Coherent X-ray Diffraction on Quantum Dots

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Or Coming Back to Crystallography

Participants of the Project

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CONTENTS

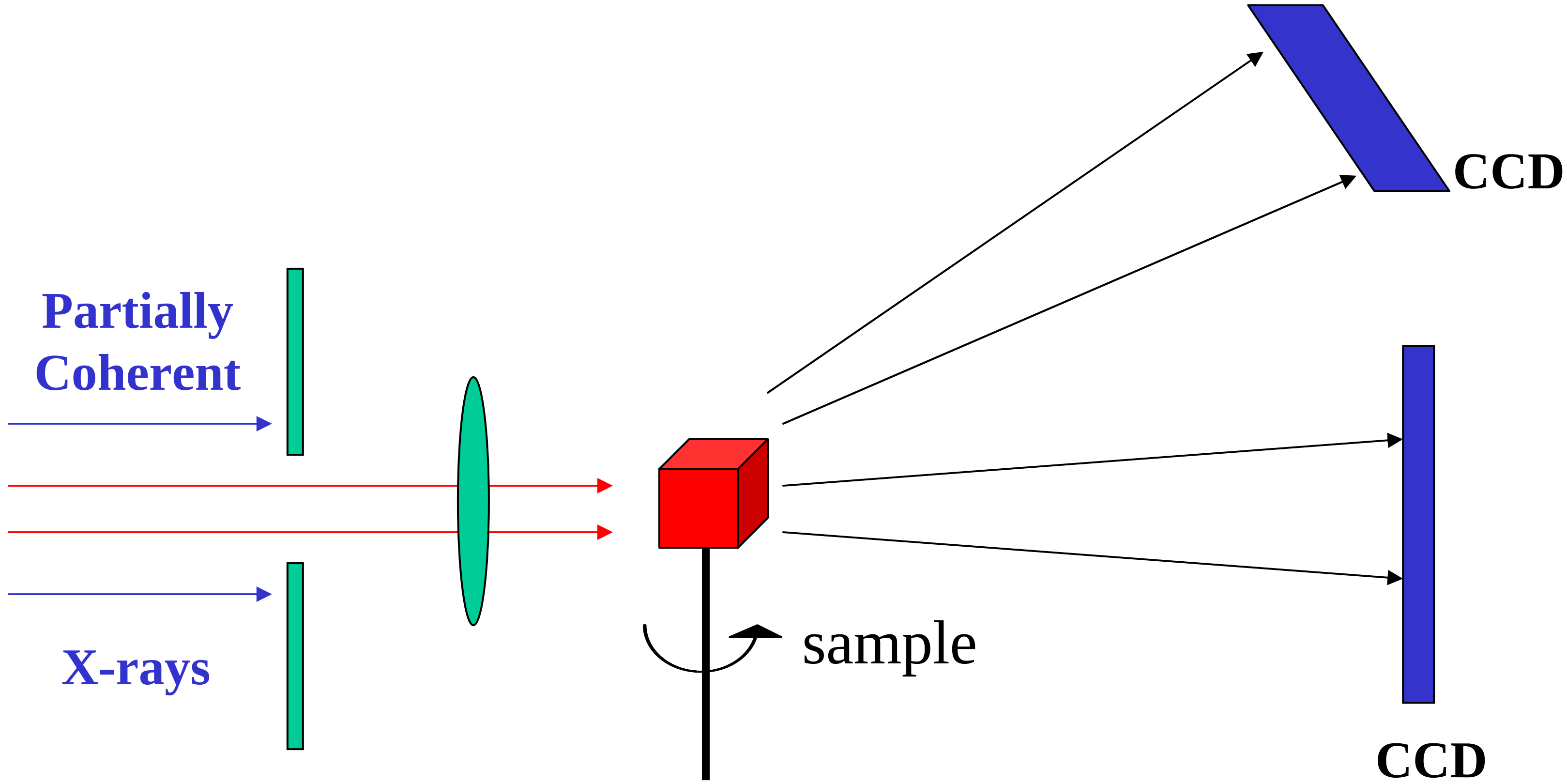
Motivations

1. **Electronic and optical properties of nano-devices depend on the structure (shape and strain)**
2. **Development of different scattering methods for imaging nano-structures is extremely important**

Imaging

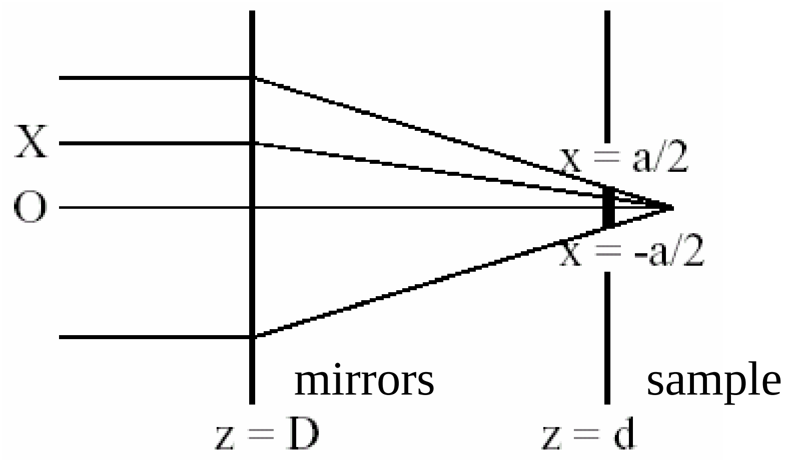
Can we compete with electron microscopy?

Coherent X-ray Diffraction or X-ray Lensless Microscopy



First approach: **Focusing Optics**

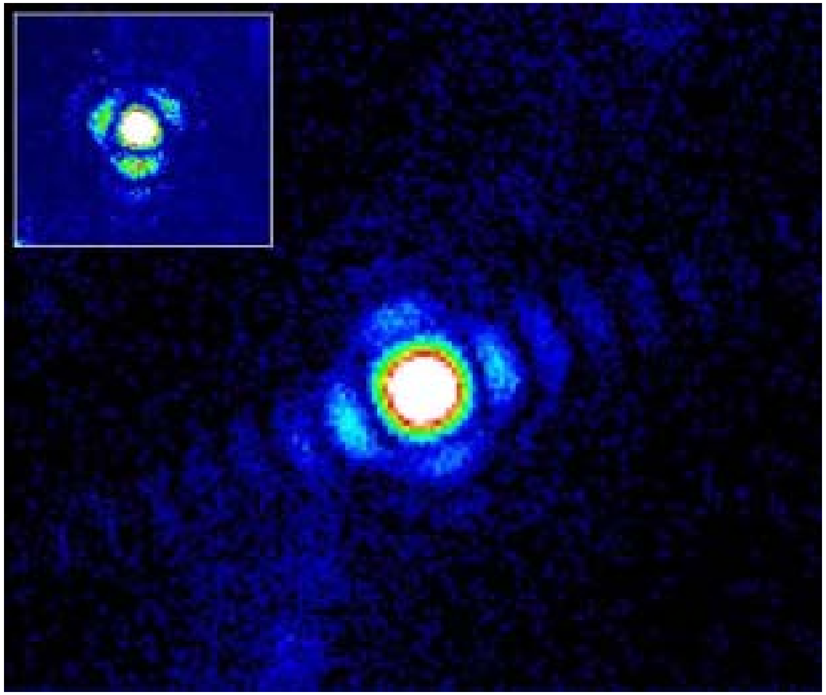
Focusing Optics
KB mirrors



100(V) × 200(H) mm

Focal spot size
1.5(H)×1.0(V) μm

Robinson *et.al.*, (2003)
Optics Express, 11, 2329



Coherent X-ray Diffraction
pattern from Ag nanocrystals
of size D=170 nm

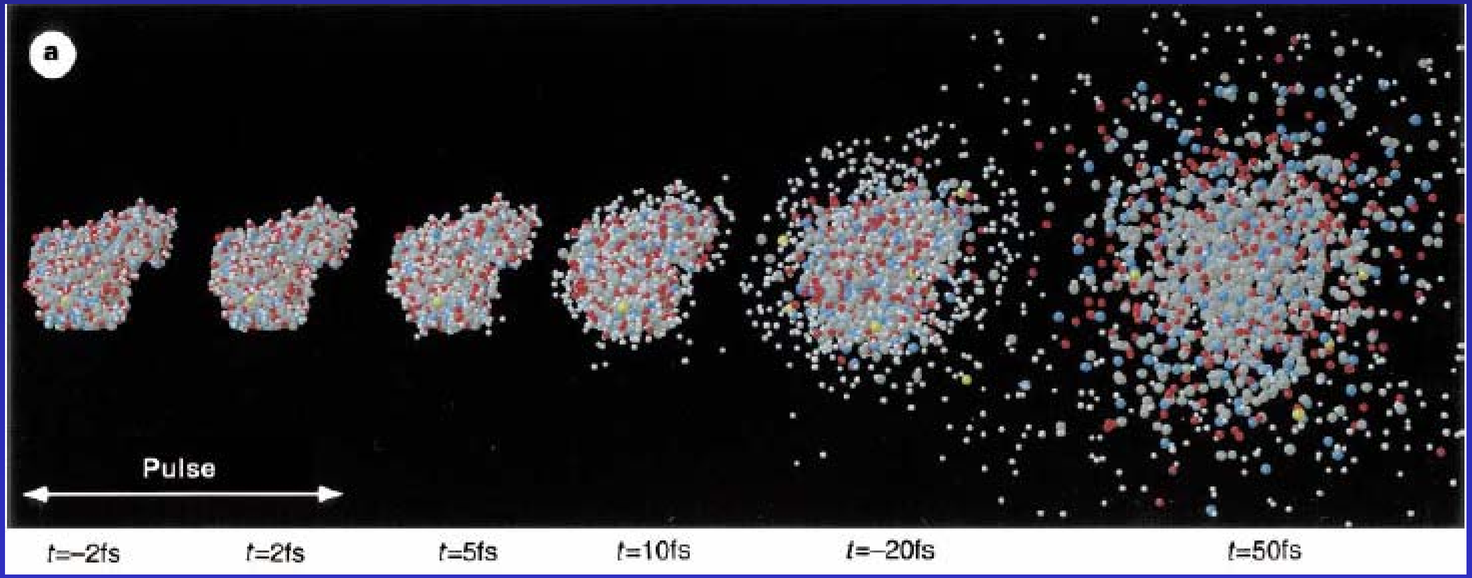
Alternative Approach: Using Periodic Array of Quantum Dots

Motivations:

