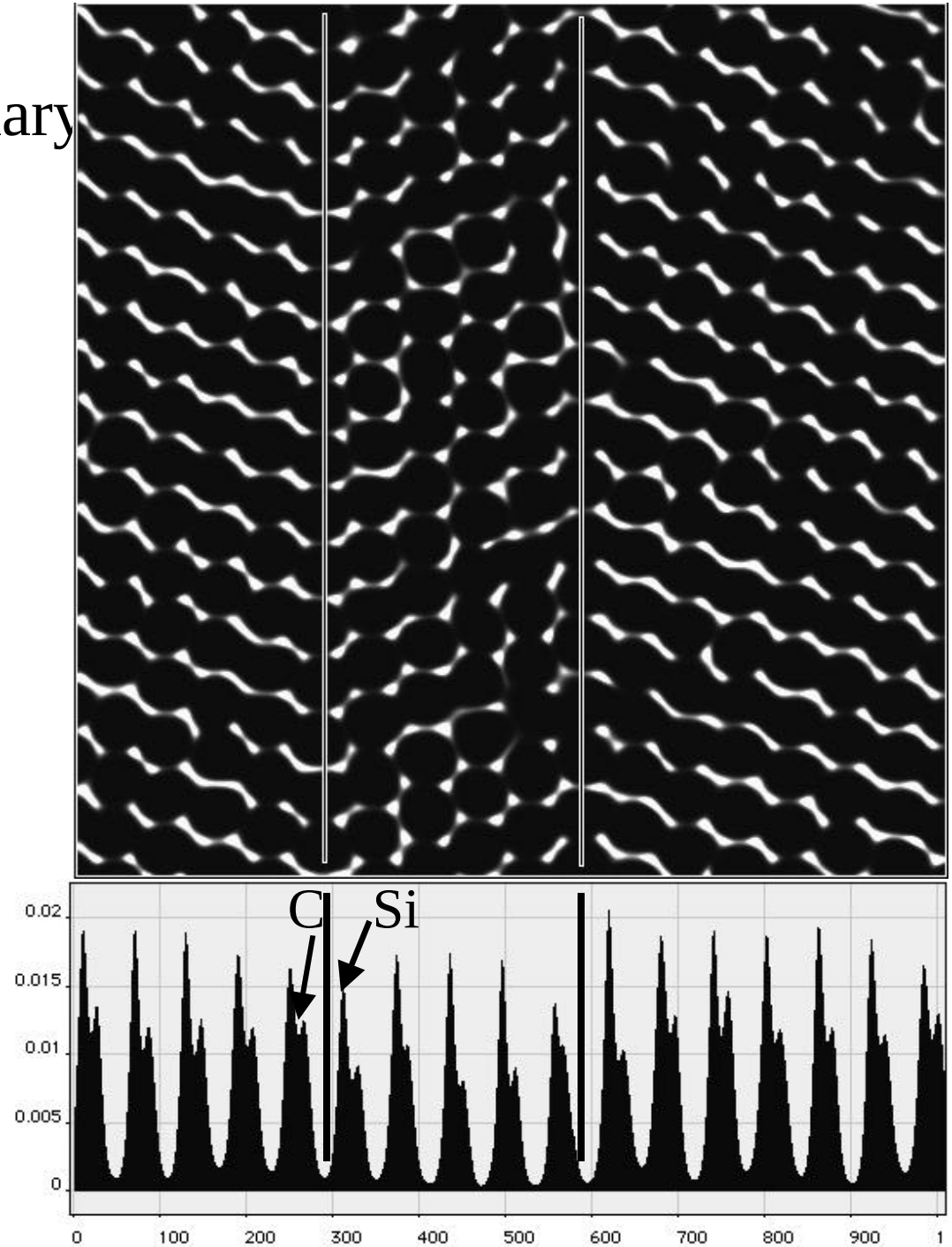


Experimental image

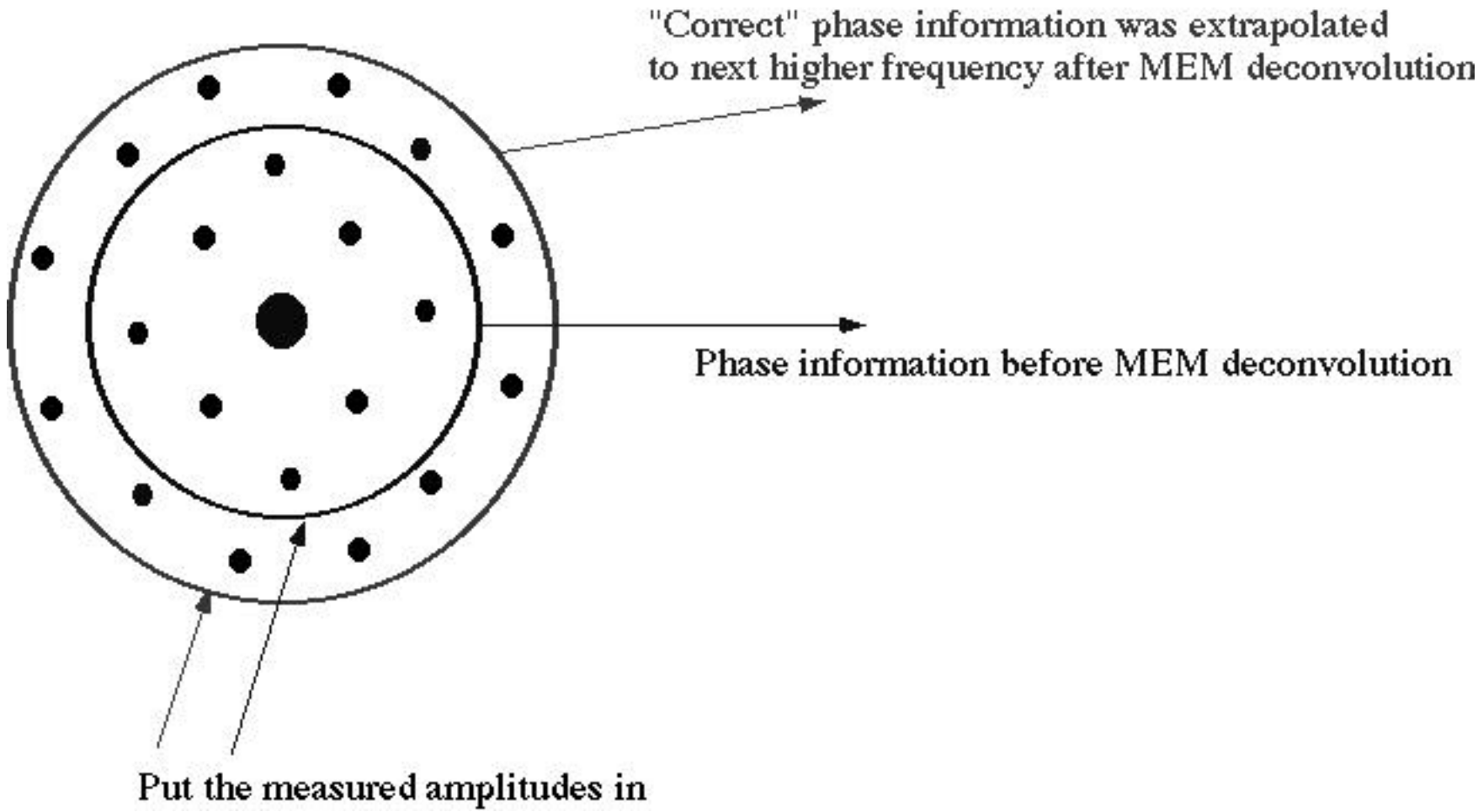


MEM image

β−SiC twin boundary

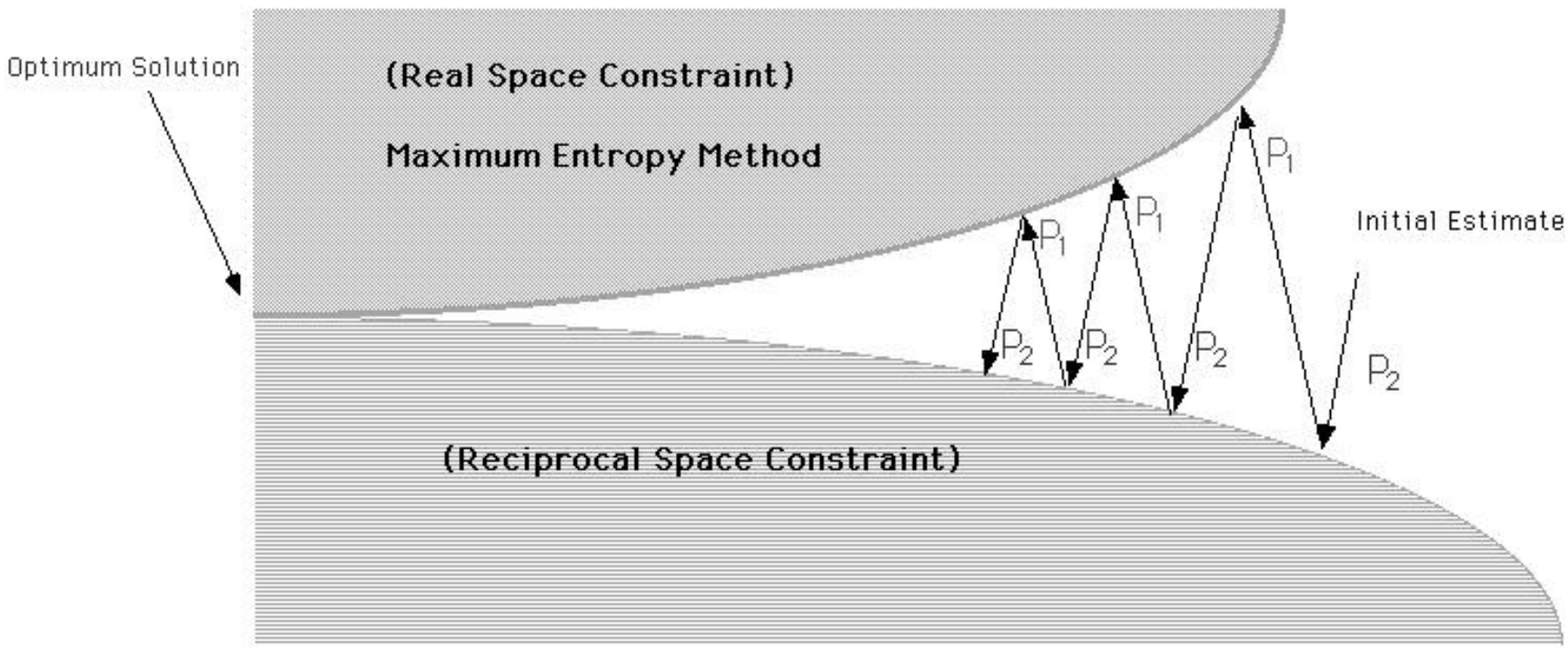


Fourier transform MEM image to reciprocal space



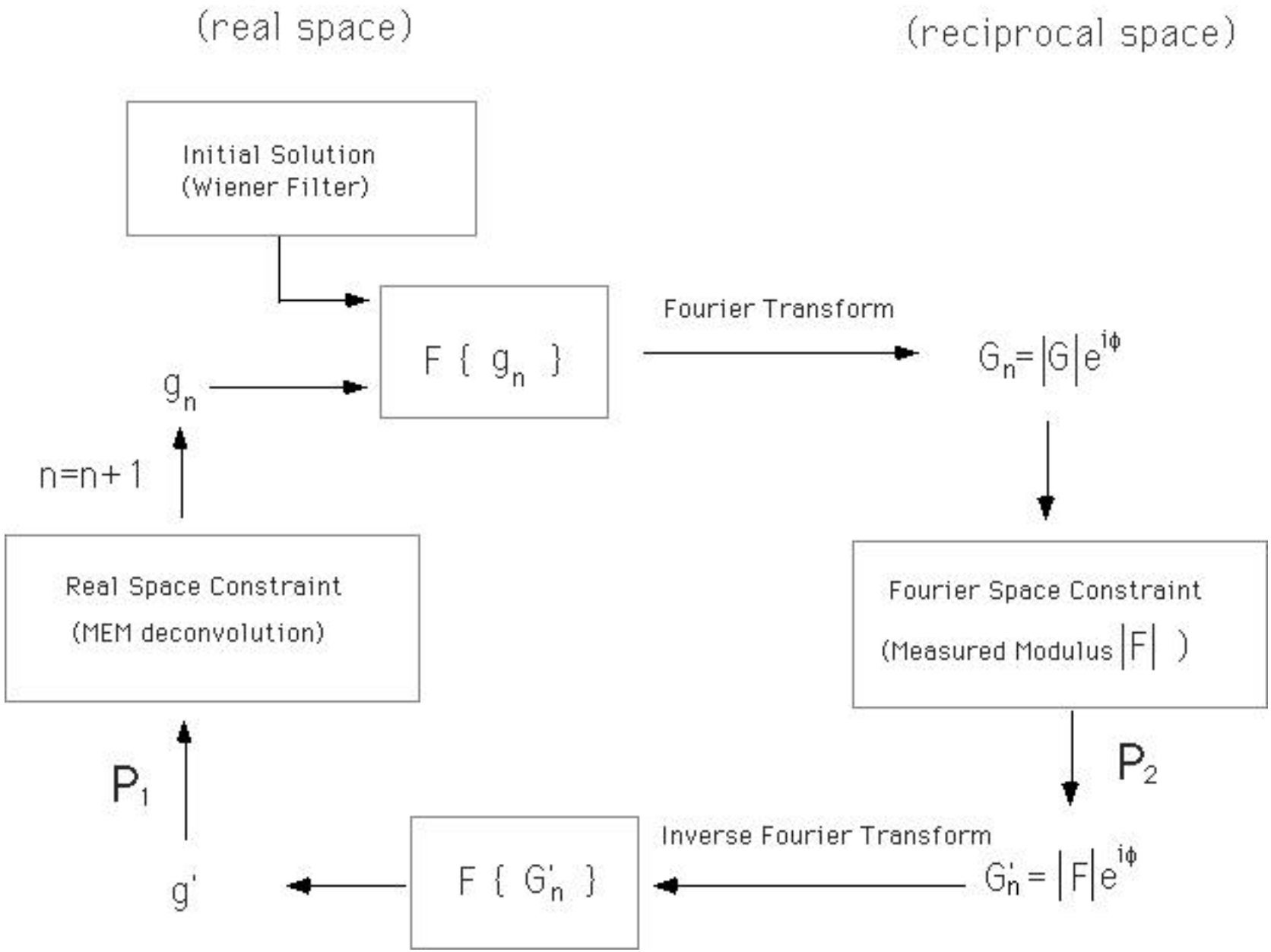
Graphic Concept of Gerchberg-Saxton Algorithm

