

The Braggs and X-ray Diffraction

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London Centre for Nanotechnology
Research Complex at Harwell

UCL Science Society Meeting
3 December 2012

Outline

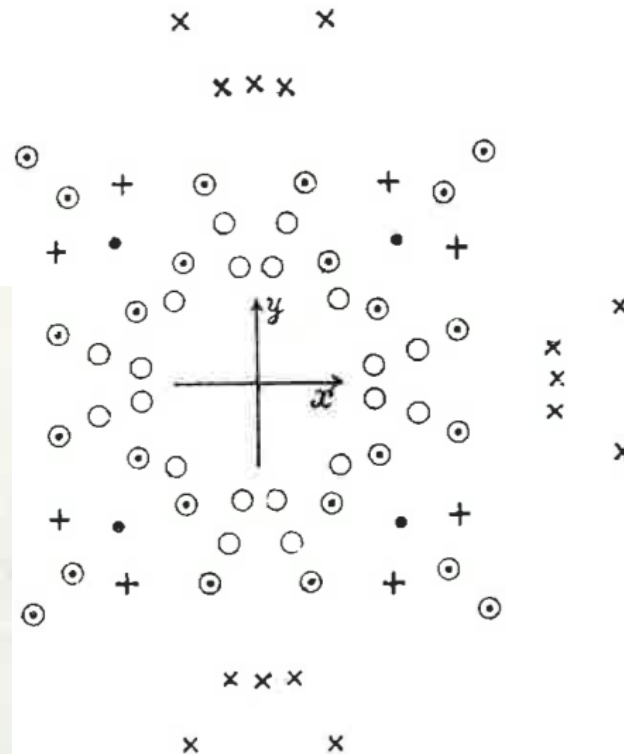
- 100 years since Bragg's Law
- X-ray Diffraction
- Properties of Diffraction
- Coherent x-ray diffraction
- Nanocrystals
- Use of nanocrystals in medicine

Max von Laue, 1879-1960

Proceedings Bavarian Academy of Sciences, 1912

Zinc Blende, ZnS, Nobel prize 1914

- $\lambda/\alpha = 0,0377$
- ⊙ $\lambda/\alpha = 0,0563$
- × $\lambda/\alpha = 0,0663$
- $\lambda/\alpha = 0,1051$
- + $\lambda/\alpha = 0,143$



W. L. Bragg 1890-1971

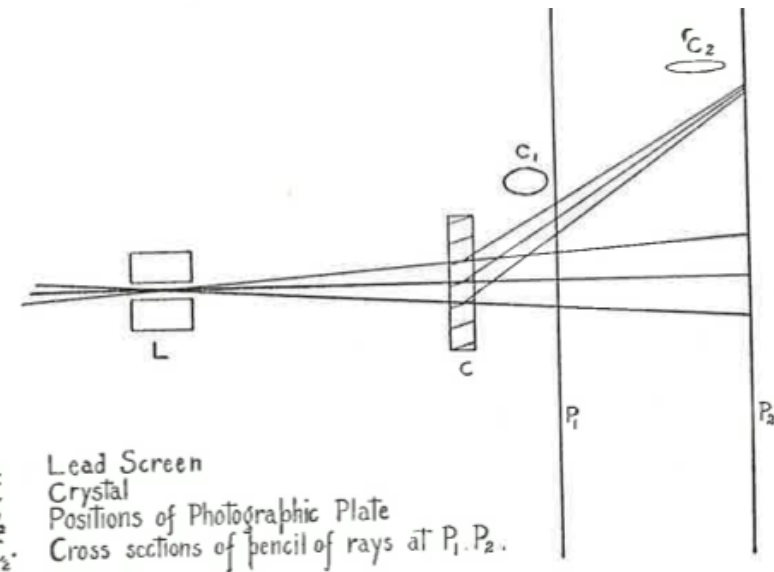
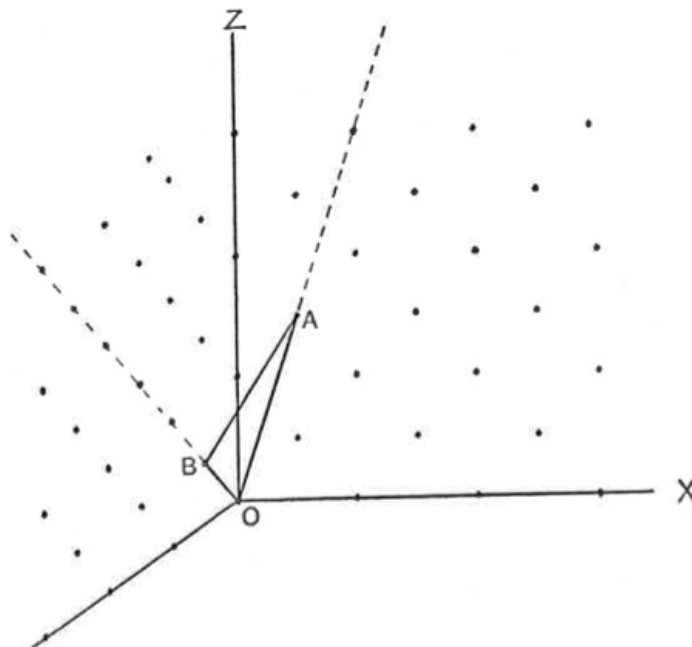
THE DIFFRACTION OF SHORT ELECTROMAGNETIC WAVES BY A CRYSTAL