Using a periodic patterned array for bio-molecules imaging

I. Vartanyants & I. Robinson, J. Synchrotr. Rad. (2003), 10, 409

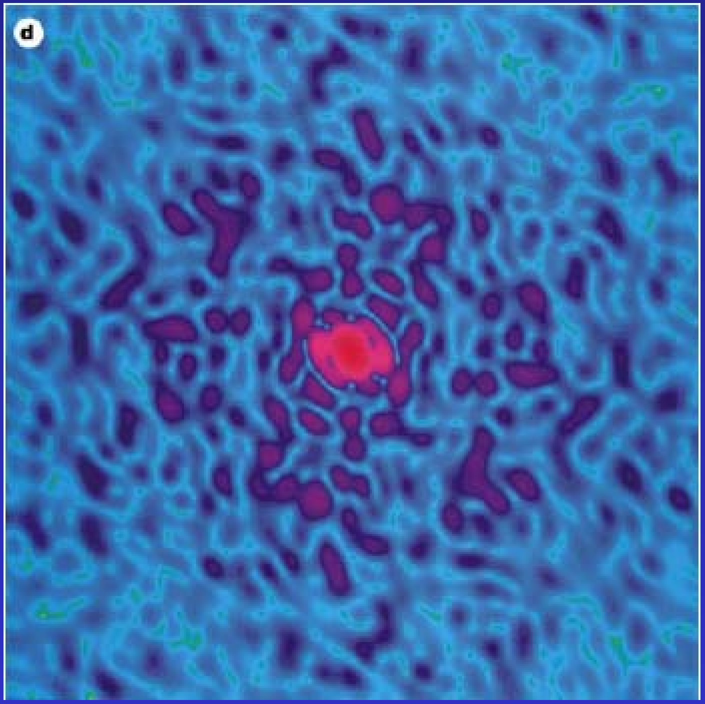
Imaging of biomolecules with femtosecond X-ray pulses



Explosion of T4 lysozyme induced by radiation damage

R. Neutze, *et al.*, Nature (2000) 406, 752

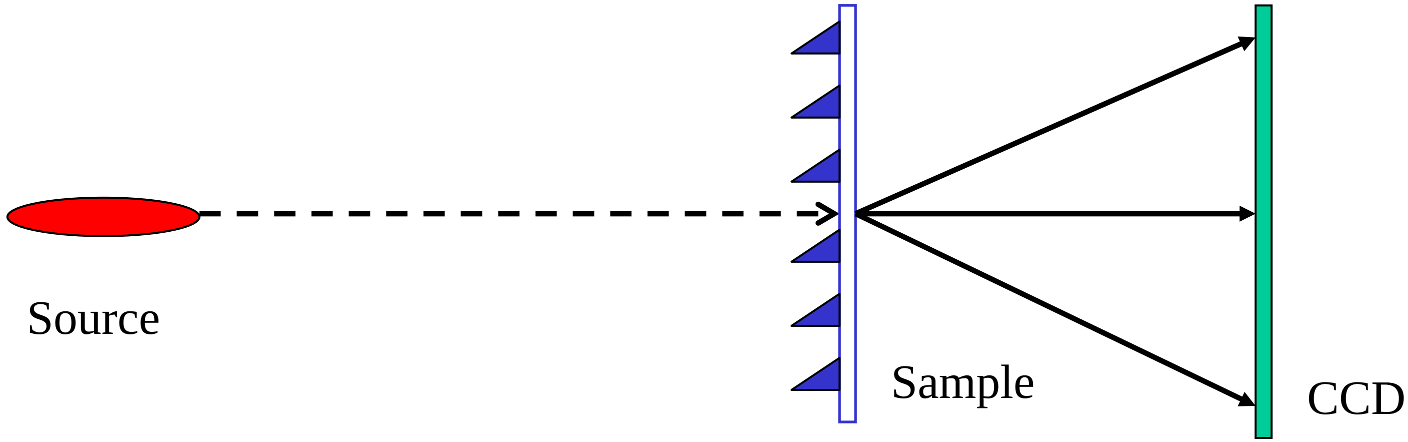
Imaging of Biomolecules with Femtosecond X-ray Pulses



Simulated continuous scattering image of a single T4 lysozyme molecule under ideal conditions without sample
movement or damage.

R. Neutze, *et al.*, Nature (2000) 406, 752

Imaging of Quantum Dots with Coherent Beams



$$\boxed{p(\mathbf{r}) = S(\mathbf{r})\cdot\left[s_z(\mathbf{r})\otimes p_\infty(\mathbf{r})\right]}$$

Electron density of periodic array of QD's

S(**r**) – shape of coherently illuminated area

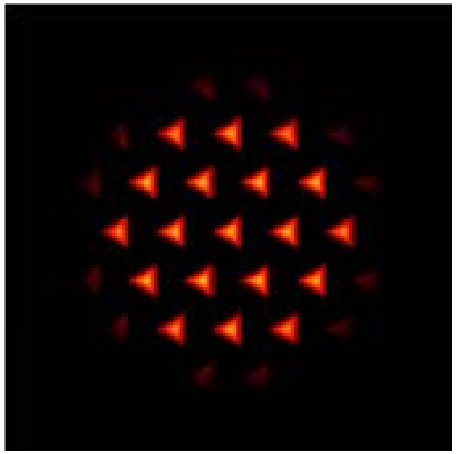
s_z(**r**) –projection of shape of one island s(**r,**z)

$$p_\infty(\mathbf{r}) = \sum_n \delta(\mathbf{r}-\mathbf{r}_n)$$

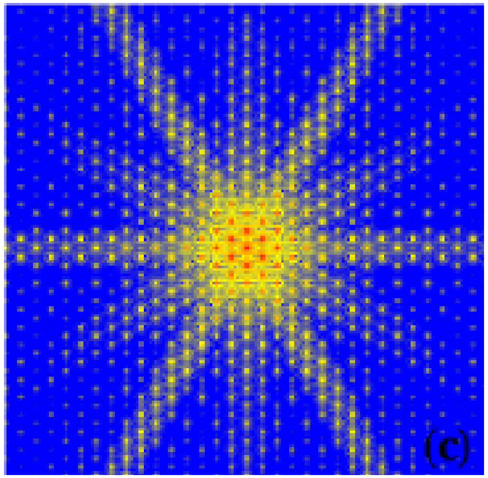
Diffracted intensity:

$$\boxed{I_{coh}(q) = \left|A_{coh}(q)\right|^2 = \sum_n \left|s_z(h_n)\right|^2 \left|S(q-h_n)\right|^2}$$

2D array of QD's and it's diffraction pattern



2D array of QD's



Diffraction pattern of 2D array

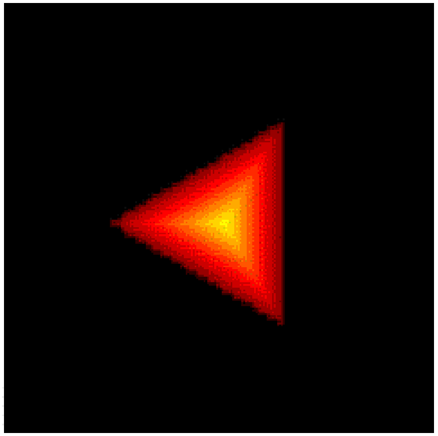
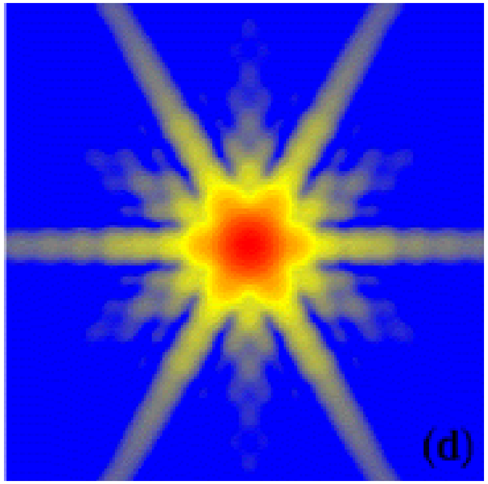
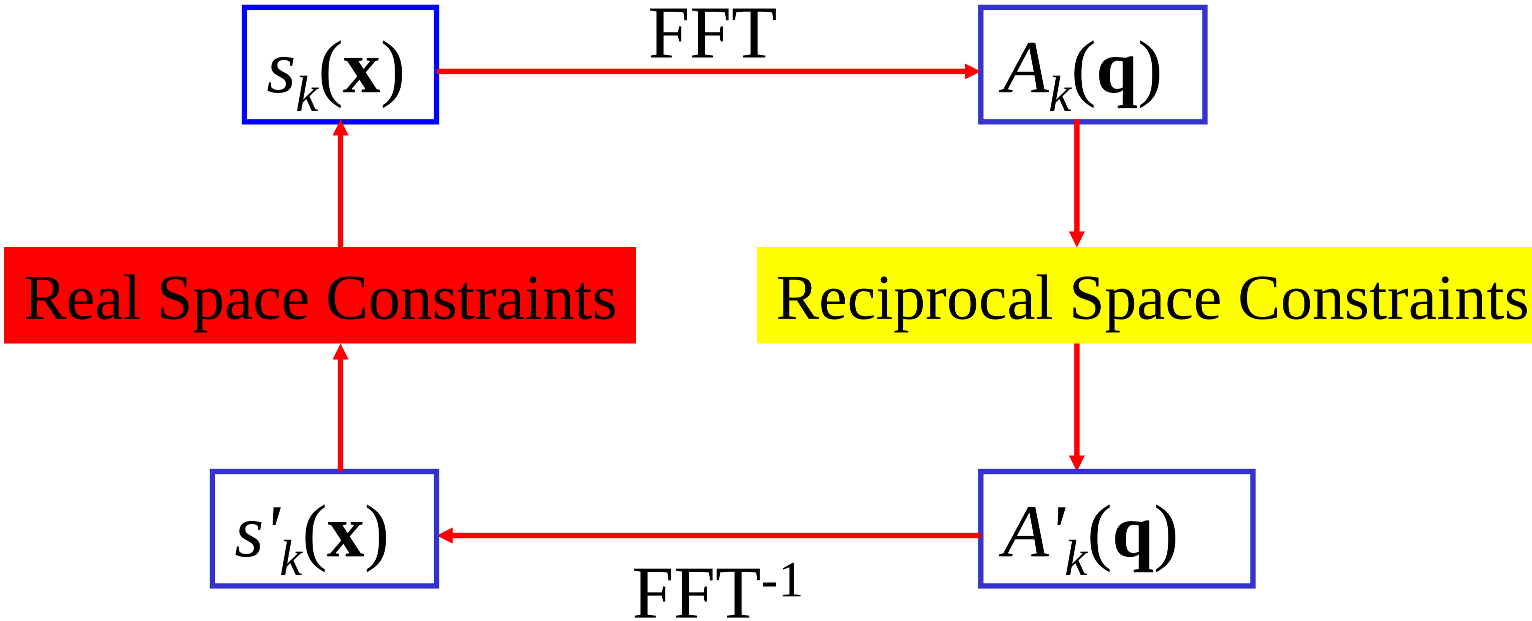


Image of individual island



Diffraction pattern of individual island

Iterative phase retrieval algorithm



Real space constraints:

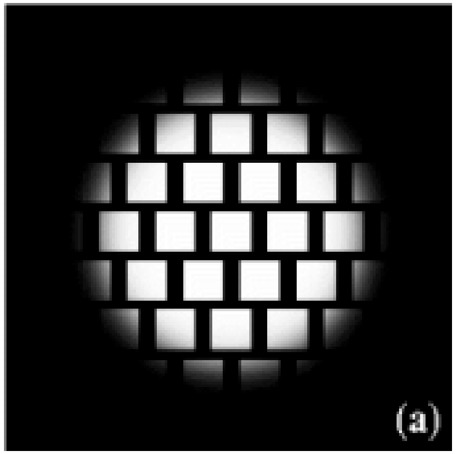
- finite support
- real, positive

Reciprocal space constraint:

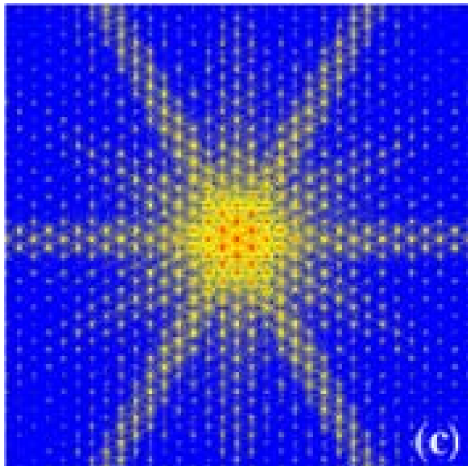
$$\left|A_k(\mathbf{q})\right| \rightarrow \sqrt{I_{exp}(\mathbf{q})}$$

J.R. Fienup, *Appl Opt.* (1982). **21**, 2758
R.P. Millane & W.J. Stroud, *J. Opt. Soc. Am.* (1997) **A14**, 568

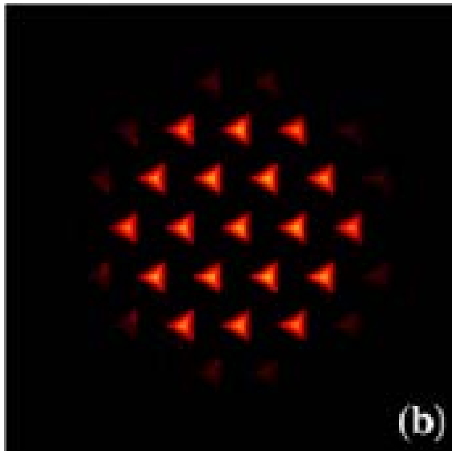
Reconstructed image of 2D array of QD's



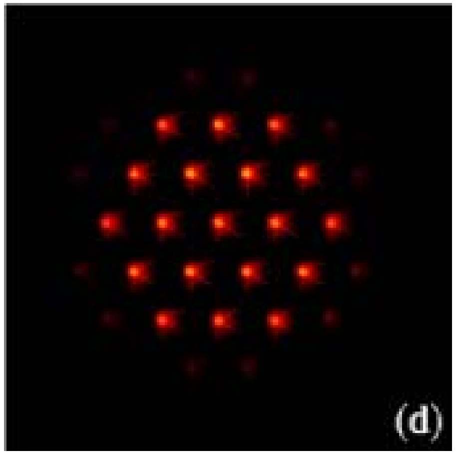
Support used for reconstruction



Diffraction intensity of reconstructed image



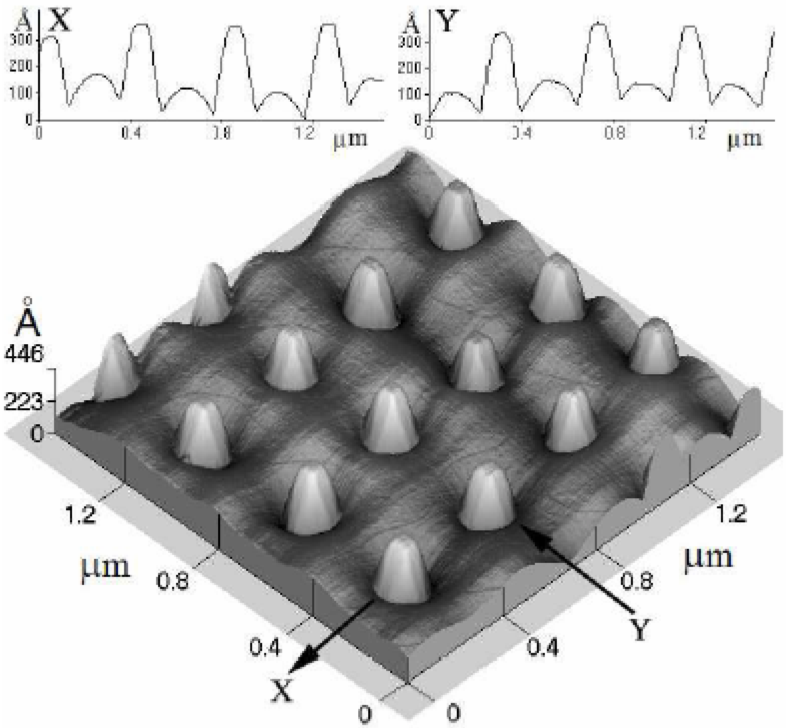
Reconstructed image



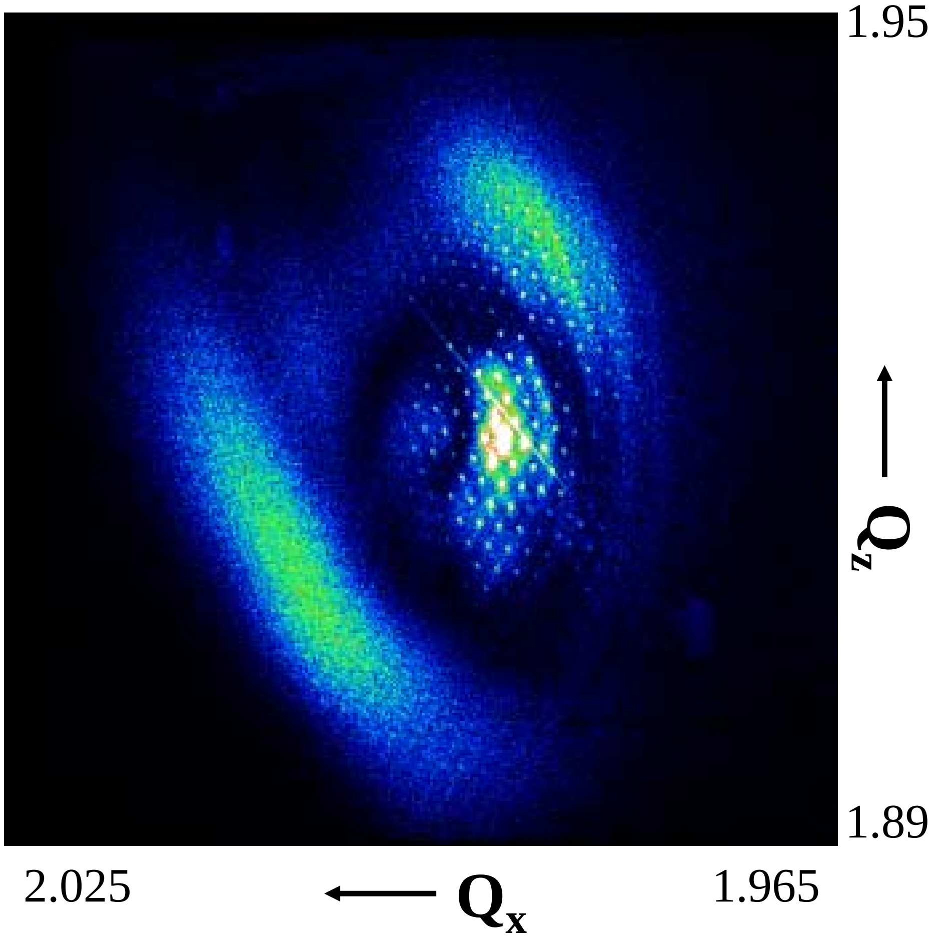
Reconstructed image with
superposition of twin images

Experiment

Experiment (Sector 34 APS)



AFM image of 2D ordered Ge islands with corresponding line scans

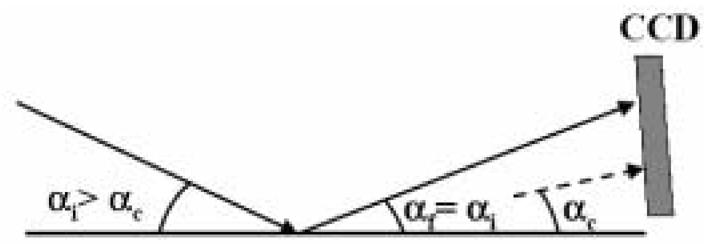


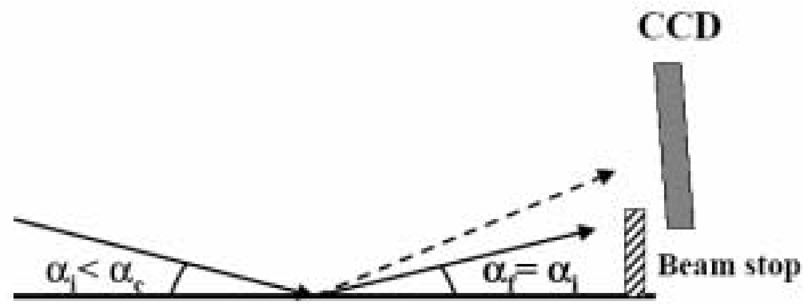
Diffraction pattern around Ge (202) peak