——— recover information from partial information of phases and amplitudes



Optimum Solution= $P_1\ P_2\ P_1\ P_2\ P_1\ P_2$ ..... $P_1\ P_2$ (Initial Estimate)

Flow Chart of Gerchberg-Saxton Algorithm



EXAMPLES

- Interfaces

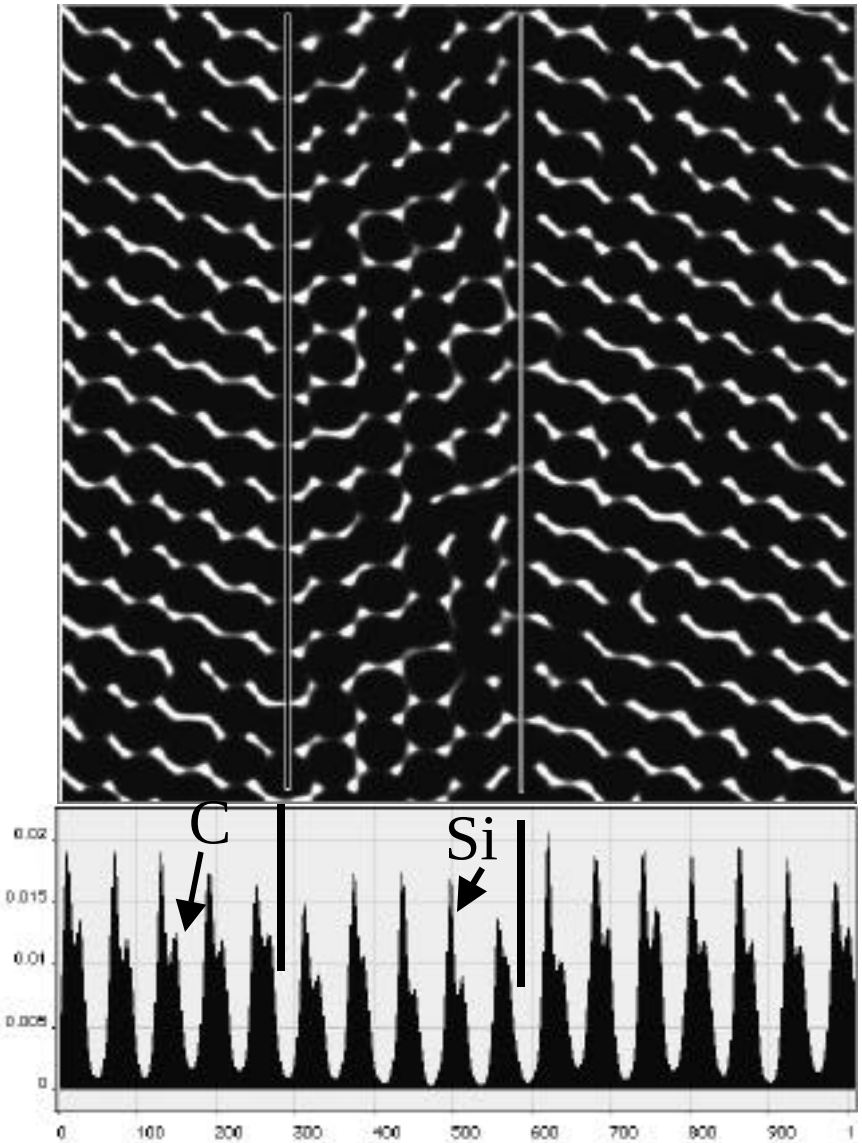
  SiC twin boundary

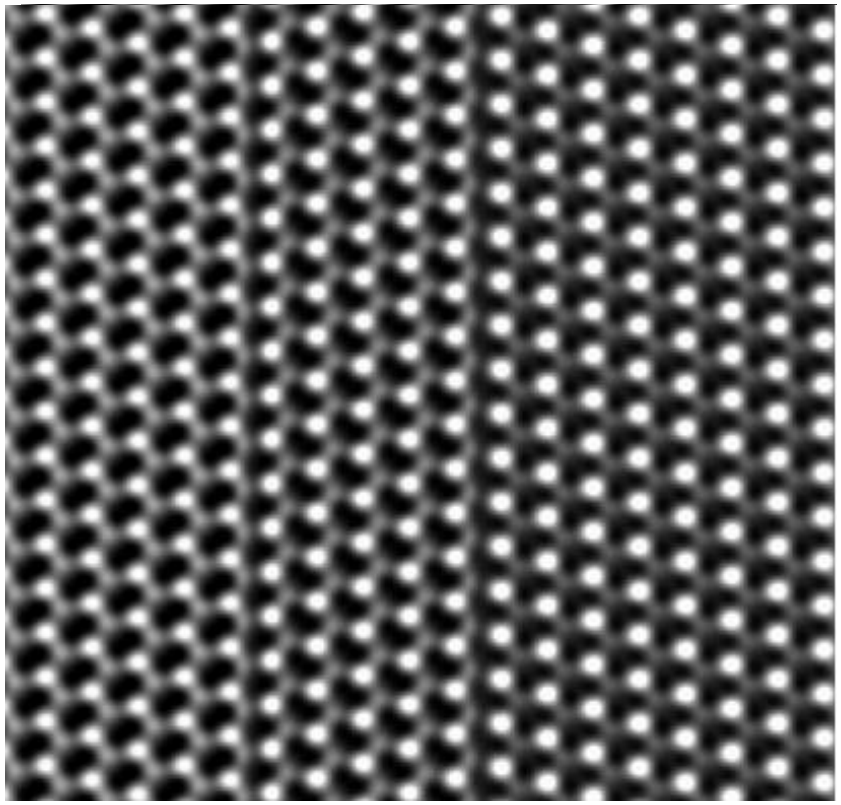
  2x1 reconstructed $NiSi_2$/Si interface