by

W. L. Bragg, B. A., Trinity College

(communicated by Prof. Sir J. J. Thomson)

(Read 11 November 1912)



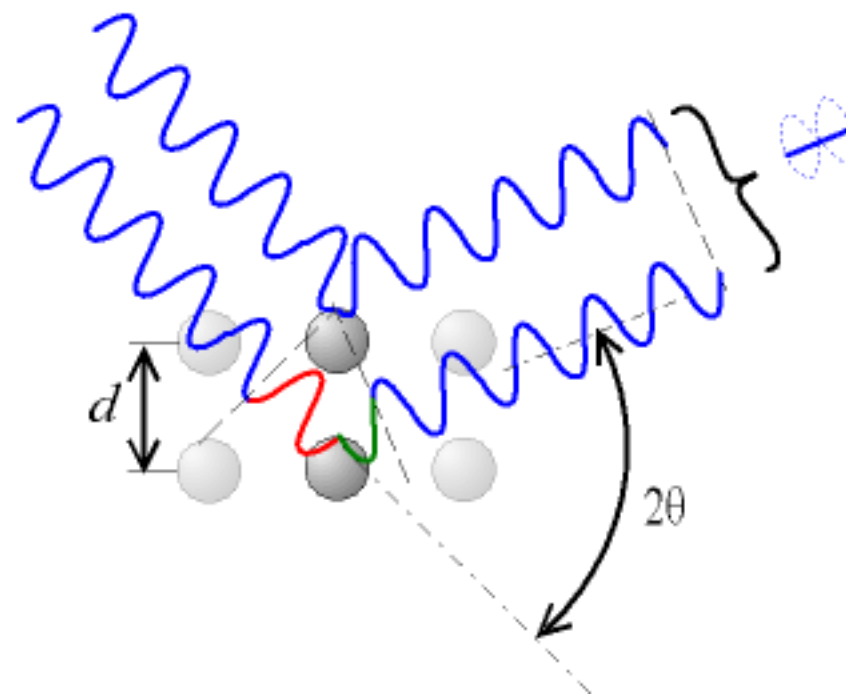
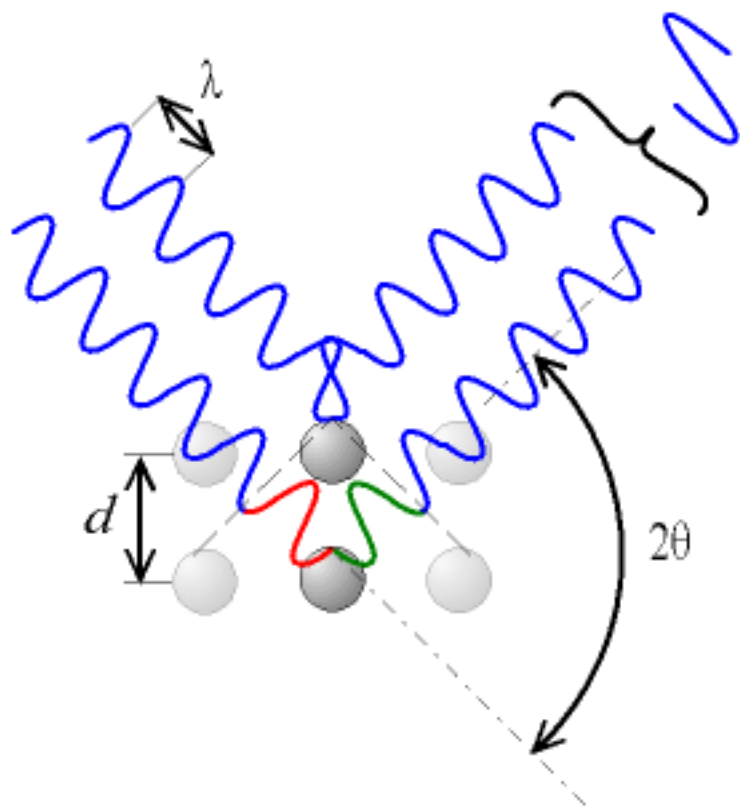
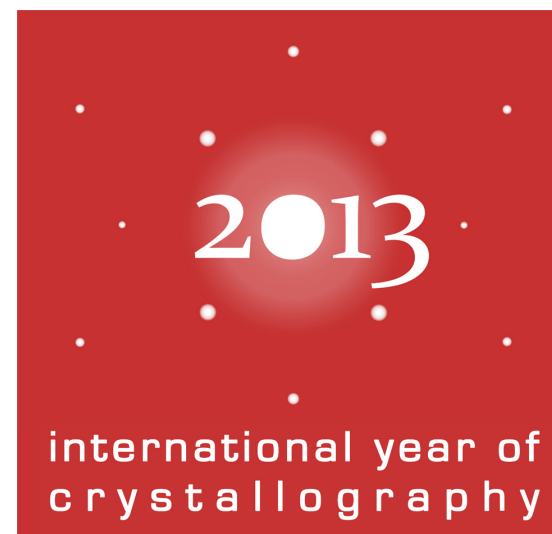
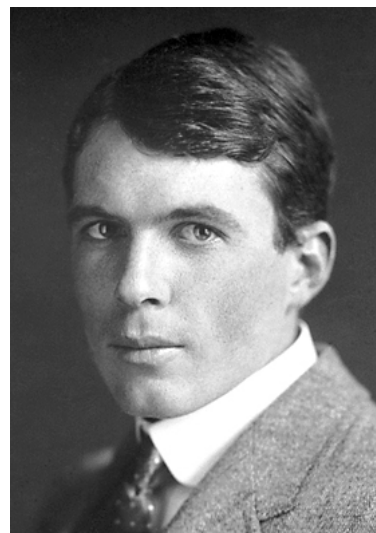
L Lead Screen
C Crystal
P₁ P₂ Positions of Photographic Plate
C₁ C₂ Cross sections of pencil of rays at P₁, P₂.