Z. Zhong & G. Bauer

I. Vartaniants *et. al.*, PRB **71**, 245302 (2005)

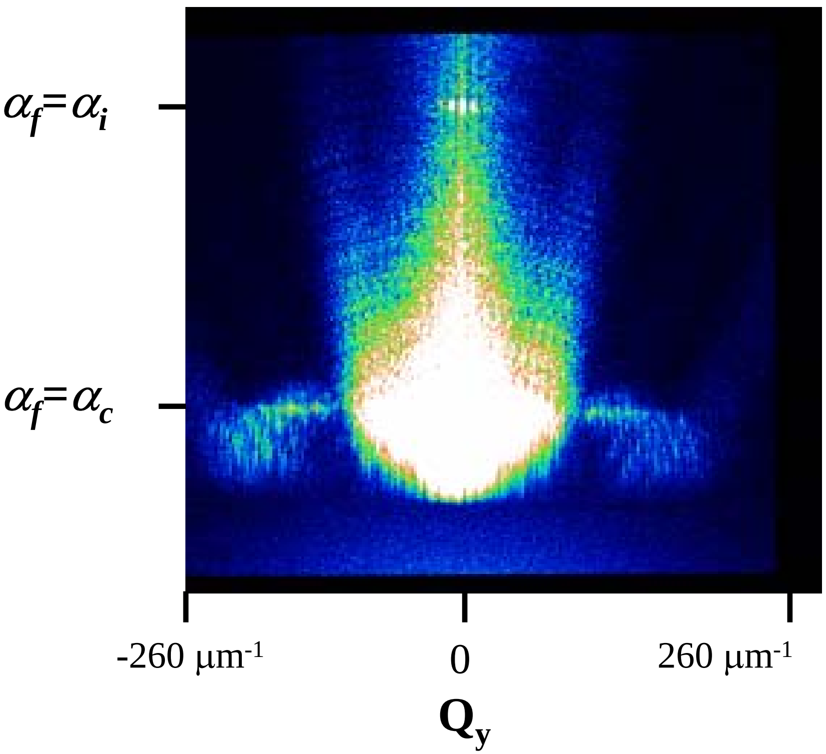
GISAXS measurements

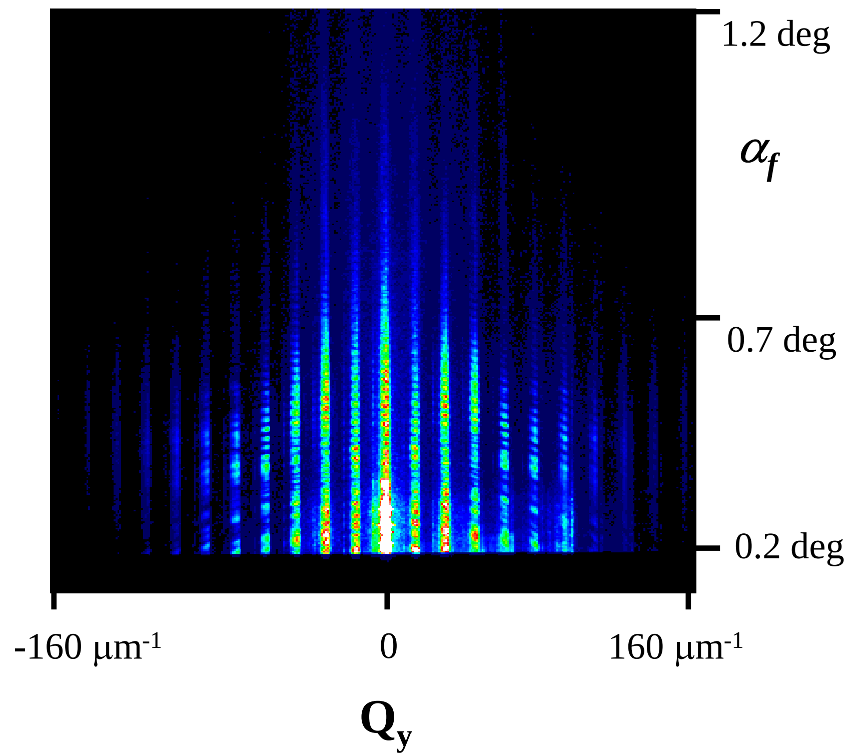




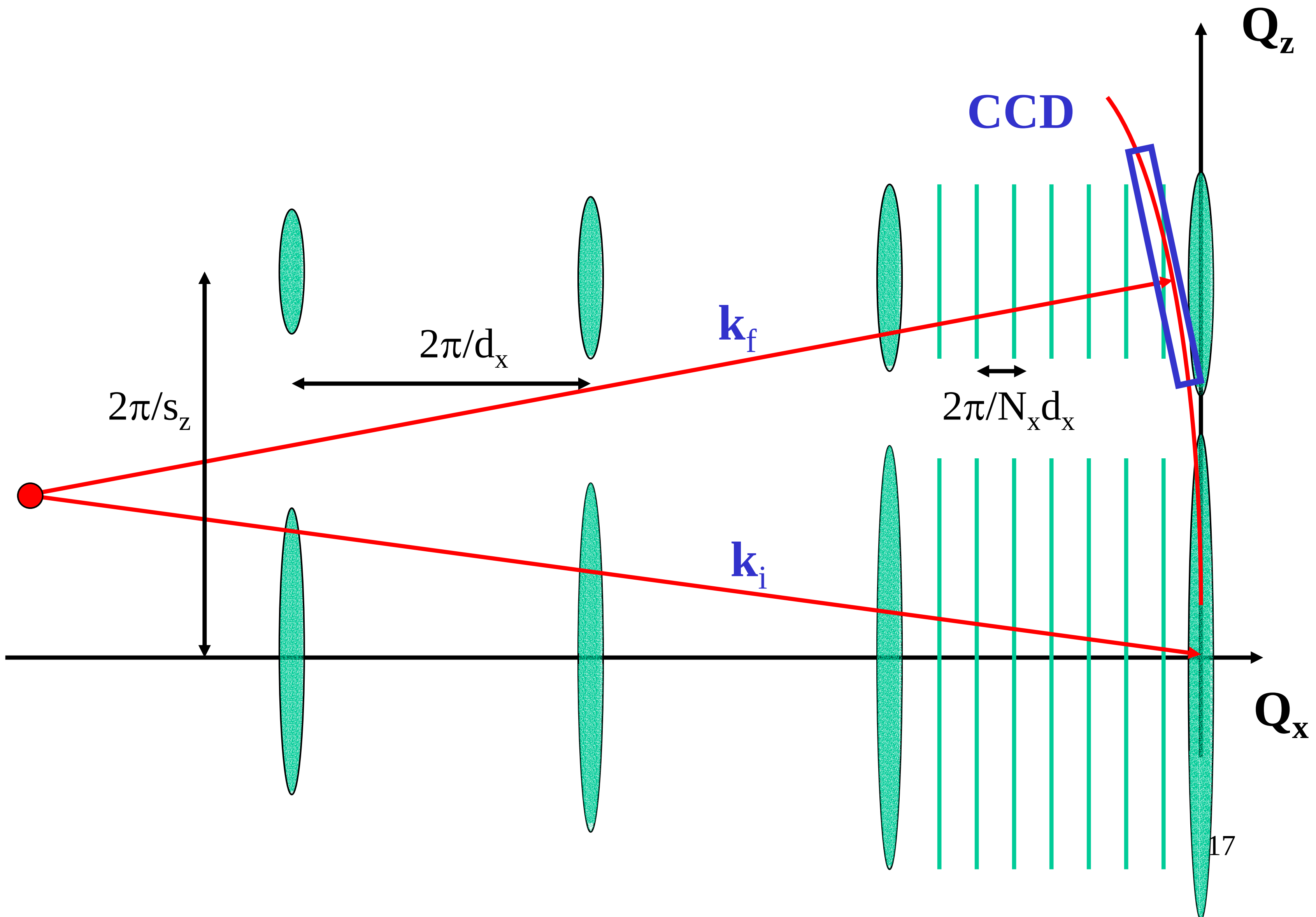
$\alpha_i > \alpha_c\,; \;\; \alpha_f < \alpha_i$