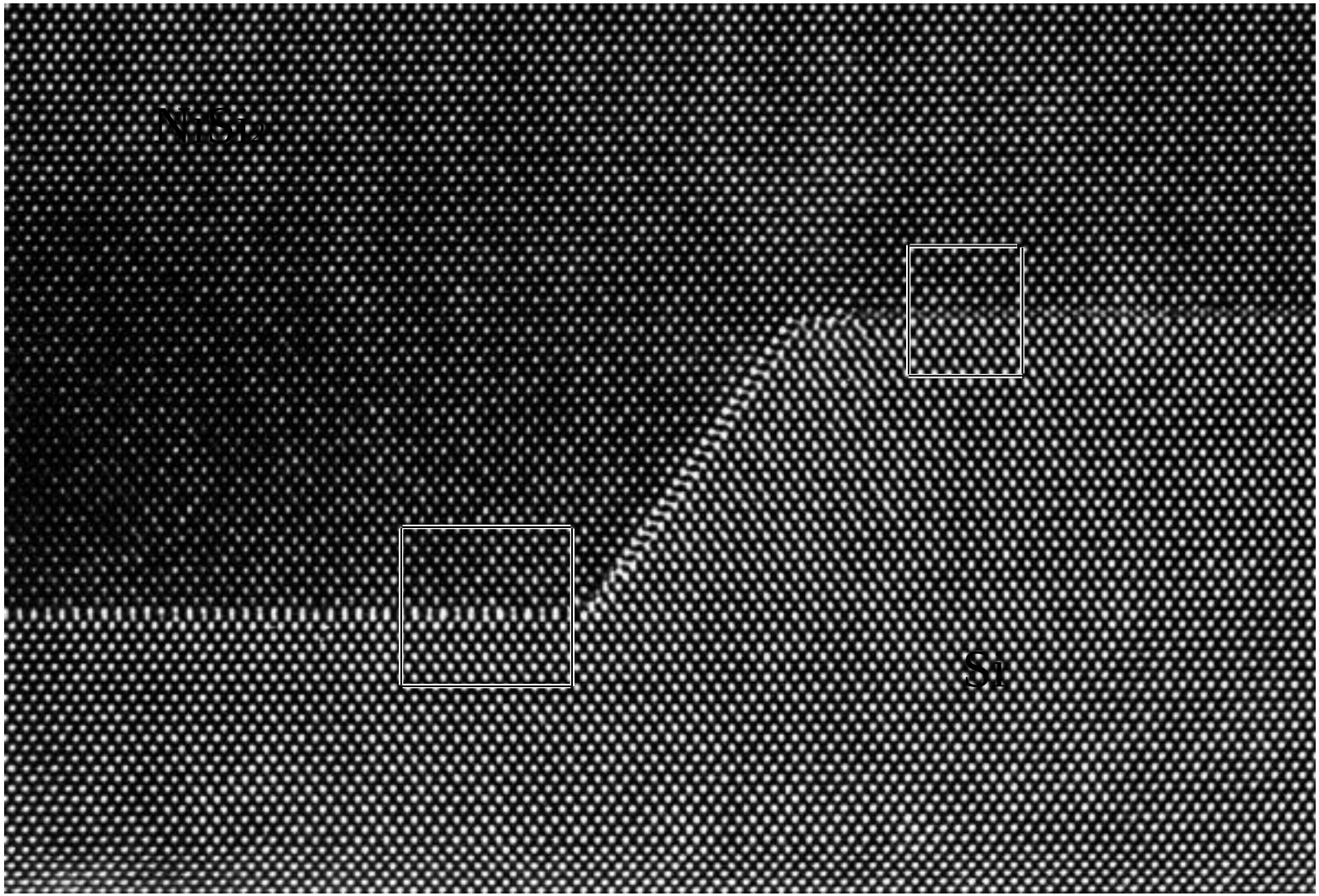
  dislocation in $NiSi_2$/Si interface

  Σ=5 TiO2 grain boundary

β−SiC twin boundary

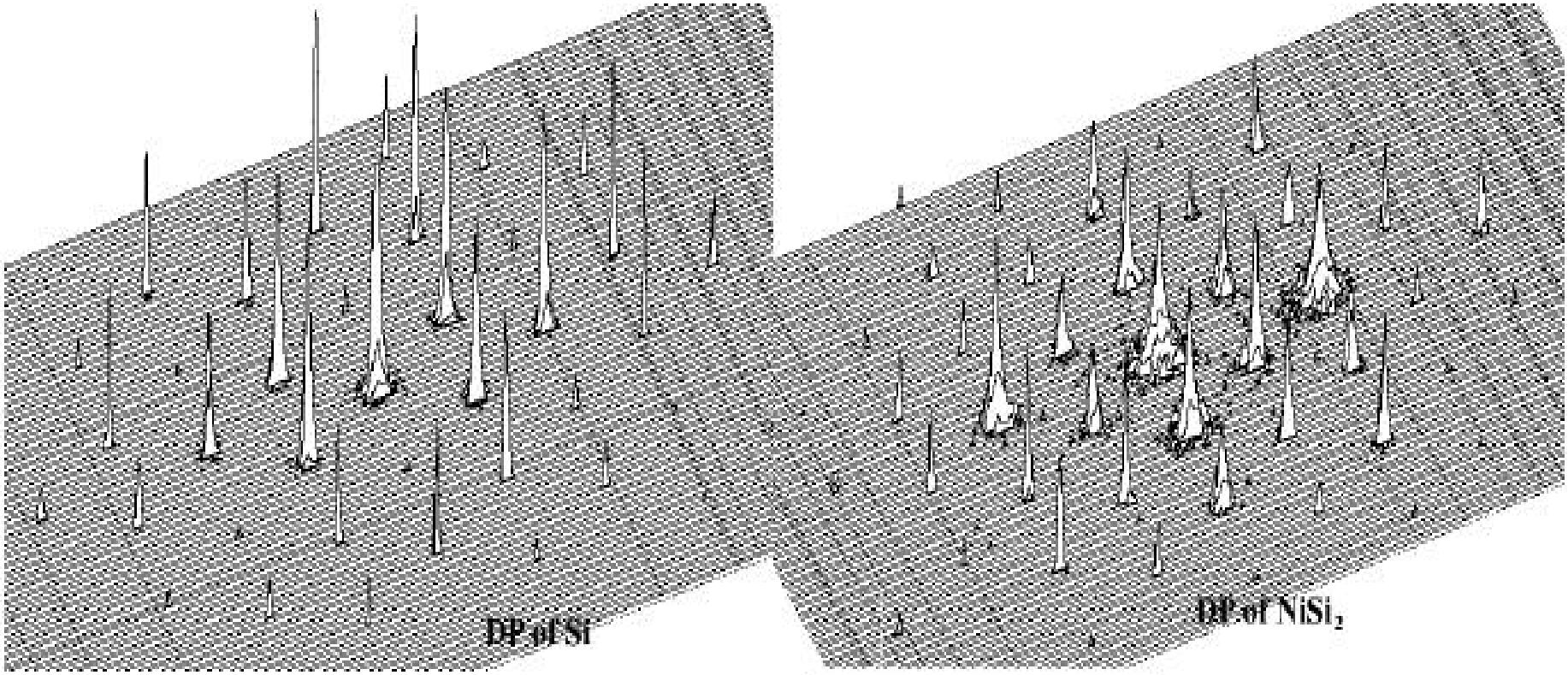


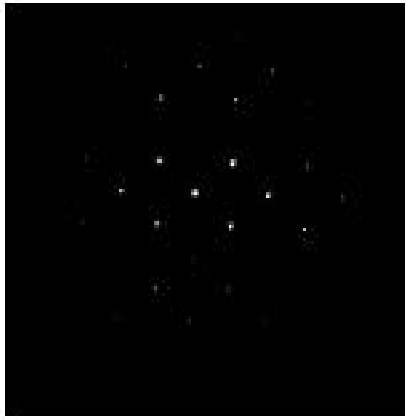


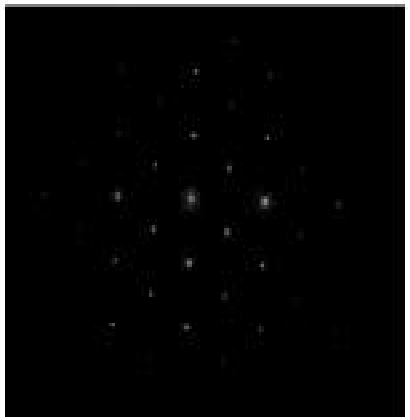


$NiSi_2$/Si Interface

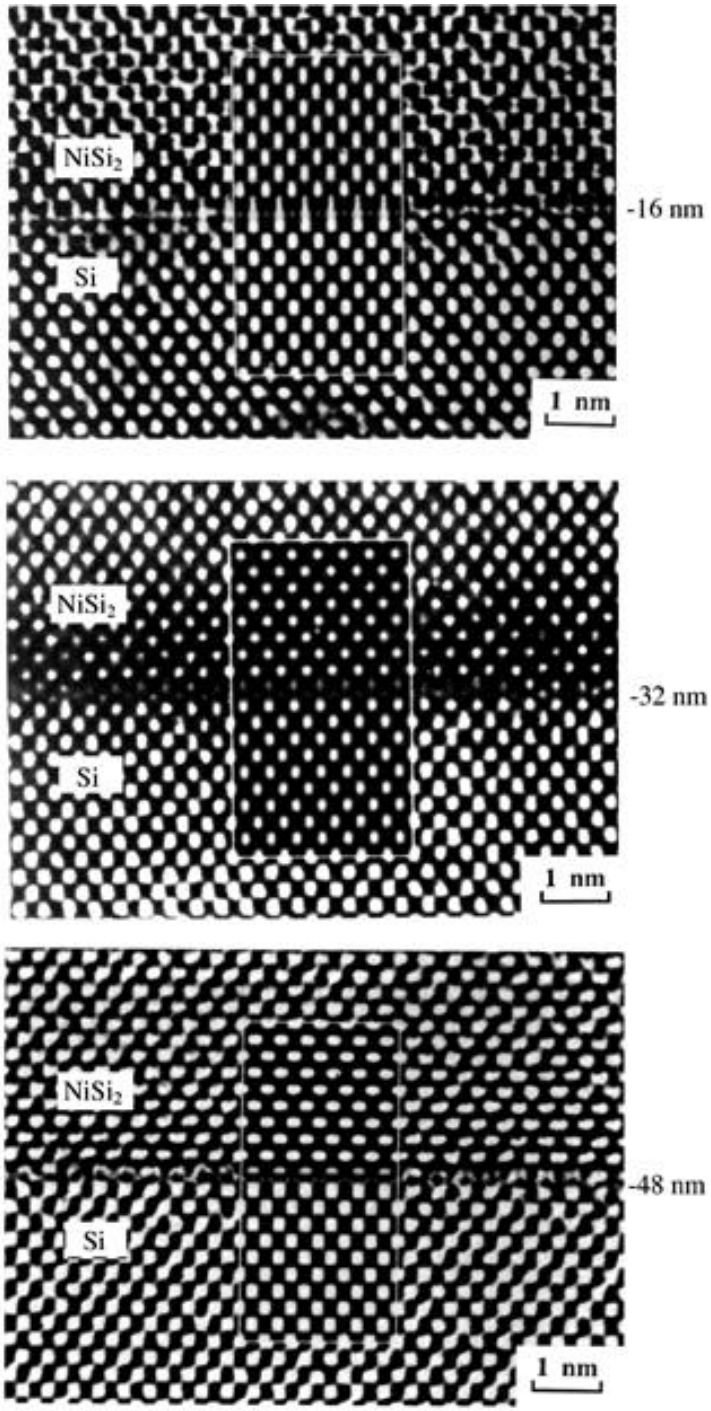
Digitized Diffraction Intensity

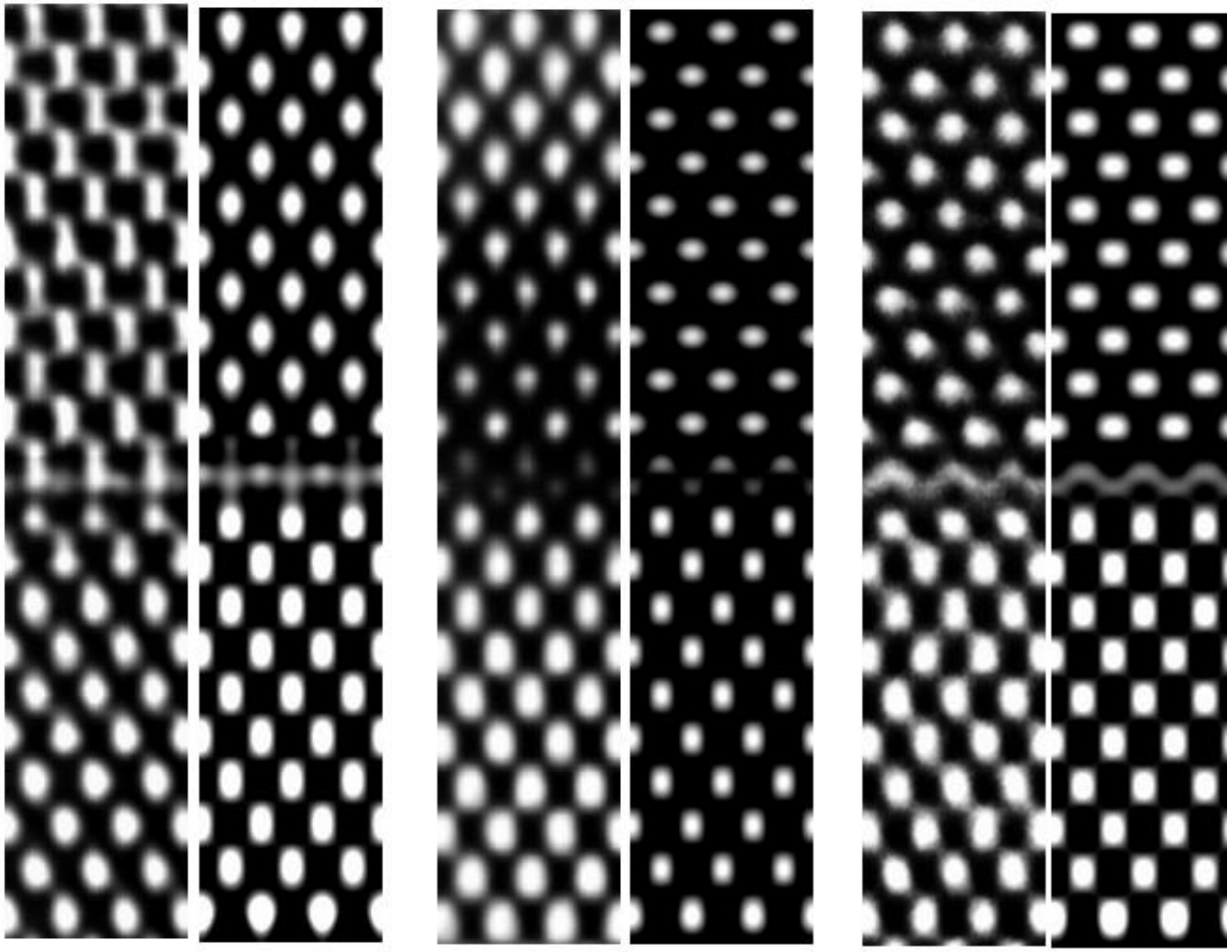




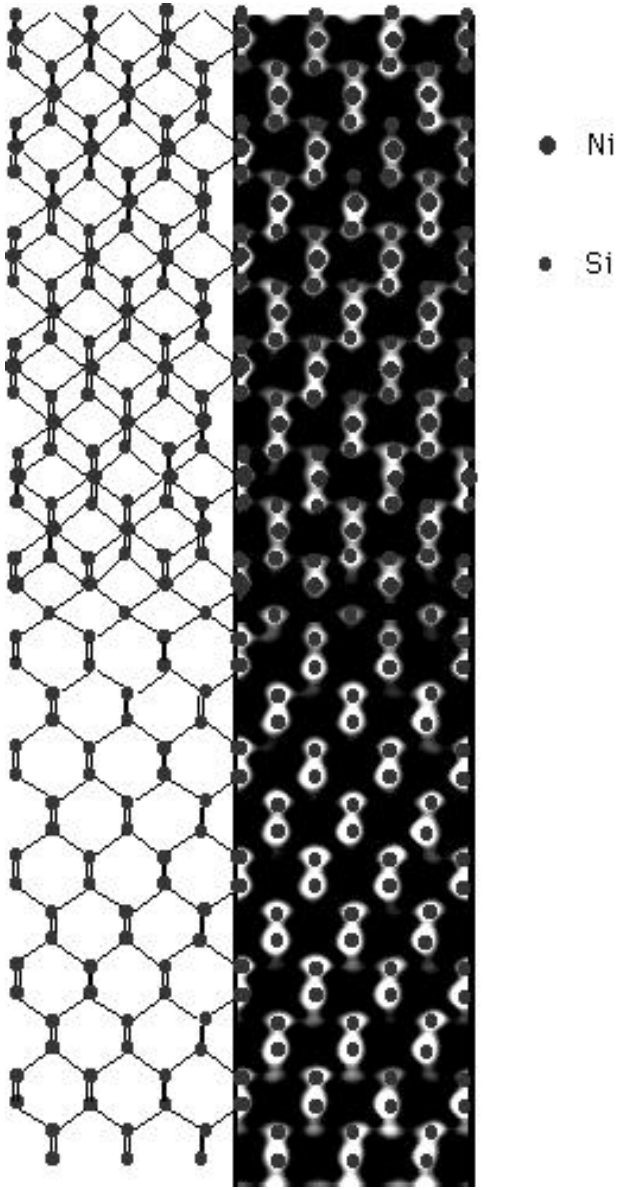