Fig. 2.

Bragg Law 1913

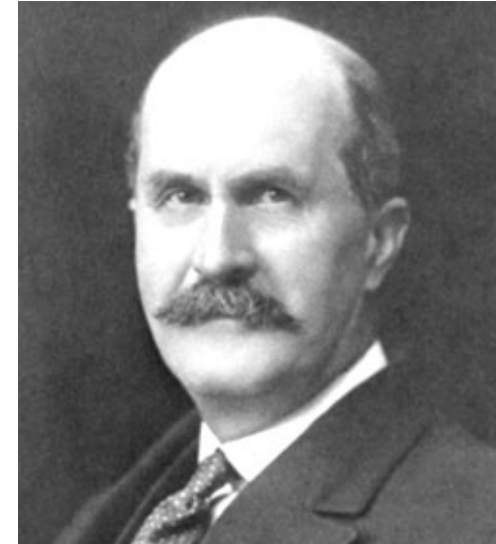
$$2d\sin\theta = \lambda$$

C D Ngoc Chan, Wikipedia



W. H. Bragg 1862-1942

- 1885 Cambridge to Adelaide
- 1890 W. L. Bragg born
- 1895 Roentgen discovered X-rays
- 1904 Ion chamber experiments
- 1912 von Laue X-ray Diffraction
- 1913 Bragg's Law published
- 1915 Quain professor at UCL
- 1915 Nobel prize
- 1939 Bragg "X-ray Microscope"
- 1953 Crick-Watson DNA model