$\alpha_i < \alpha_c; \;\; \alpha_f > \alpha_i$



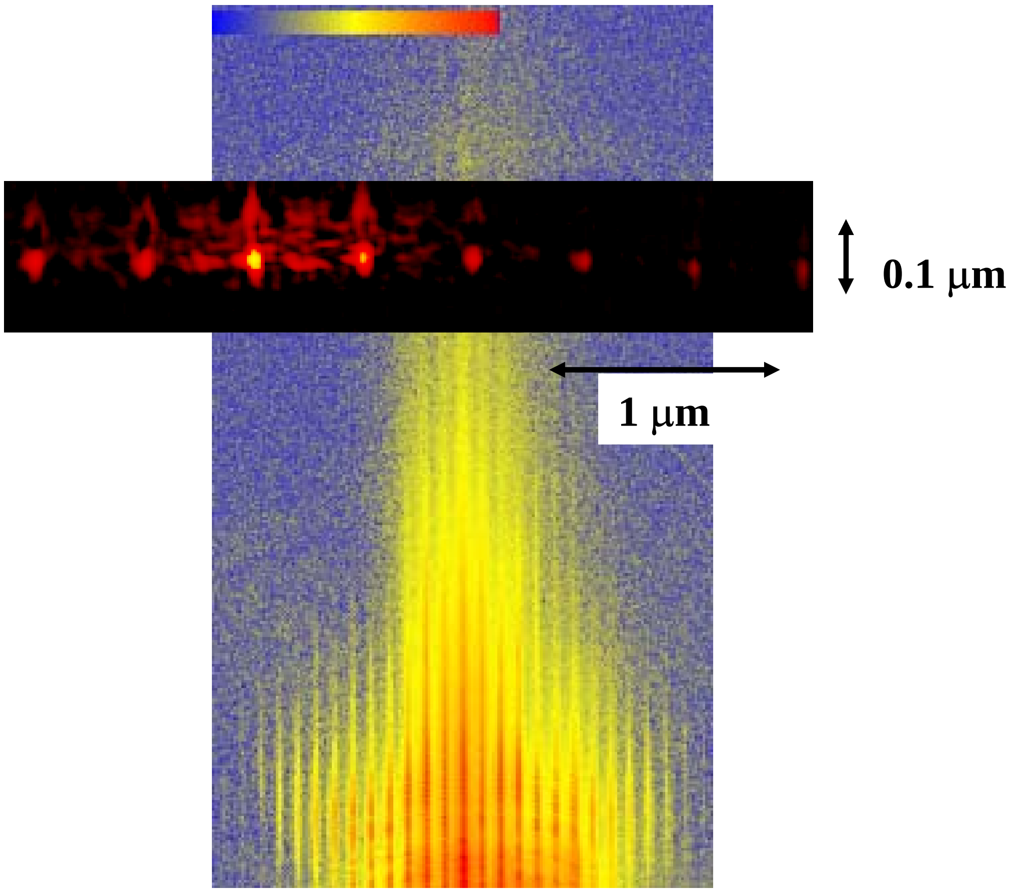


Ewald sphere construction

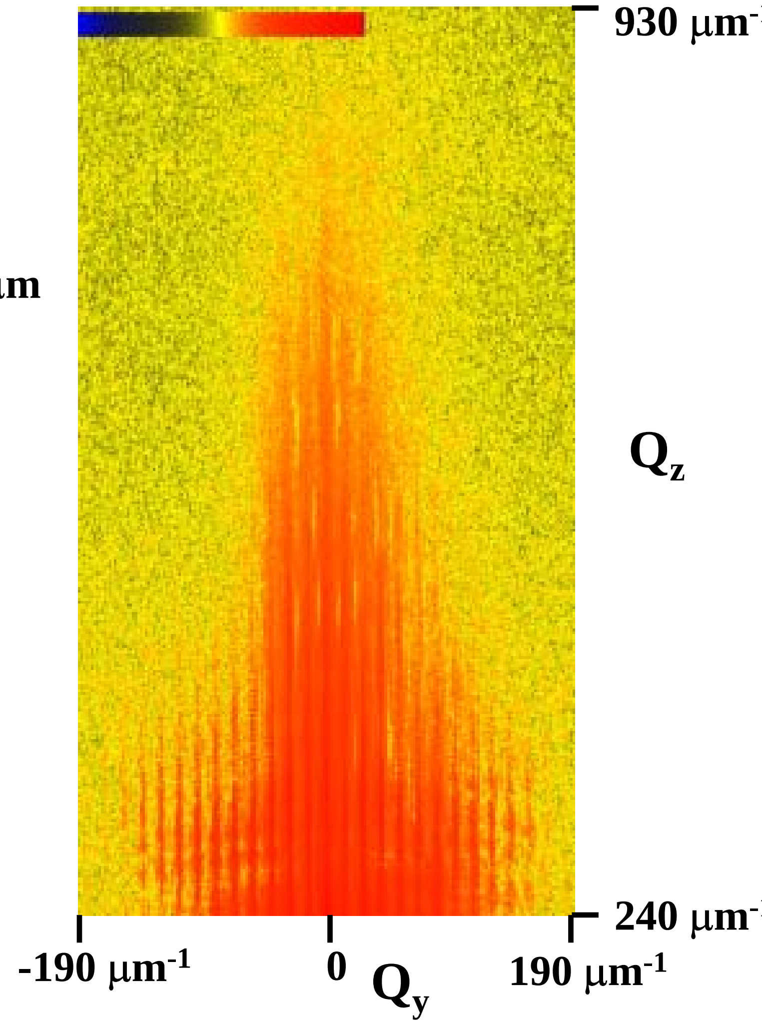


Reconstruction of quantum dot shape

GISAXS measurements ($\alpha_i < \alpha_c$)

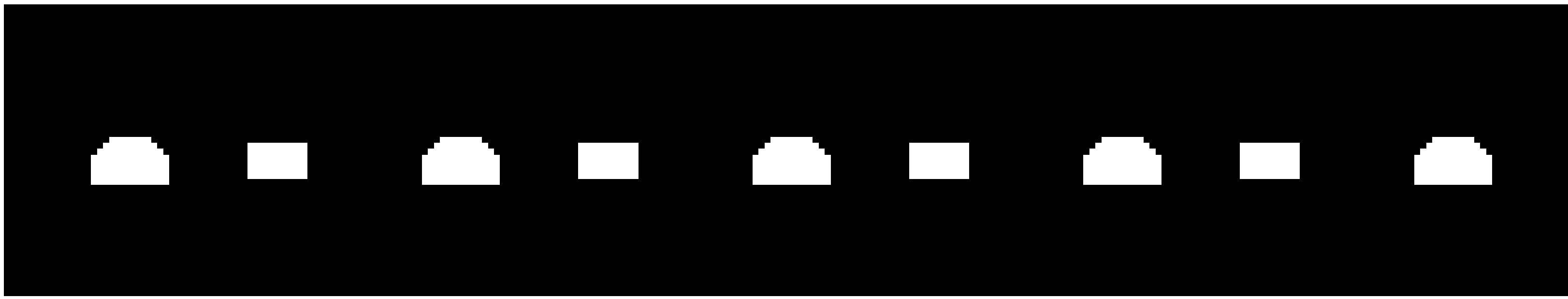


Experimental Data
(Log scale)

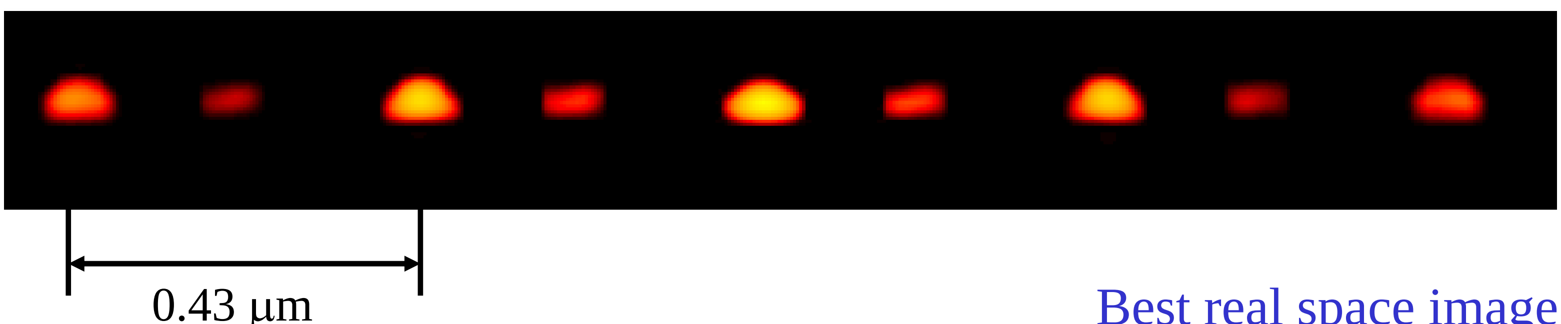


Reconstruction

Reconstruction of quantum dot shape
GISAXS measurements ($\alpha_i < \alpha_c$)



Final support



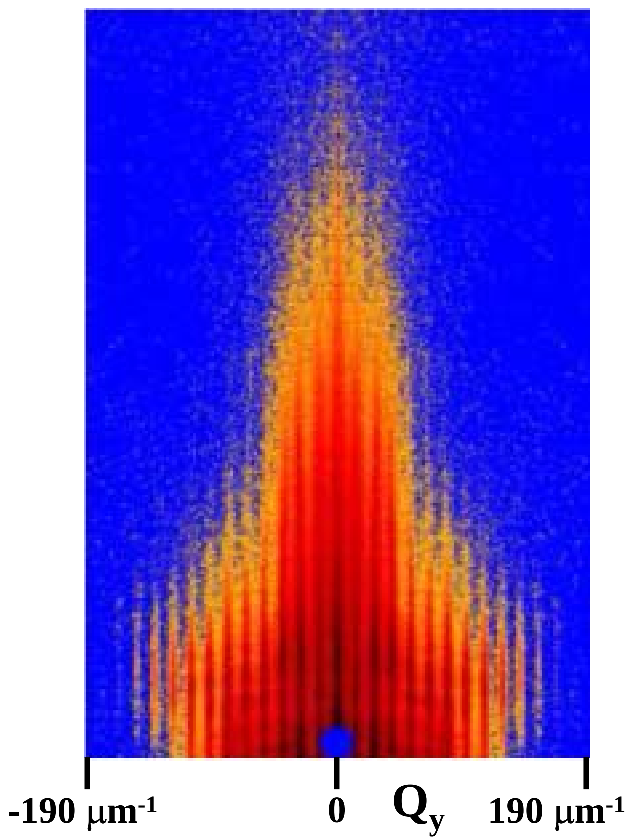
Best real space image

Comparable with resolution in electron microscopy

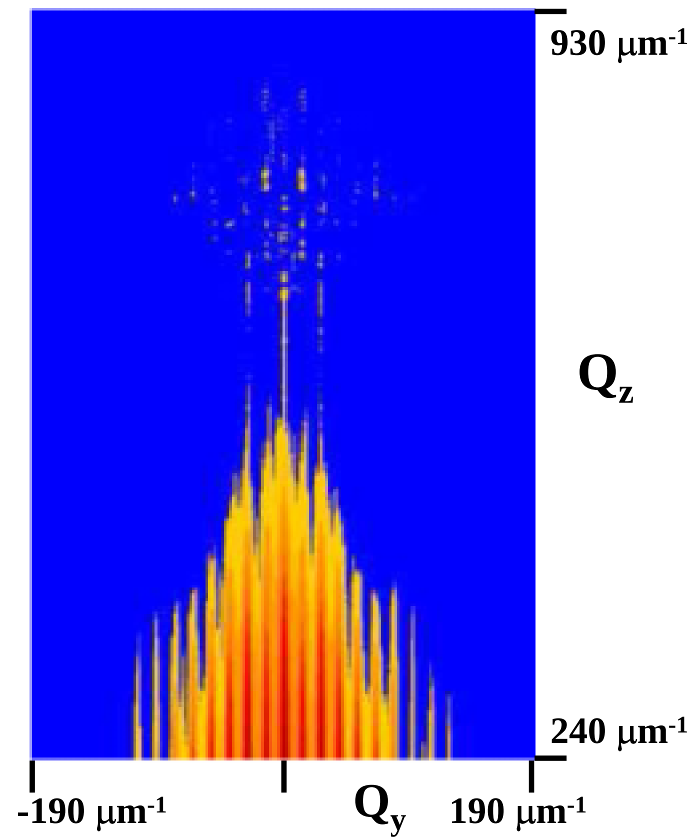
Average size: 128(H)×45(V) nm
Resolution: 20(H) ×5(V) nm

Reconstruction of quantum dot shape

GISAXS measurements ($\alpha_i < \alpha_c$)



Experimental Data
(Log scale)