Through focus images of $NiSi_2$/(001)Si Interface





(a) -16 nm (b) -32 nm (c) -48 nm



Left are experimental images
Right are the simulated images
using MEM image

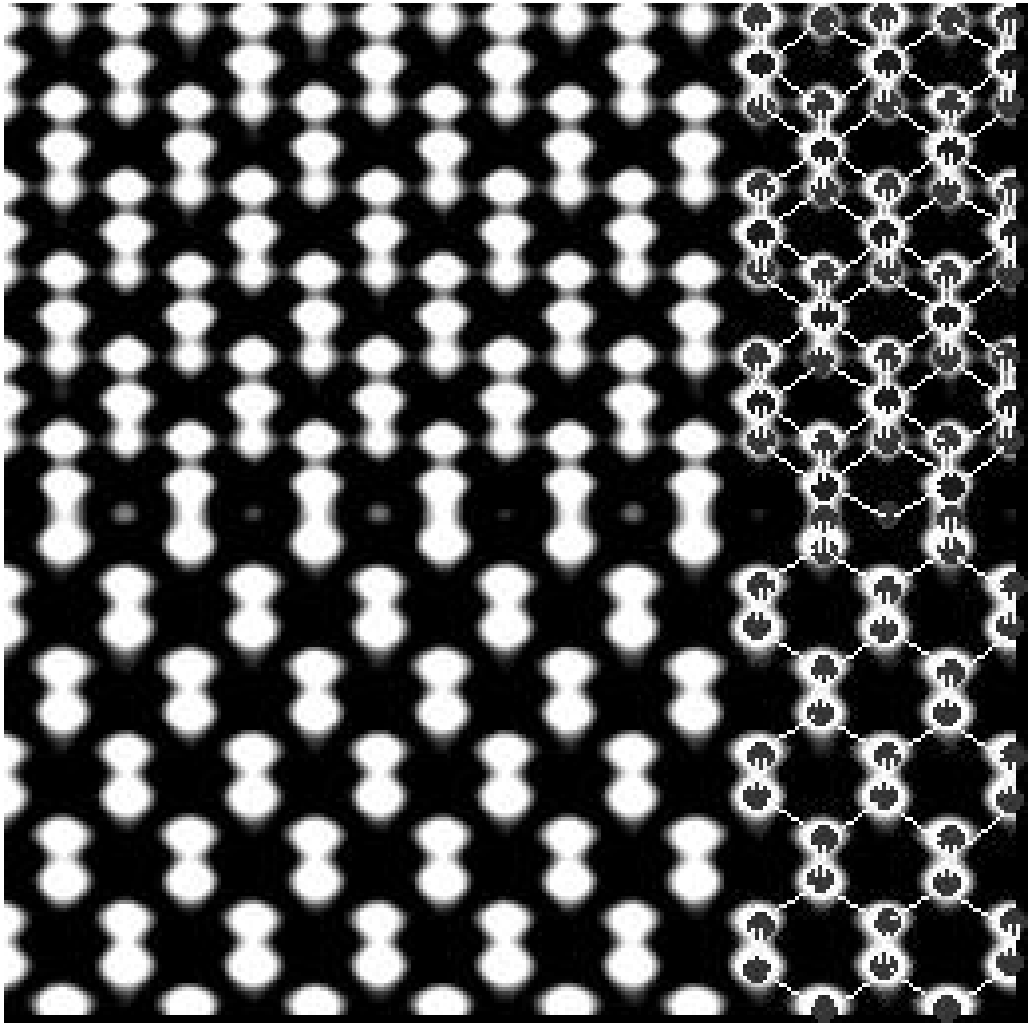
MEM image

2x1 reconstructed $NiSi_2$/Si interface

Experimental Image

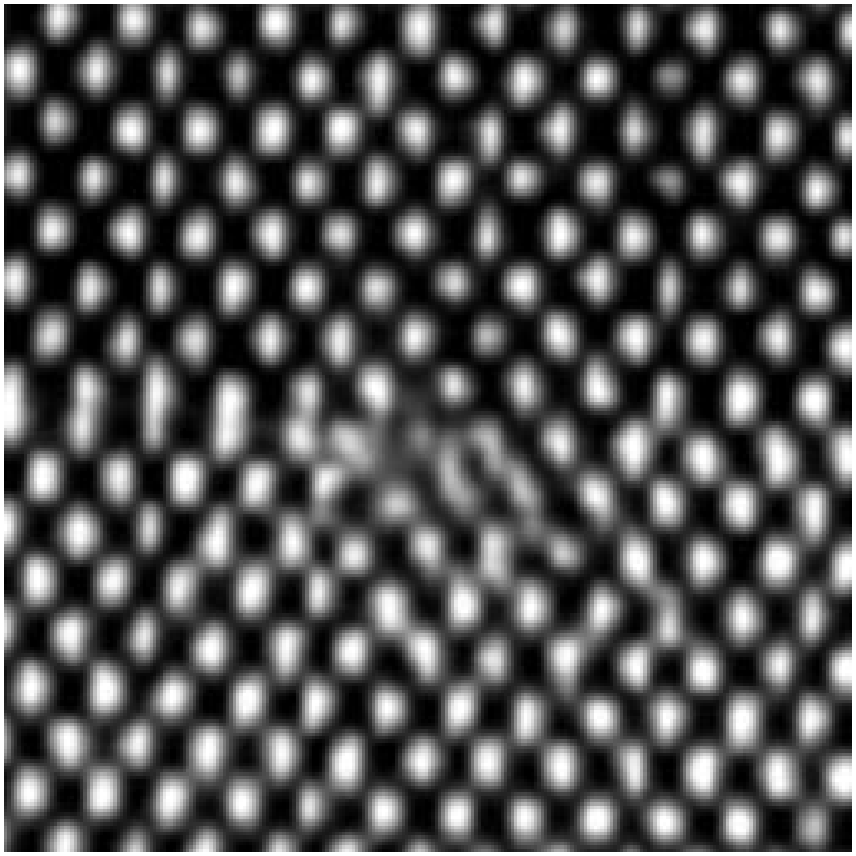
Predicted Image

2x1 reconstructed $NiSi_2$/Si interface



MEM image

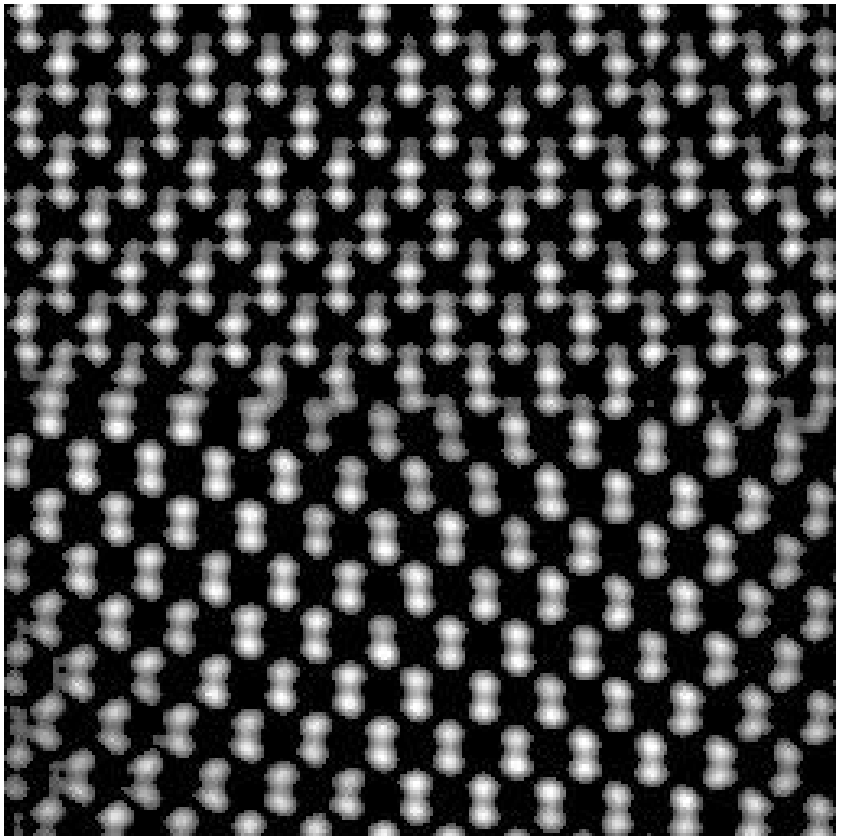
Interfacial dislocation at $NiSi_2$/Si interface