Nobel prizes in X-ray Crystallography

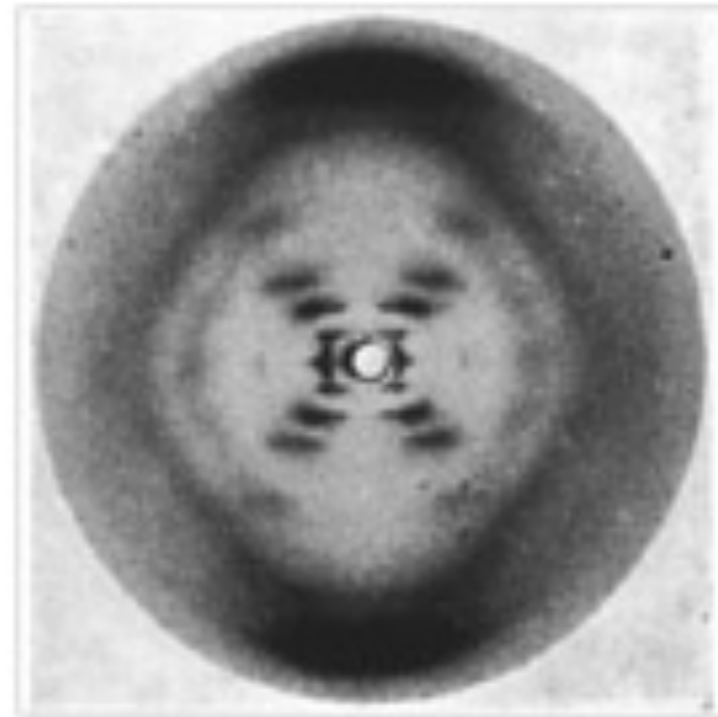
- 2012 Chemistry R. J. Lefkowitz and B. K. Kobilka G-protein-coupled receptors
- 2011 Chemistry D. Shechtman Discovery of quasicrystals
- 2009 Chemistry V. Ramakrishnan, T. A. Steitz and A. E. Yonath Ribosome
- 2006 Chemistry R. D. Kornberg Molecular basis of eukaryotic transcription
- 2003 Chemistry R. MacKinnon Potassium channels
- 1994 Physics C. Shull and N. Brockhouse Neutron diffraction
- 1988 Chemistry J. Deisenhofer, R. Huber and H. Michel Photosynthetic reaction centre
- 1985 Chemistry H. Hauptman and J. Karle Direct methods for crystal structures
- 1982 Chemistry A. Klug Nucleosome structure
- 1976 Chemistry W. N. Lipscomb Structure of boranes
- 1971 Physics D. Gabor Holography

Nobel prizes in X-ray Crystallography (continued)