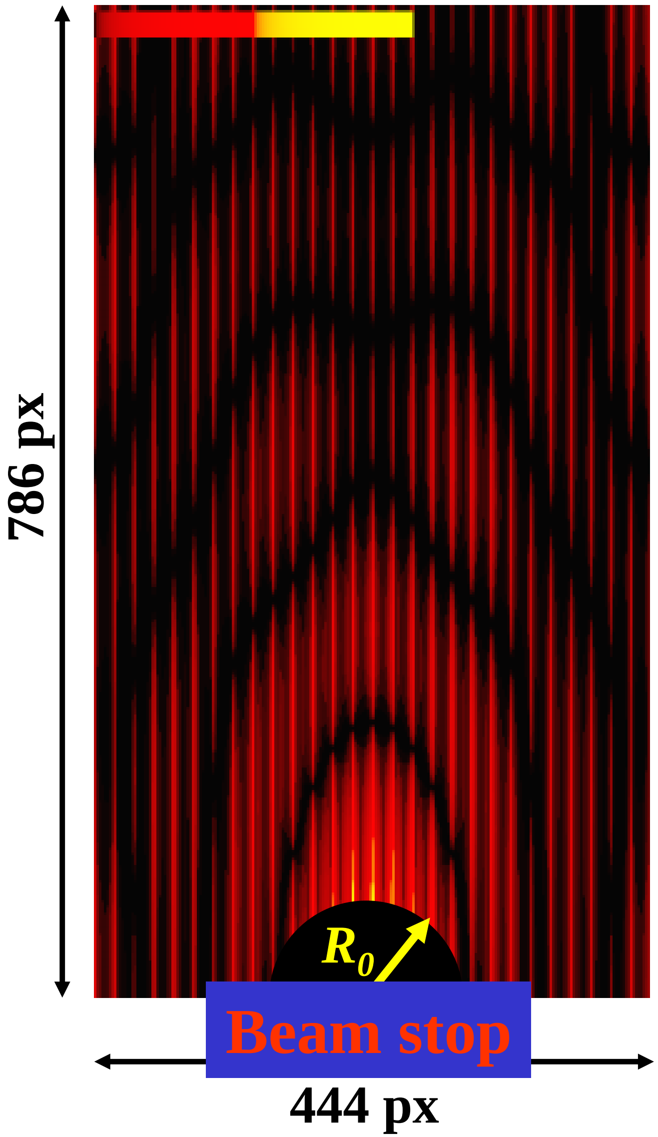


Reconstruction

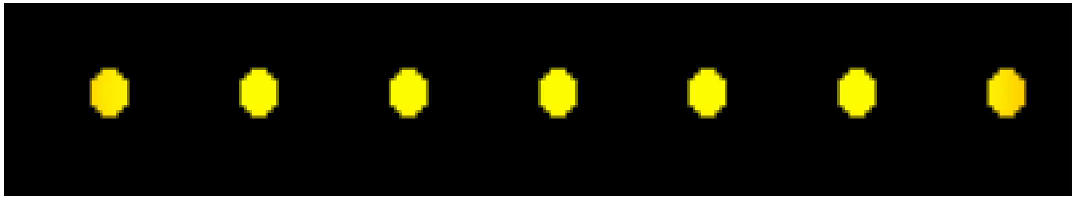
Questions
Problems
Future Directions

Simulation of diffraction pattern

Beam stop effects

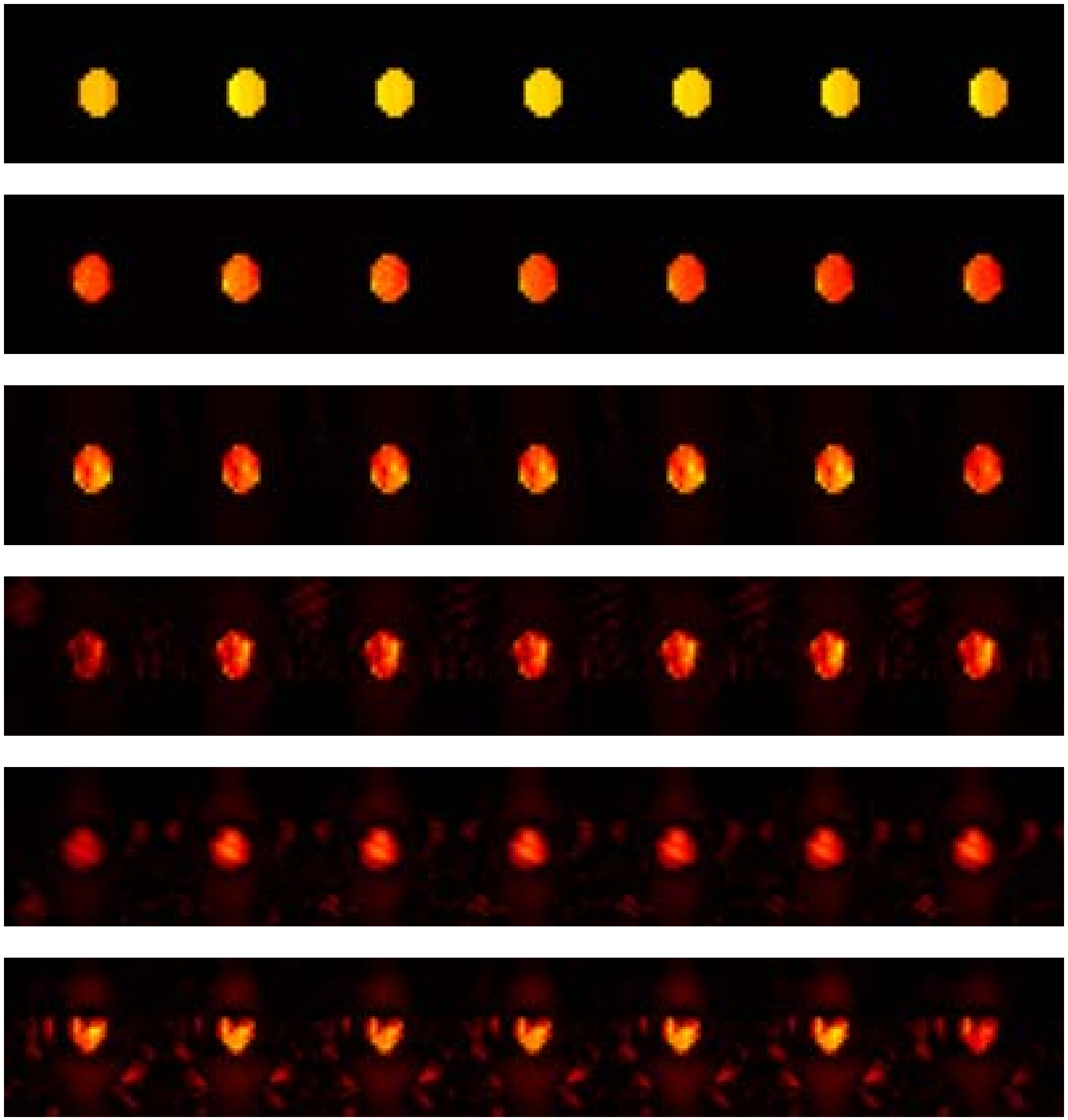


An array of quantum dots used for simulation



Simulated diffraction pattern

Test Reconstructions for the Different Size of the Beam Stop



R_0=0 px

R_0 =10 px

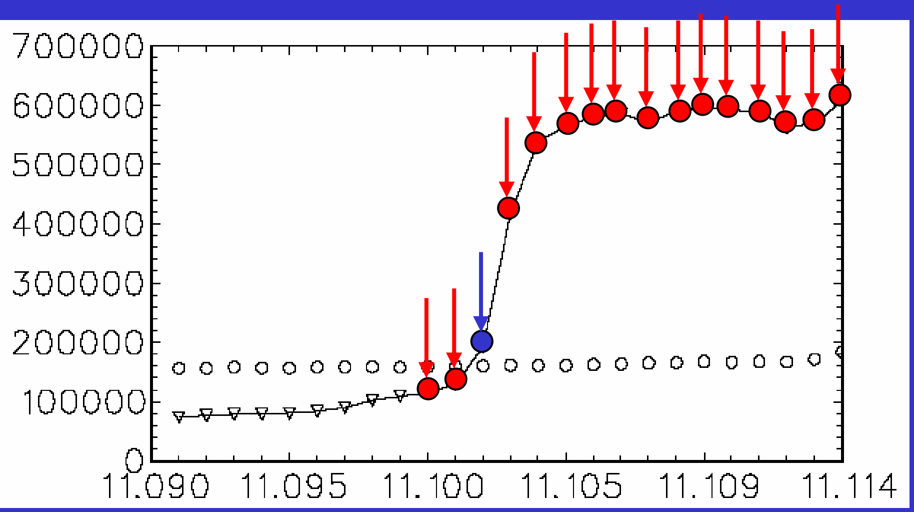
R_0 =20 px

R_0 =30 px

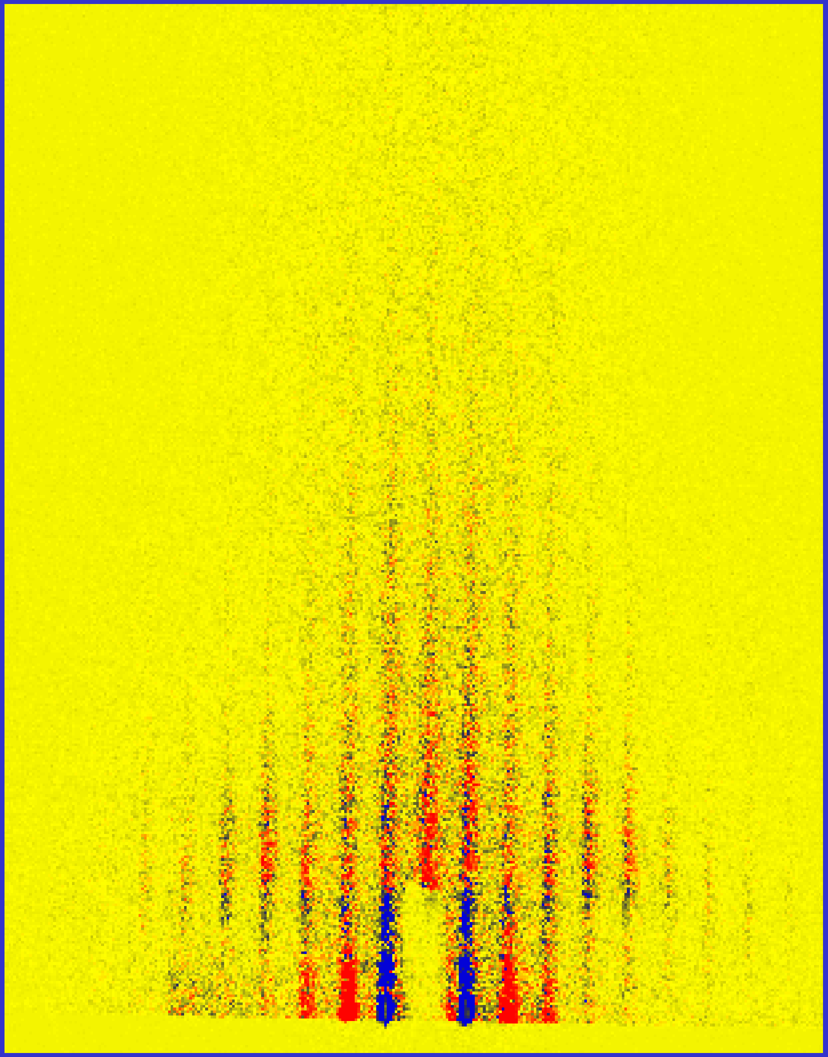
R_0 =40 px

R_0 =50 px

Anomalous Scattering @ Ge K-edge

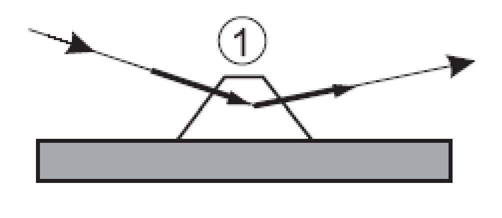


Energy E(keV)