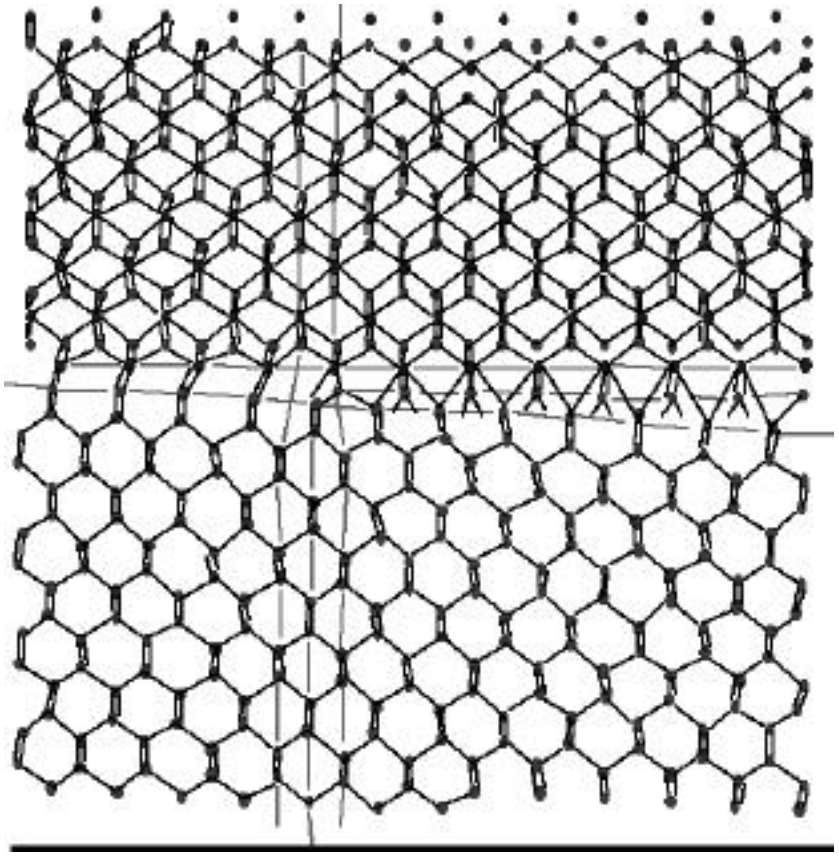
Experimental Image

Predicted Image

Interfacial dislocation at $NiSi_2$/Si interface



MEM image

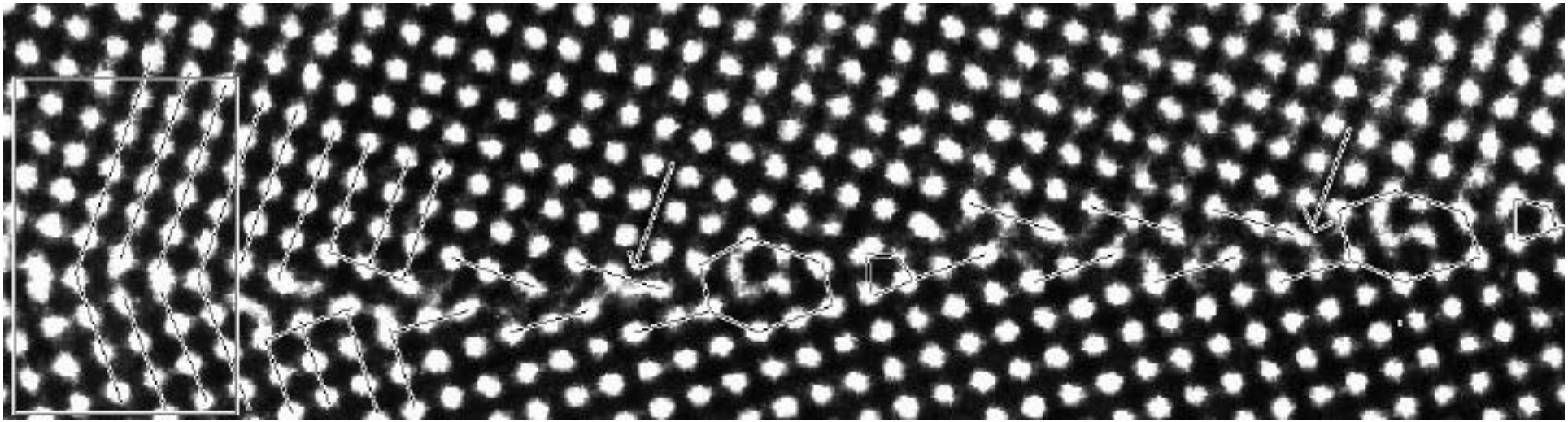


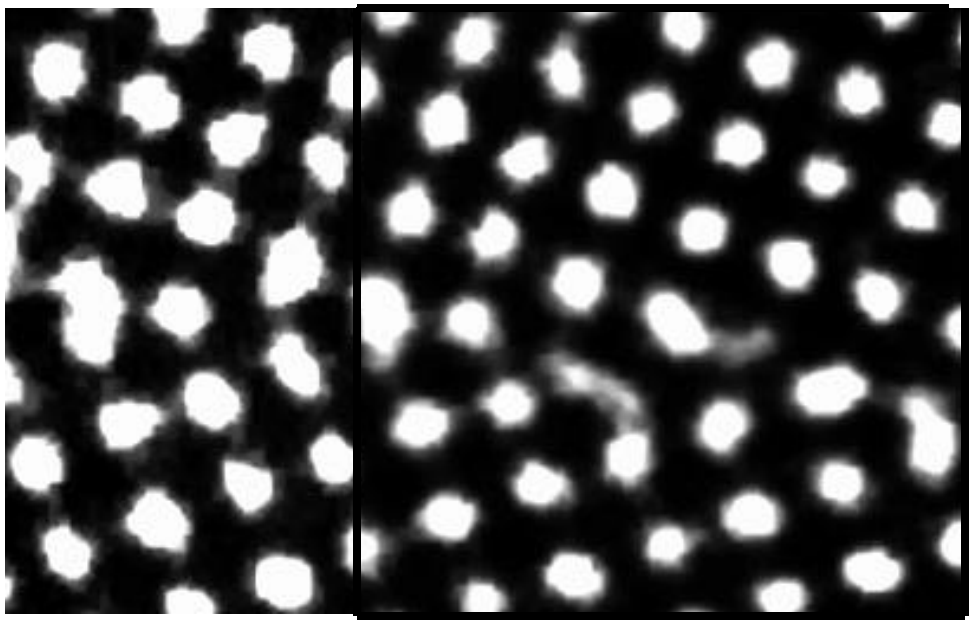
Schematically Structure

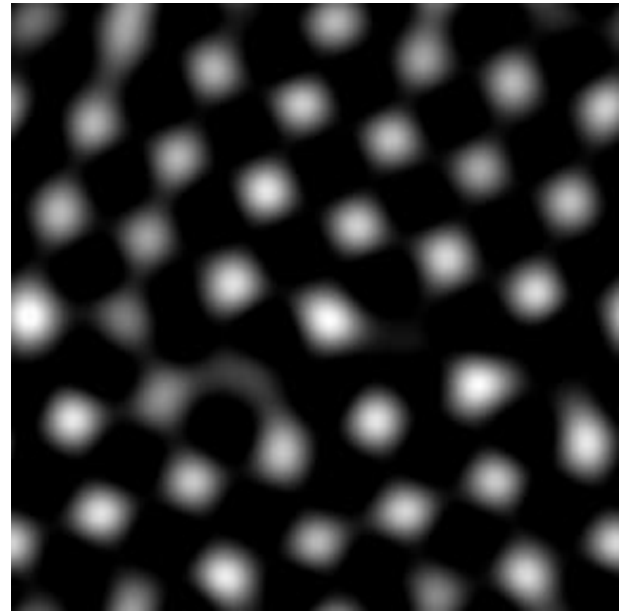
EXAMPLES

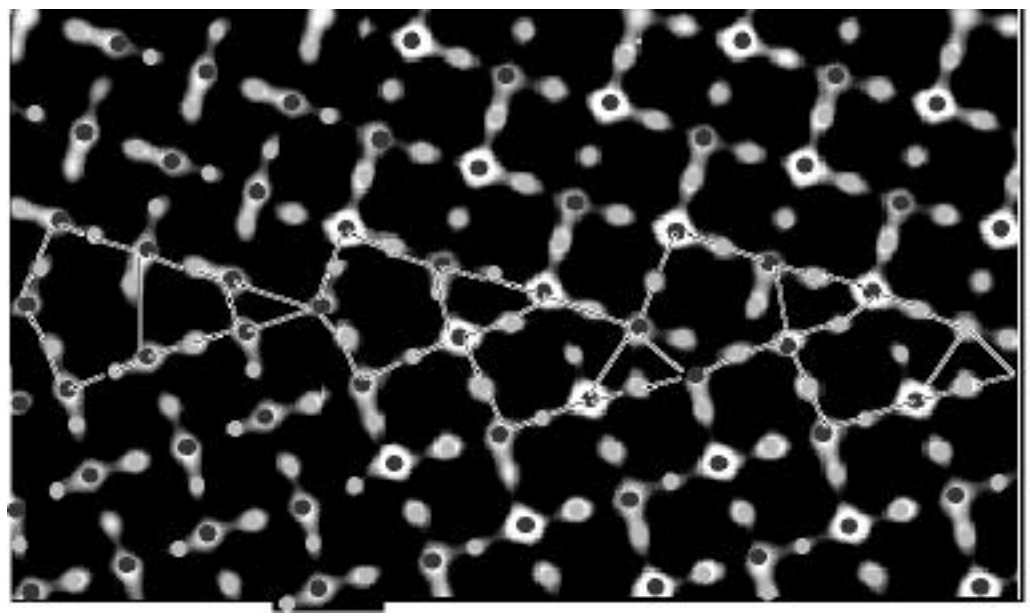
- Σ5 Grain Boundary of TiO_2

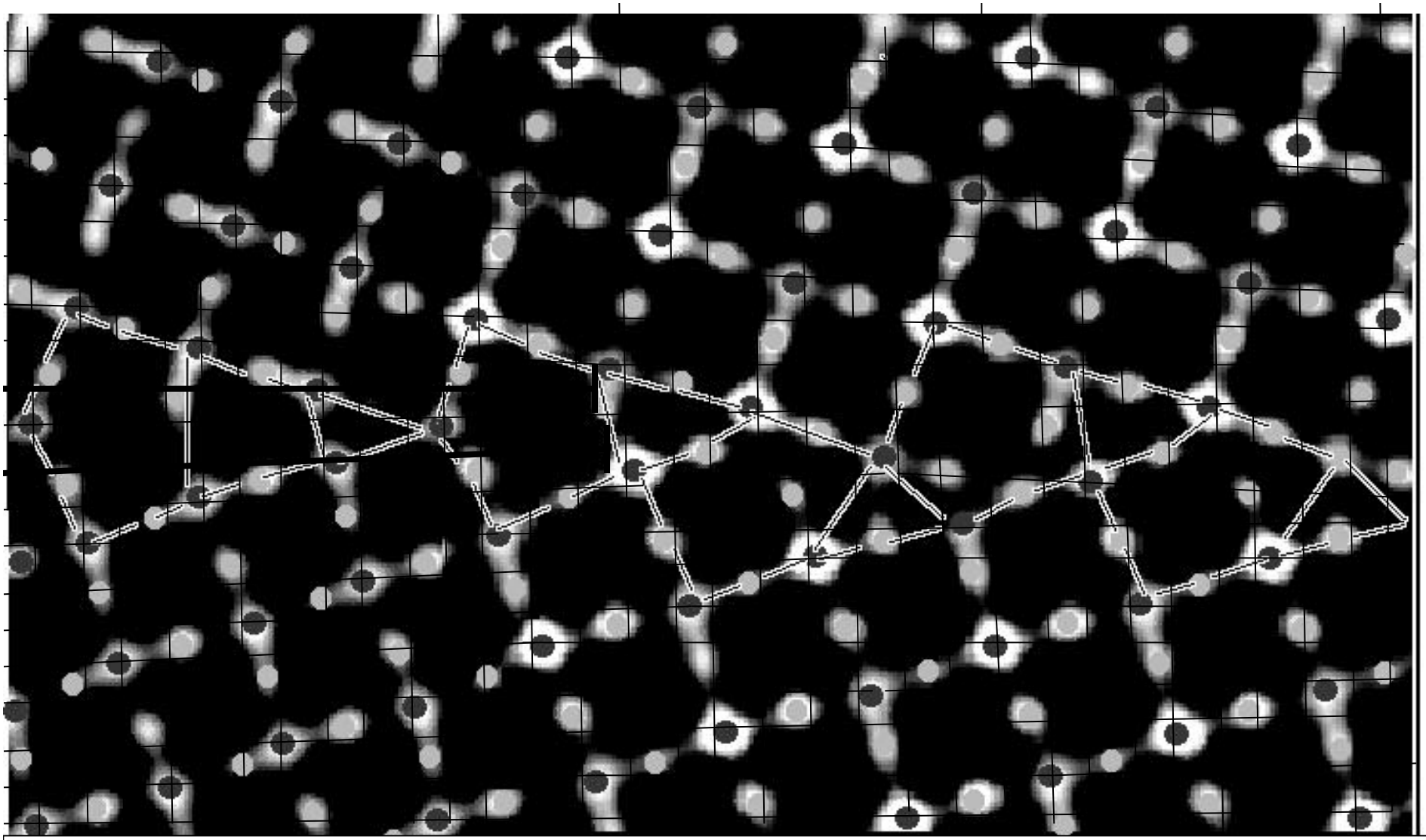
Symmetrical Segment
Asymmetrical Segment