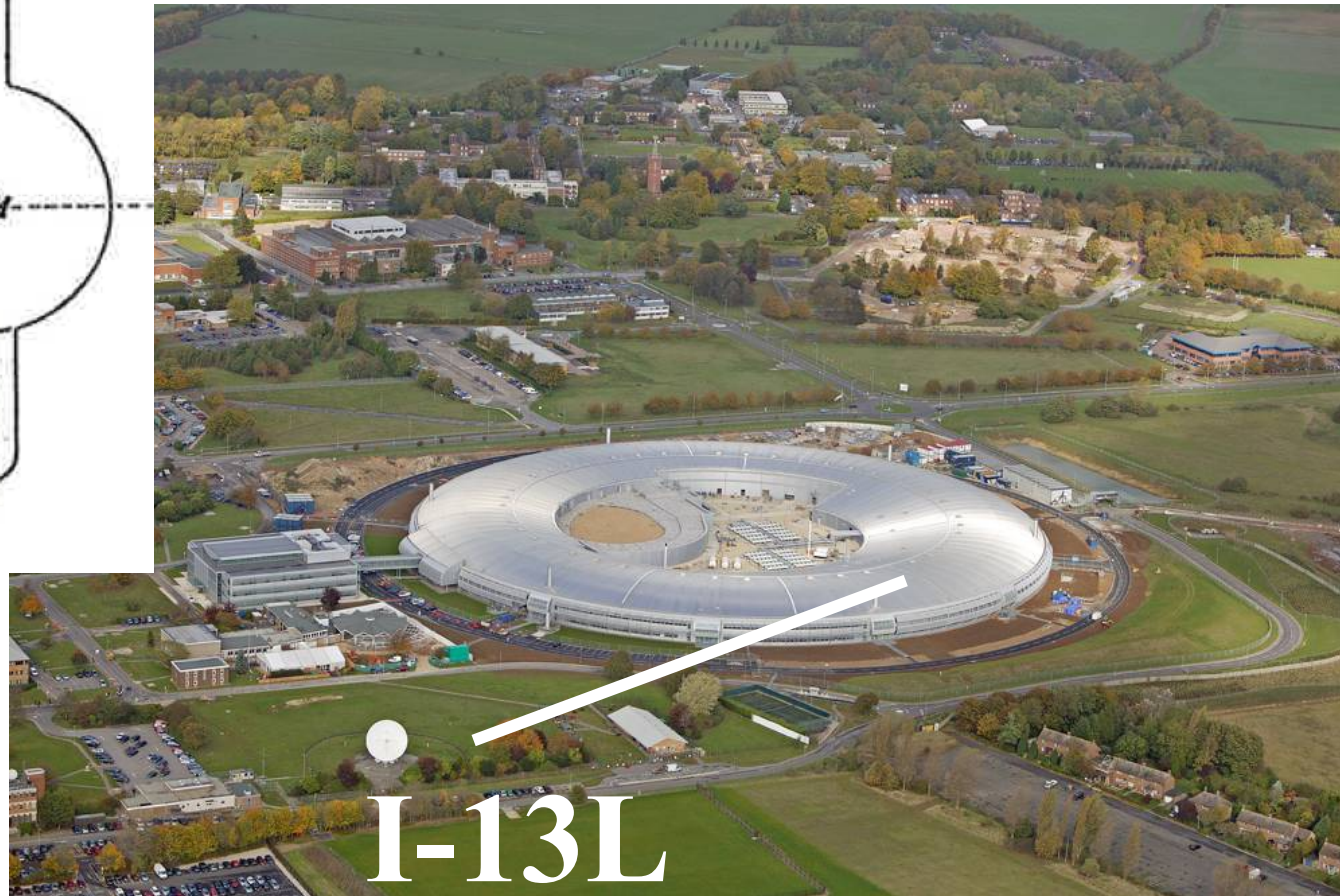
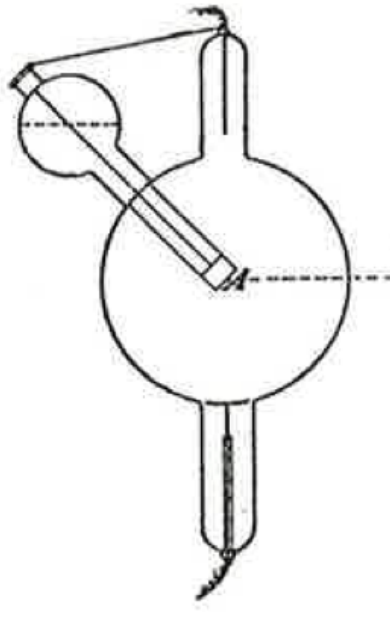
- 1964 Chemistry D. Hodgkin Vitamin B12
- 1962 Physiology/Medicine F. Crick, J. Watson and M. Wilkins Structure of DNA
- 1962 Chemistry J. C. Kendrew and M. Perutz Structures of globular proteins
- 1954 Chemistry L. C. Pauling Nature of the chemical bond
- 1946 Chemistry J. B. Sumner Enzymes can be crystallised
- 1937 Physics C. J. Davisson and G. Thompson Diffraction of electrons
- 1936 Chemistry P. J. W. Debye Diffraction of X-rays and electrons in gases
- 1915 Physics W. H. Bragg and W. L. Bragg Determination of crystal structure
- 1914 Physics M. von Laue Diffraction of X-rays by crystals
- 1901 Physics W. C. Röntgen Discovery of X-rays

Diffraction as Fourier Transform

Rosalind Franklin's DNA "photo 51" 1952



Diamond Light Source (Harwell)