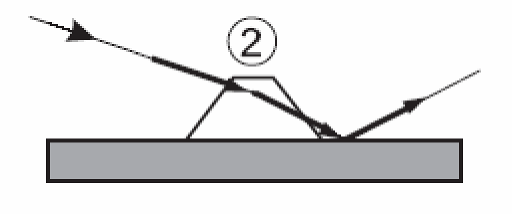


In this way we hope to separate Ge and Si contributions

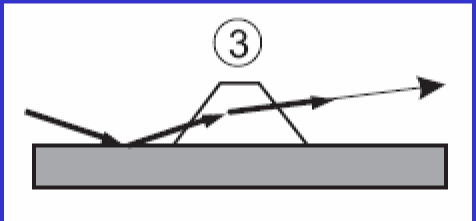
Simulations Using DWBA Theory



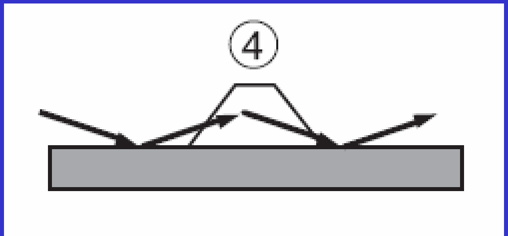
$$A_1(\mathbf{q}) = \int_{island} \chi_0(\mathbf{r}) e^{i(\mathbf{q}_{\parallel}+\mathbf{q}_1^{\perp})\cdot\mathbf{r}} dV$$



$$A_2(\mathbf{q}) = R(\alpha_f) \int_{island} \chi_0(\mathbf{r}) e^{i(\mathbf{q}_{\parallel}+\mathbf{q}_2^{\perp})\cdot\mathbf{r}} dV$$



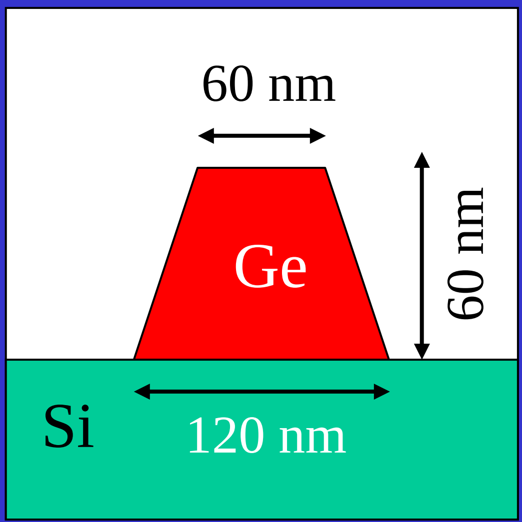
$$A_3(\mathbf{q}) = R(\alpha_i) \int_{island} \chi_0(\mathbf{r}) e^{i(\mathbf{q}_{\parallel}+\mathbf{q}_3^{\perp})\cdot\mathbf{r}} dV$$

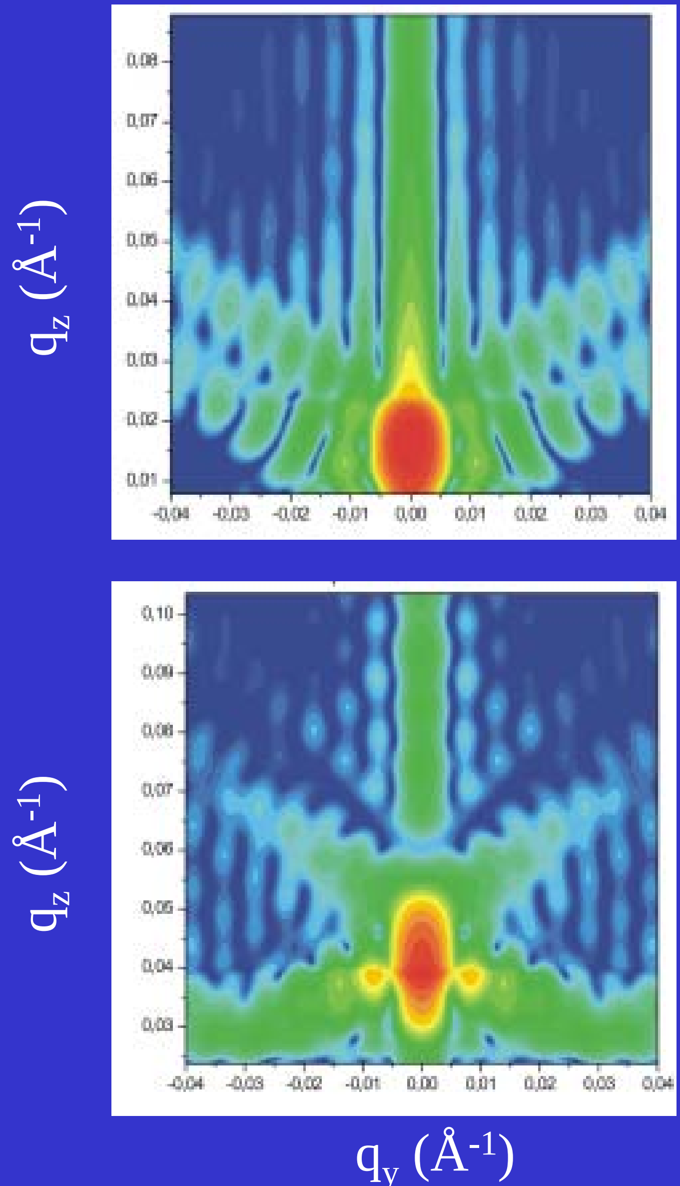


$$A_4(\mathbf{q}) = R(\alpha_i) R(\alpha_f) \int_{island} \chi_0(\mathbf{r}) e^{i(\mathbf{q}_{\parallel}+\mathbf{q}_4^{\perp})\cdot\mathbf{r}} dV$$

M. Schmidbauer *et al.*, Phys. Rev. B (2005) **71**, 115324

Simulations Using DWBA Theory



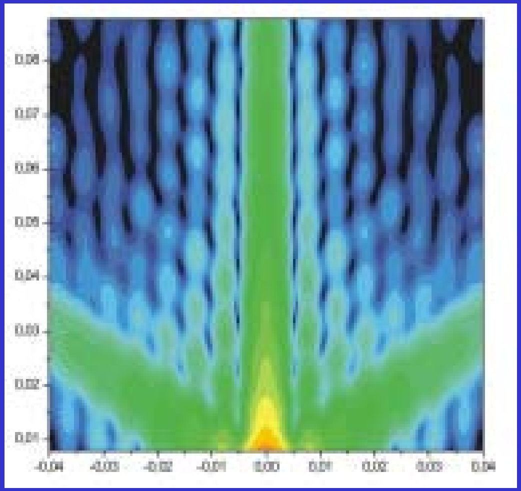


α_i=0.1°

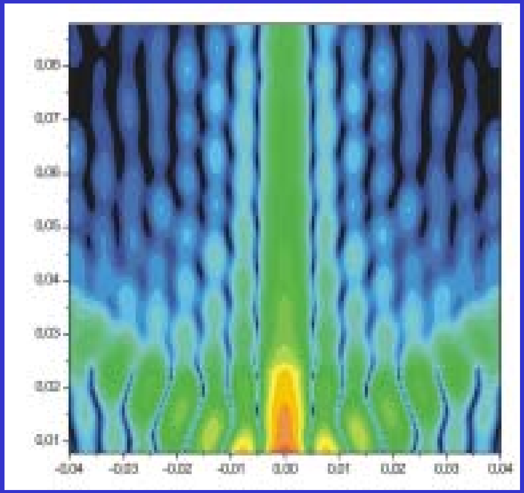
α_i=0.3°

D. Grigoriev, *HU Berlin*

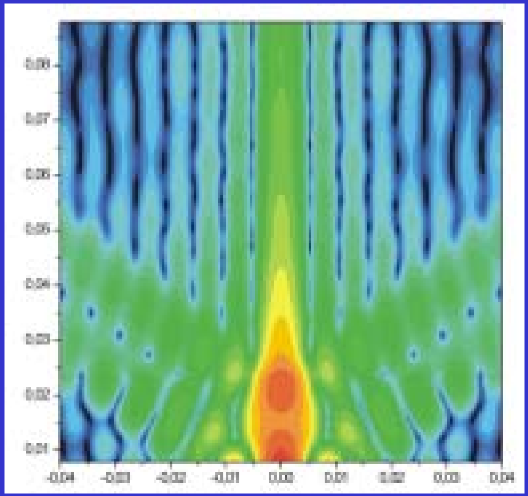
Simulations Using DWBA Theory



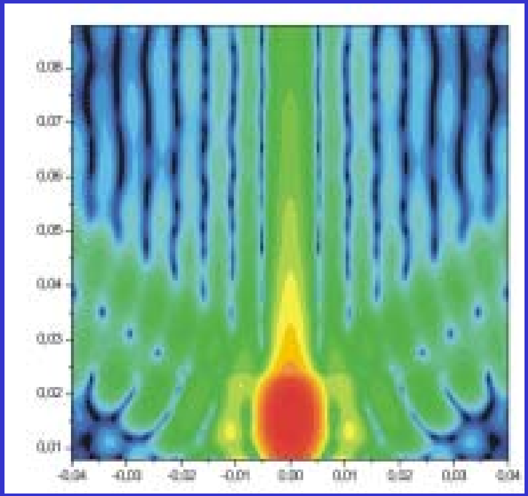
$I(\mathbf{q})=|A_1(\mathbf{q})|^2$



$I(\mathbf{q})=|A_1(\mathbf{q})+ A_4(\mathbf{q})|^2$



$I(\mathbf{q})=|A_1(\mathbf{q})+ A_2(\mathbf{q})+ A_4(\mathbf{q})|^2$



$I(\mathbf{q})=|A_1(\mathbf{q})+ A_2(\mathbf{q})+ A_3(\mathbf{q})+ A_4(\mathbf{q})|^2$

Conclusions and Outlook

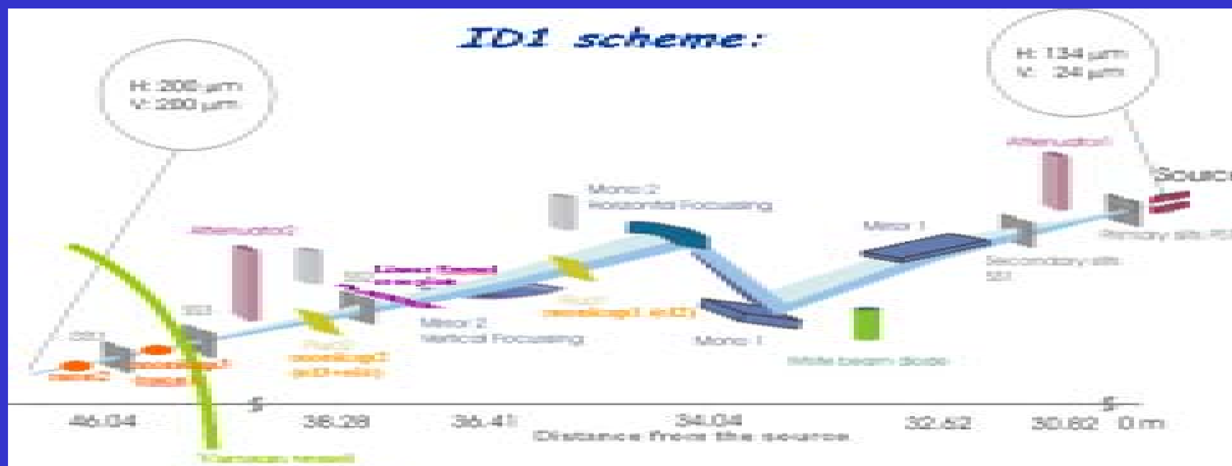
- Periodic systems of quantum dots can be effectively imaged with coherent x-rays with **nanometer** resolution
- Coherent X-ray Diffraction on **buried** quantum dot systems
- Coherent X-ray Diffraction on a patterned **biological** samples (viruses, molecules and etc.)