DSC lattice---

Conclusions

- Sub-0.1nm resolution can be achieved from indirect microscopy method

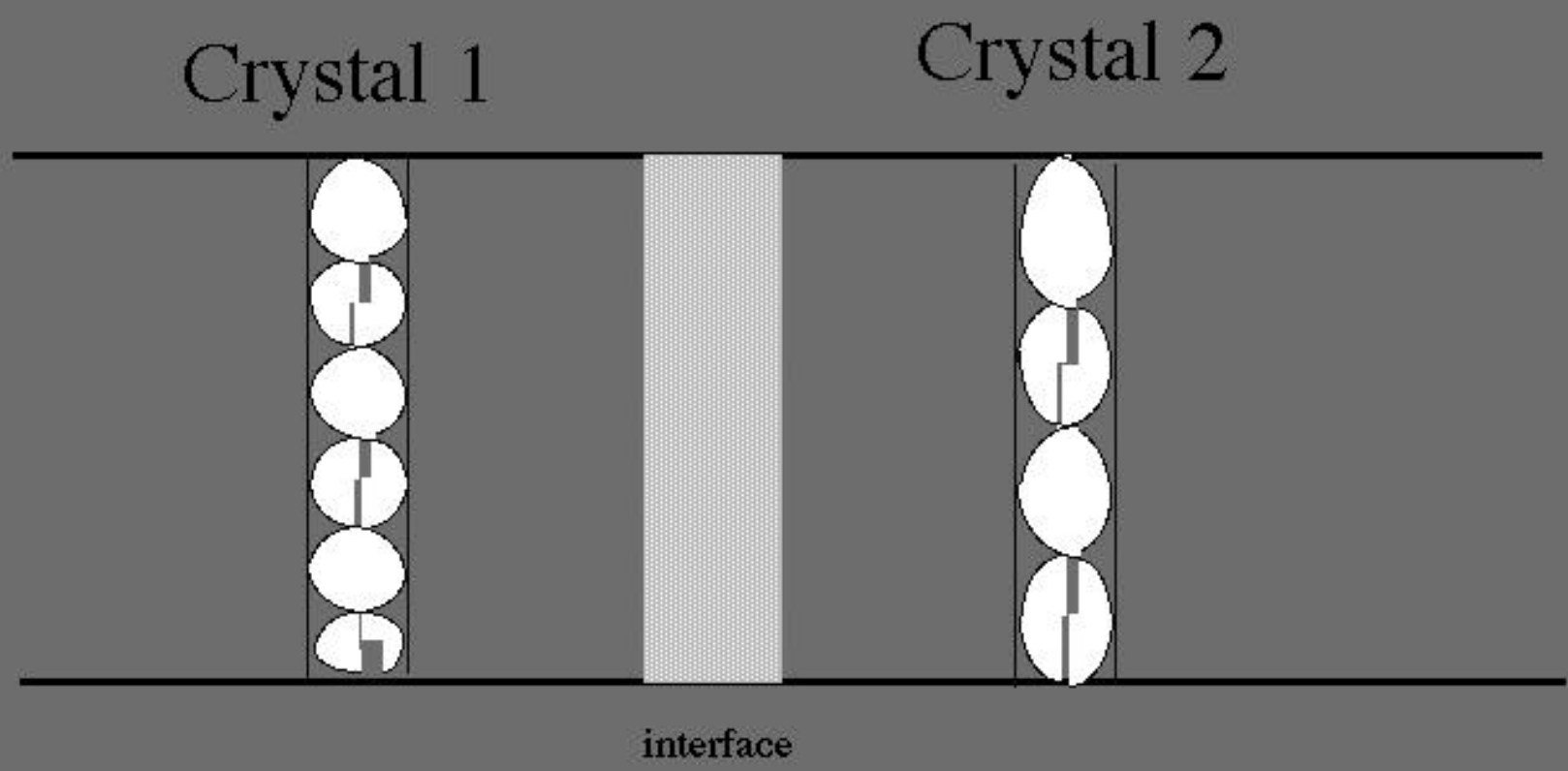
Problems remain unsolved:-

- Time costing
- the intensity of solution does not have simple relationship with atomic number
- Resolution ? Precision ?

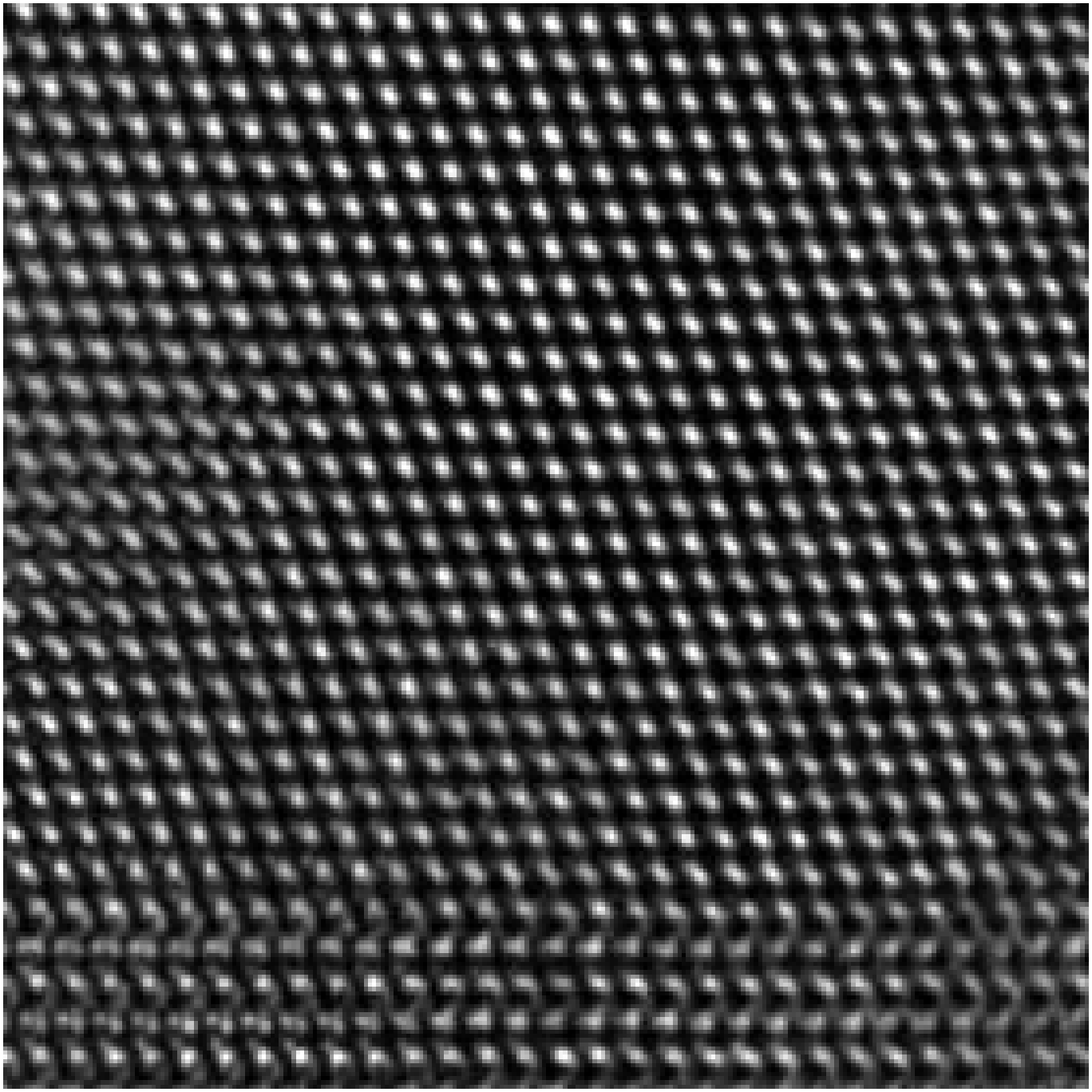
Current Work:

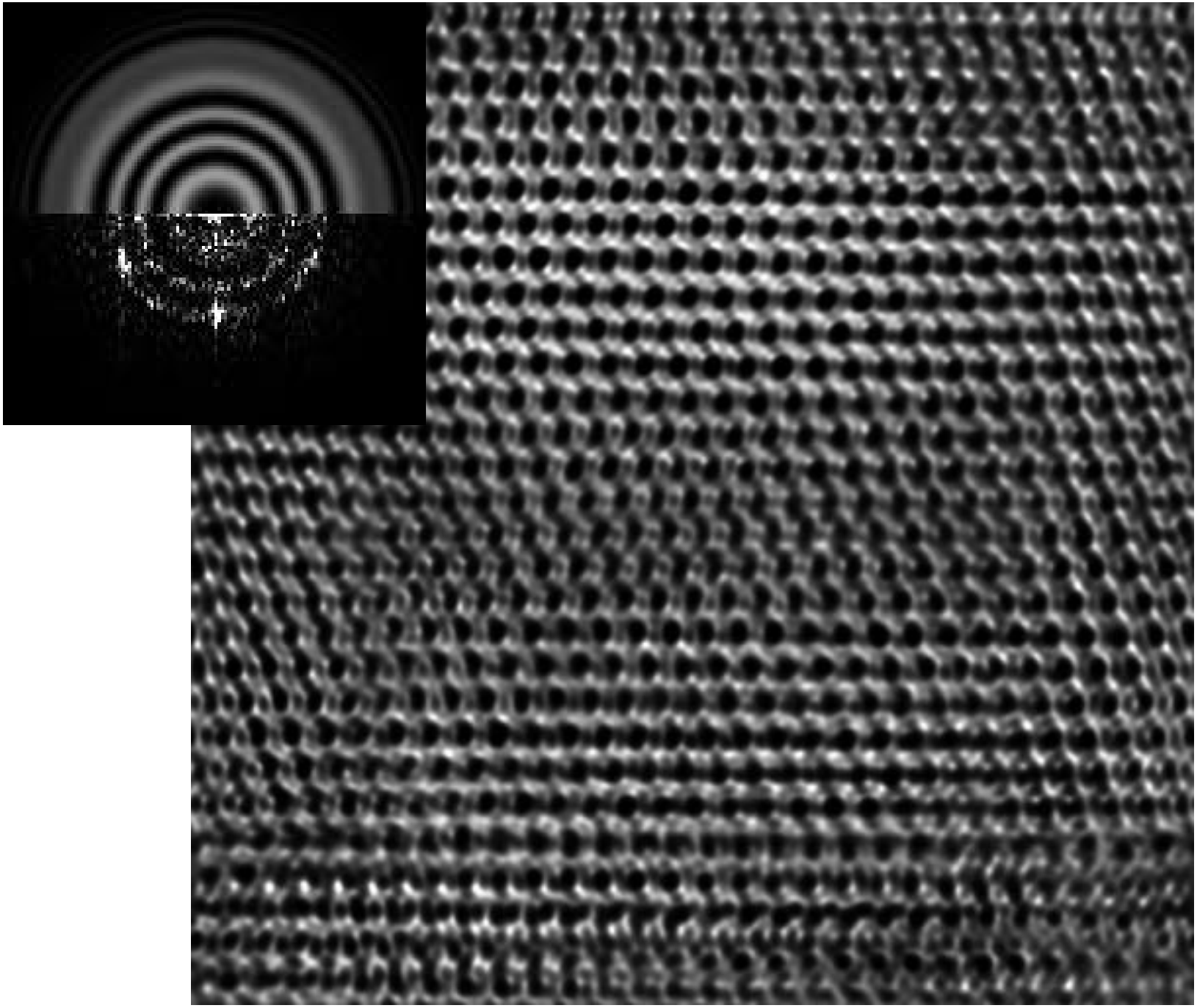
Possibility of automation

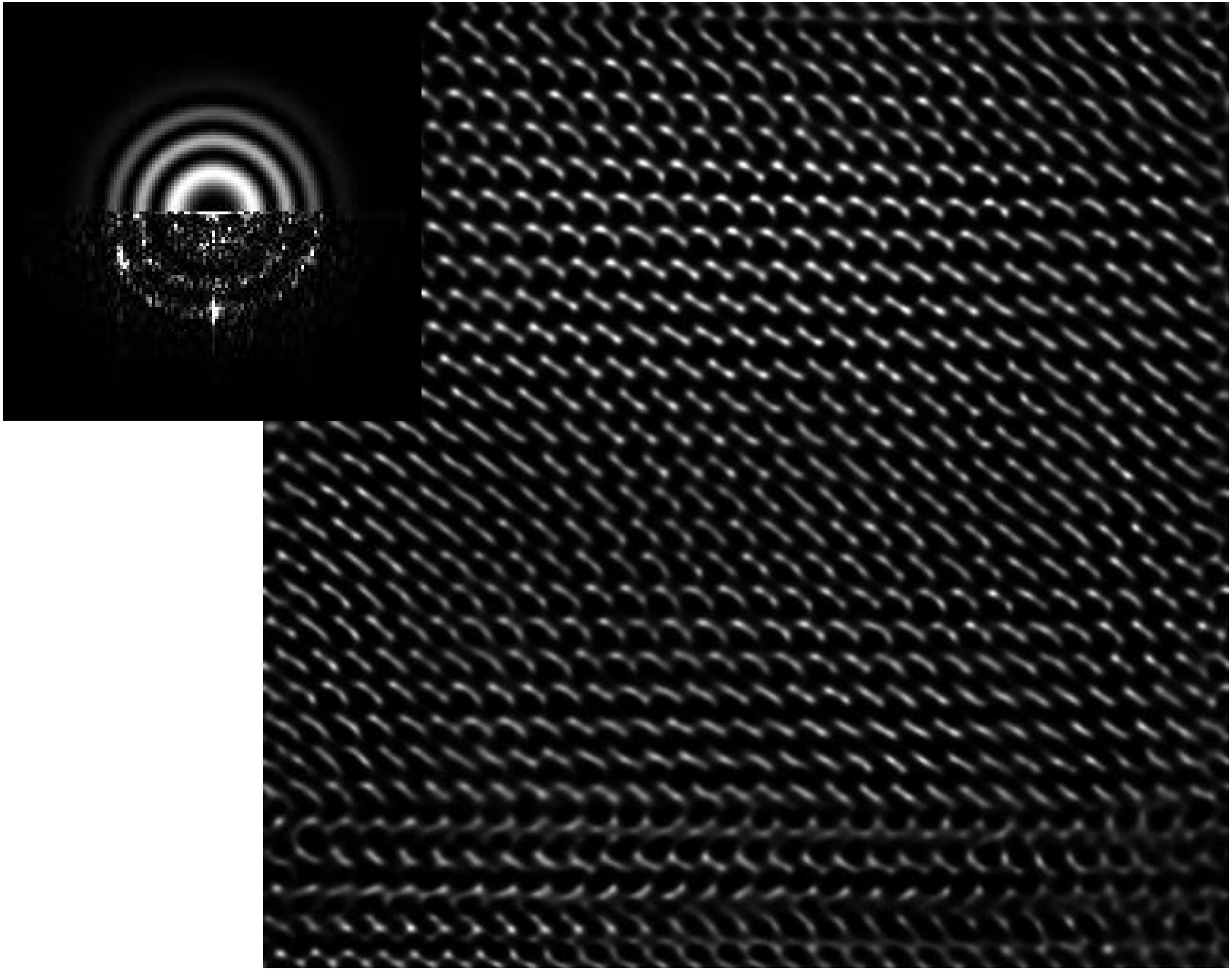
Schematic Representation of Electron Channeling



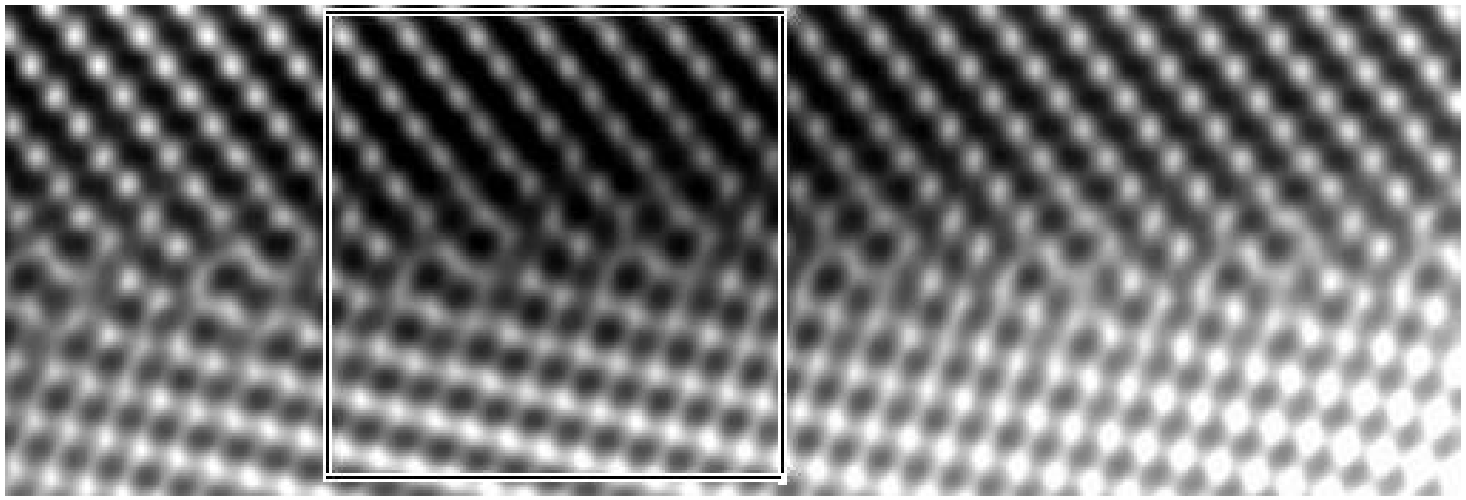
Van Dyck & Op deBeek(1996), Ultramicroscopy,64, 99-107



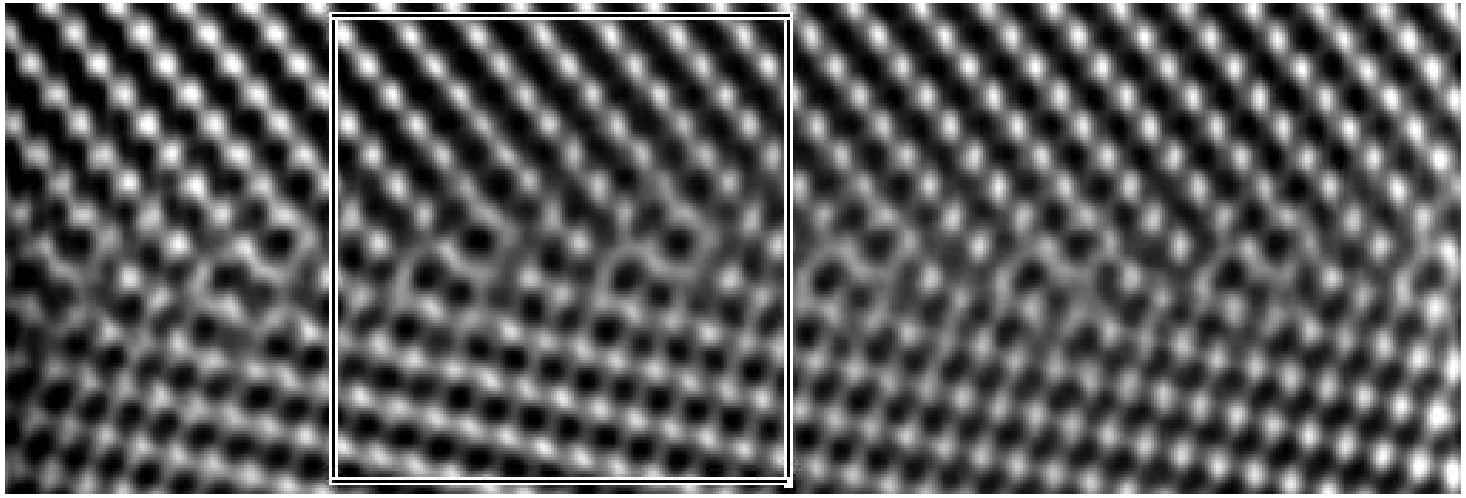




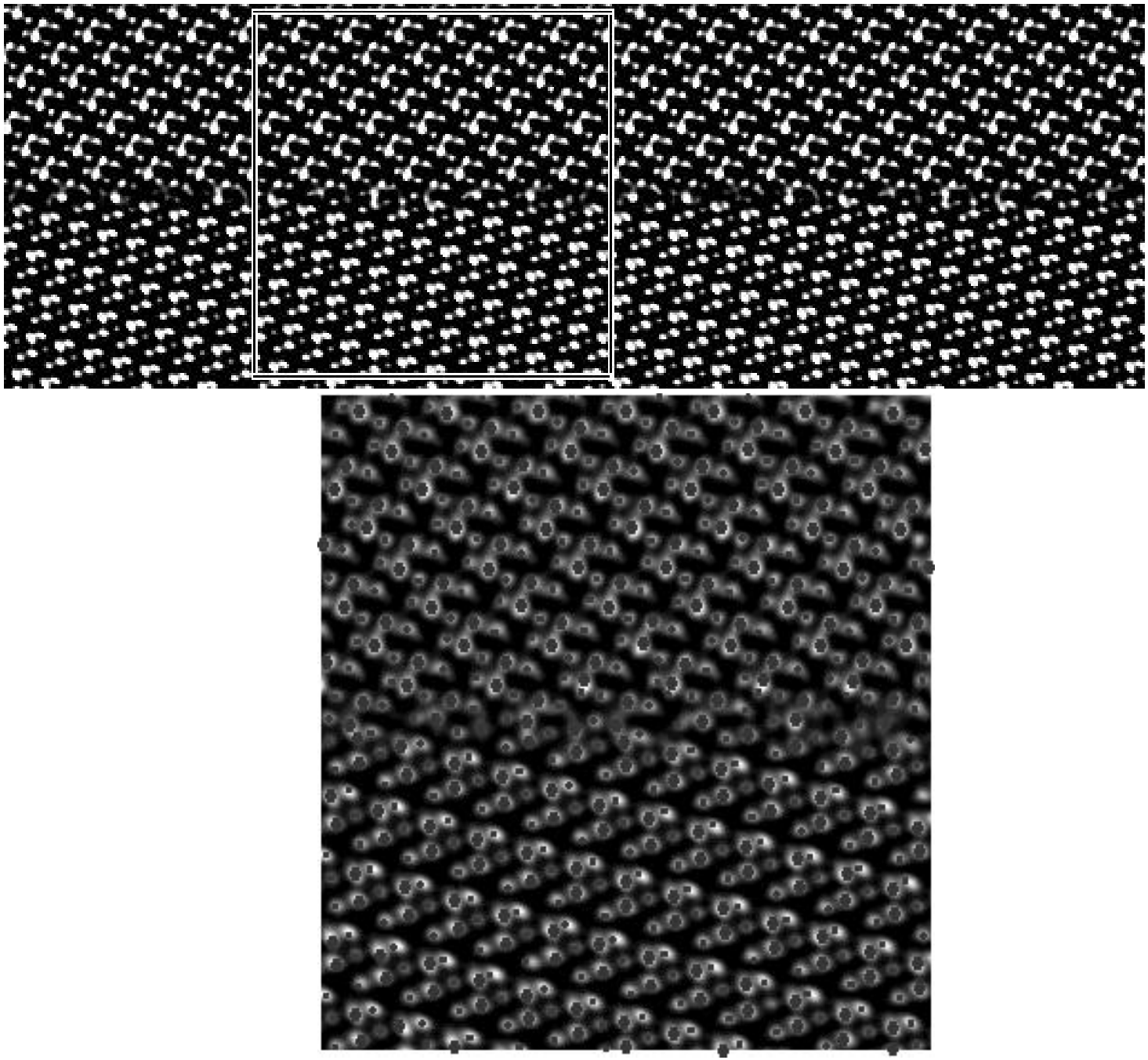
Al_2O_3 Σ=11 $(01\bar{1}1)/(01\bar{1}\bar{1})$