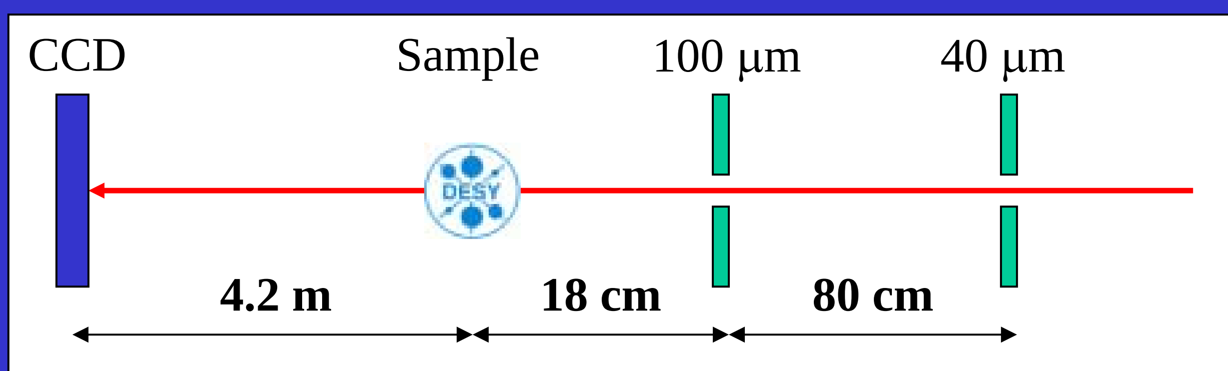
Coherent X-ray Diffraction Project at HASYLAB

Andreas Schropp
Christian Schroer
Edgar Weckert

Experiment on ID-01 in ESRF

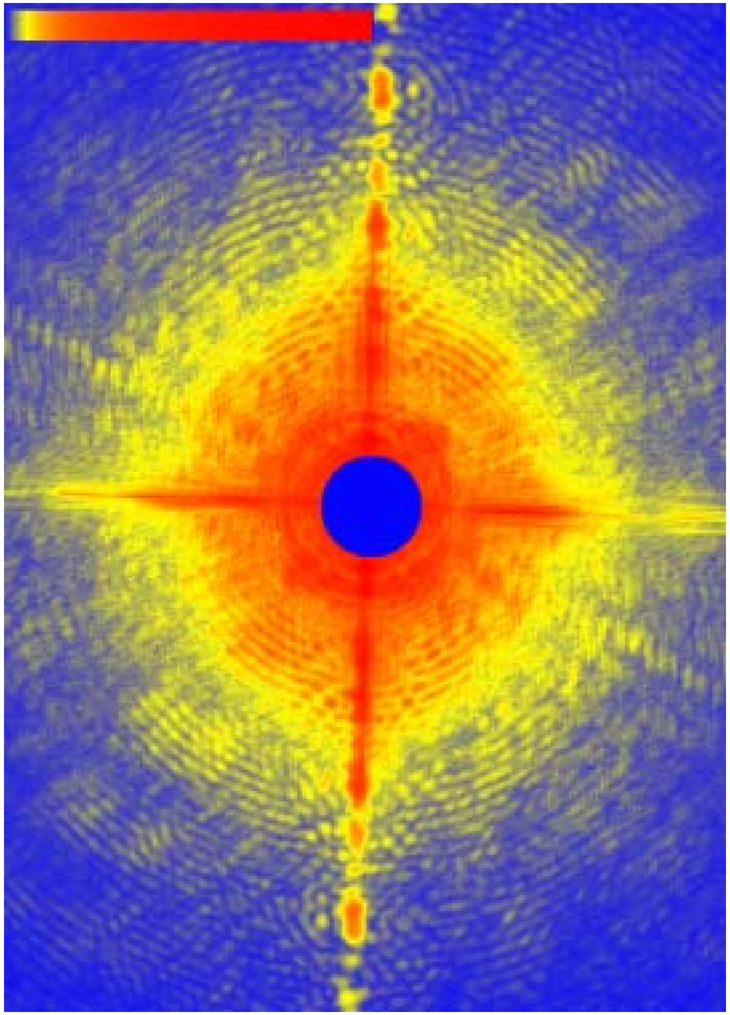
Staff of ID-01: Hartmut Metzger
Christian Mocuta,
Peter Boesecke



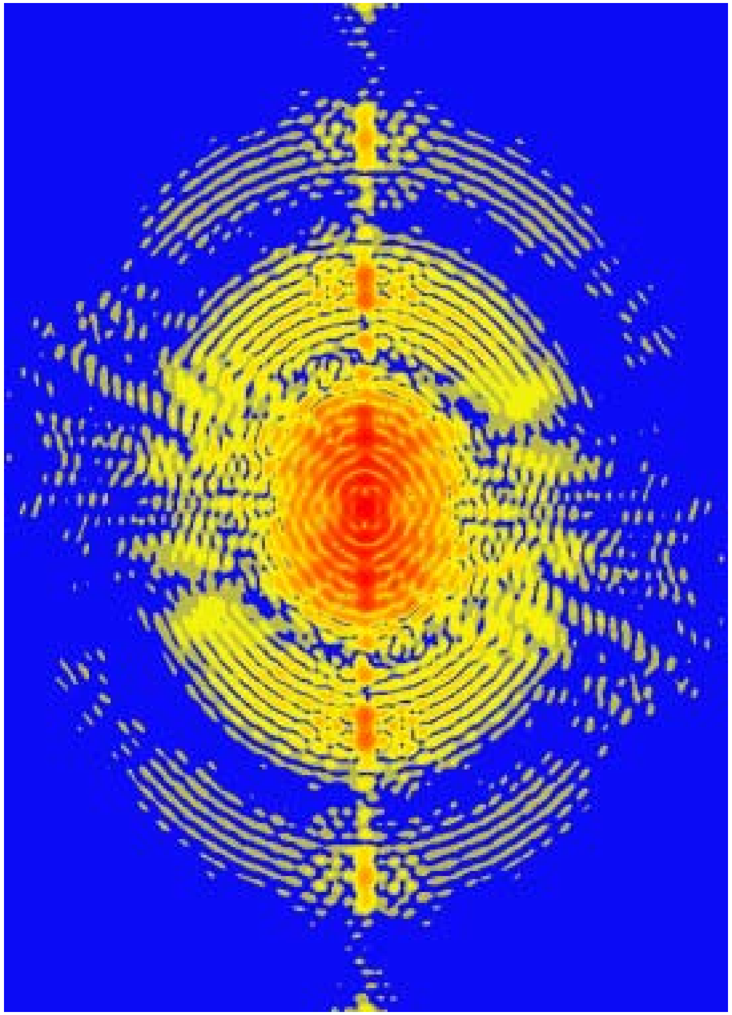


Diffraction Pattern Measured @ 7 keV

700 px (120 μm^{-1})

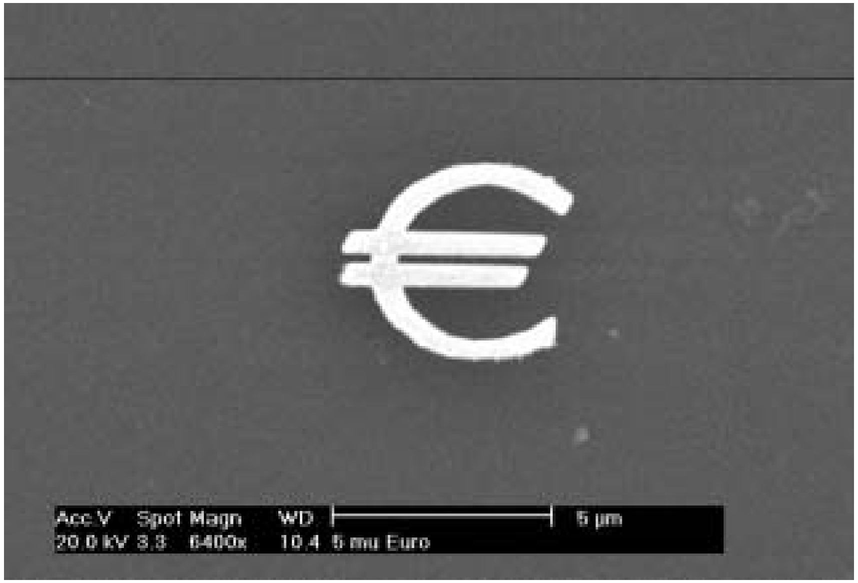


500 px (85 μm^{-1})

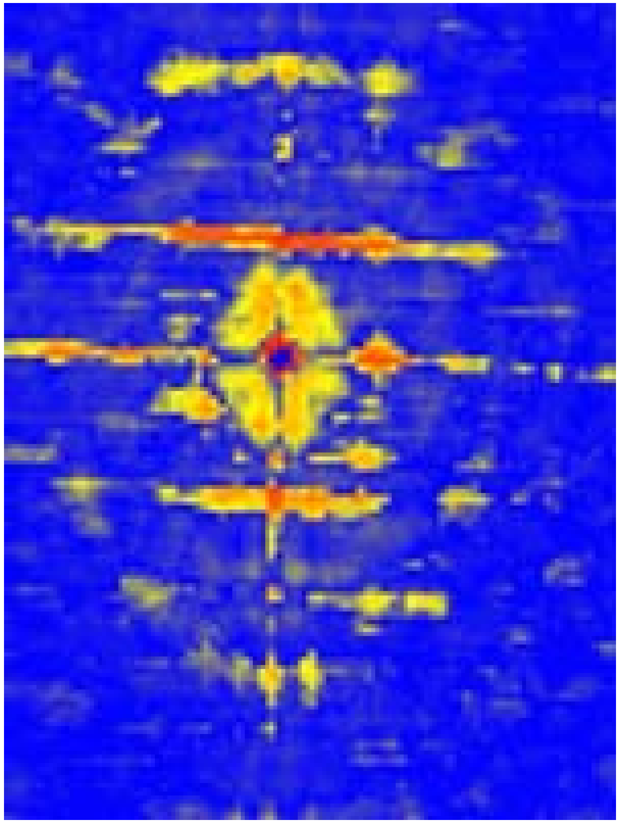


Simulation

Samples



Electron Microscopy



First Results of Reconstruction

O. Kuparova, ***II Physikalishes Institut, Aachen***

Thank you for your attention