Experimental Image

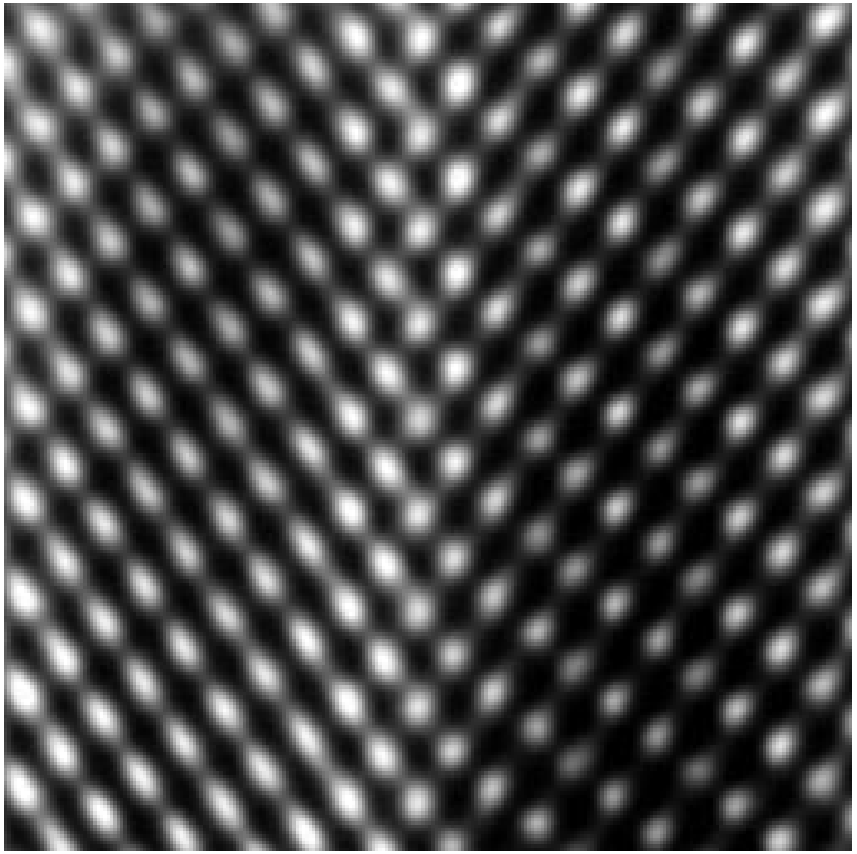


Predicted Image

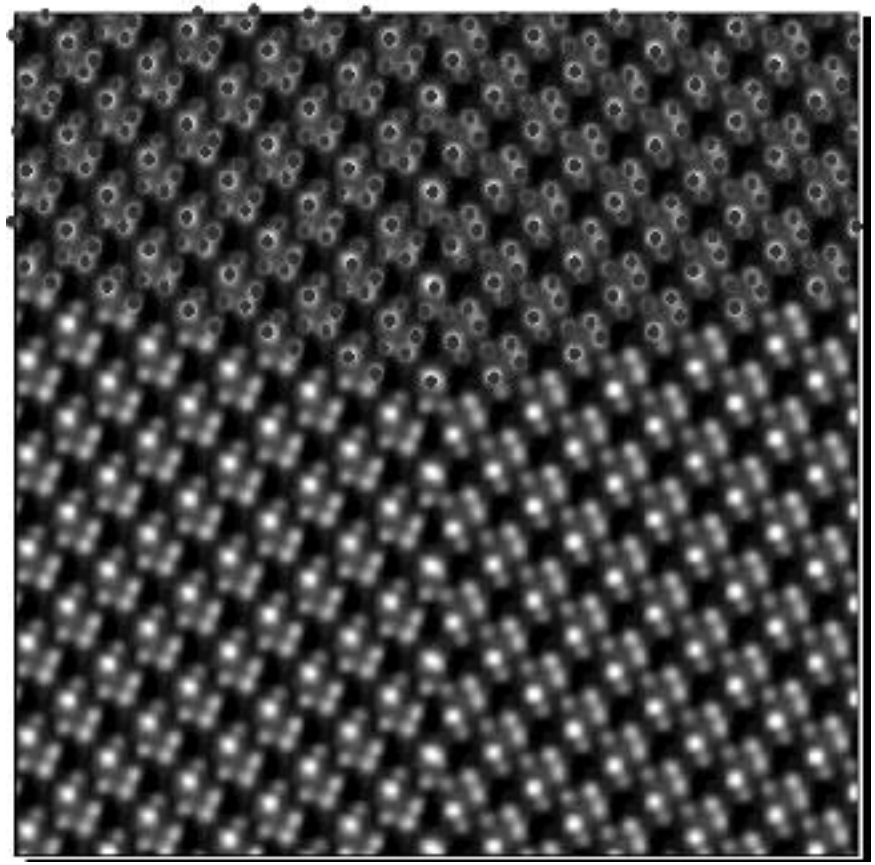


MEM image

Al_2O_3 Σ=11 $(01\bar{1}1)/(01\bar{1}1)$

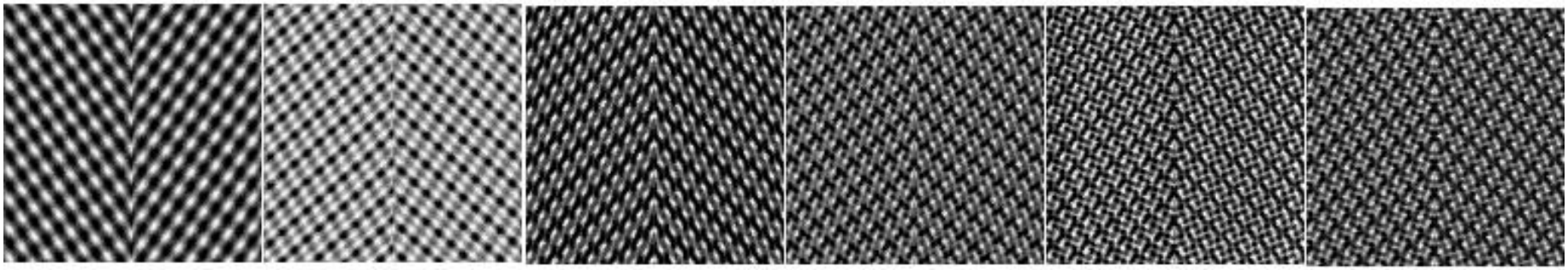


Experimental Image

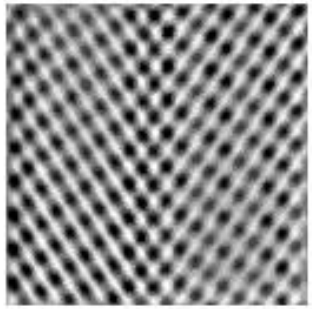


MEM image

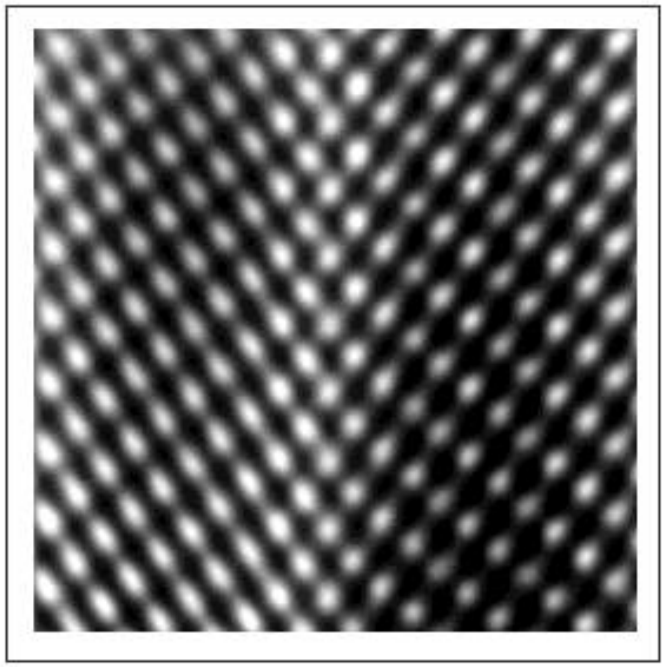
Resolution Extension for Σ11 Grain Boundary of Al_2O_3



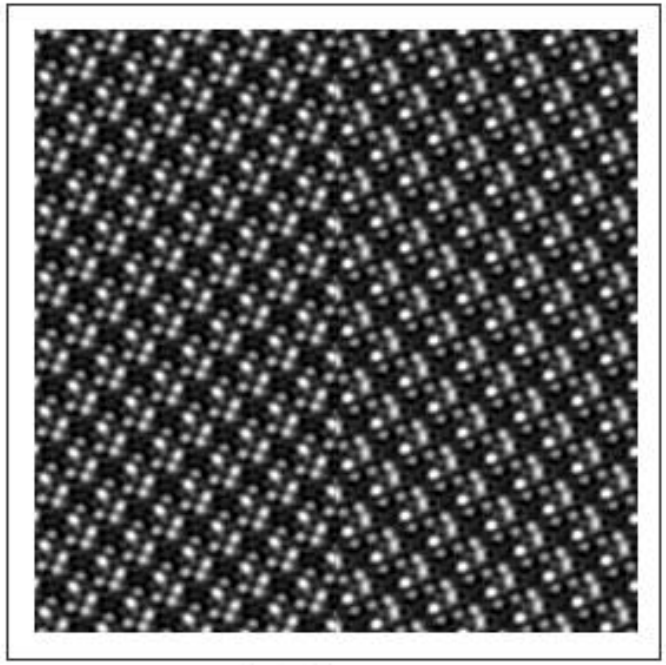
0.18 nm ($5.5\ nm^{-1}$) | 0.15 nm ($6.5\ nm^{-1}$) | 0.14nm ($7.5\ nm^{-1}$) | 0.12nm ($8.5\ nm^{-1}$) | 0.11nm ($9.5\ nm^{-1}$) | 0.086nm ($11.5\ nm^{-1}$)



Wiener Filtered Image



Experimental Image



0.083 nm ($13.5\ nm^{-1}$)