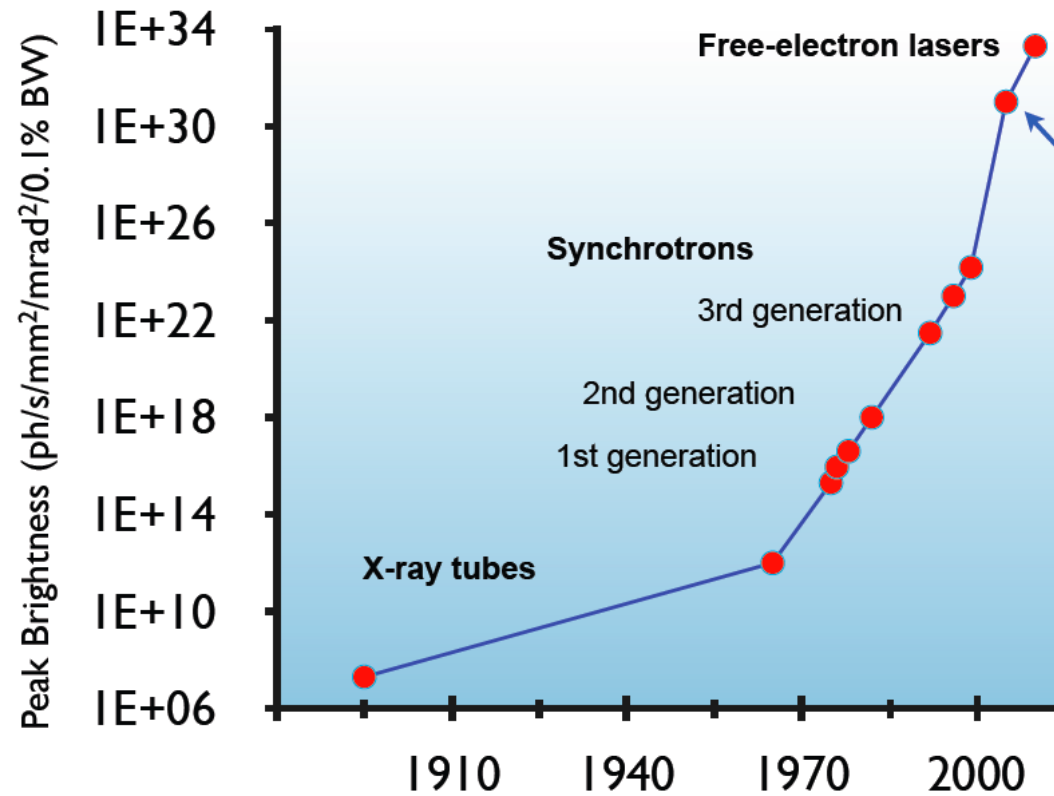
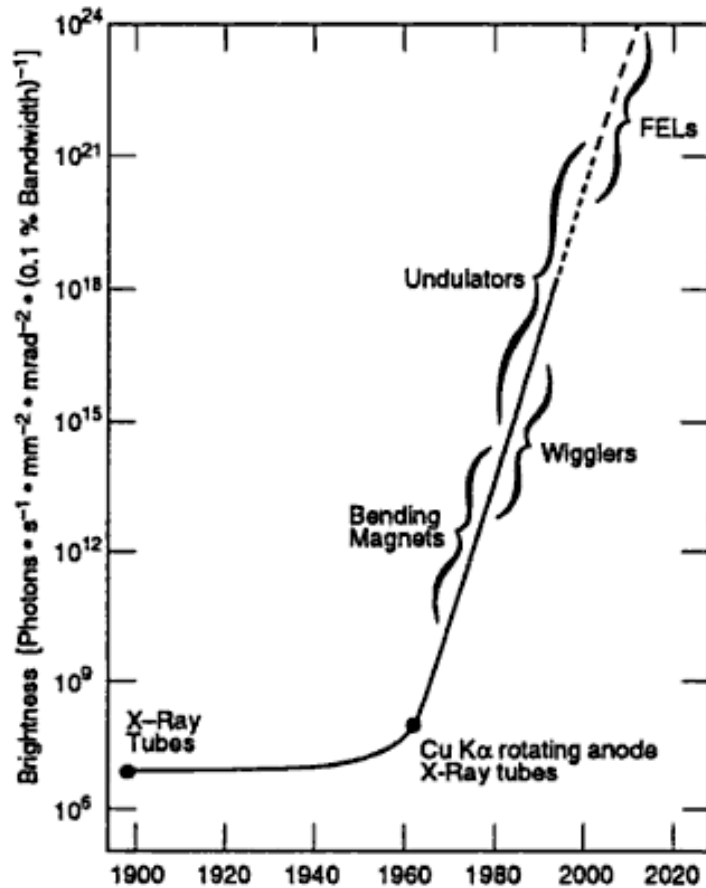


I-13L

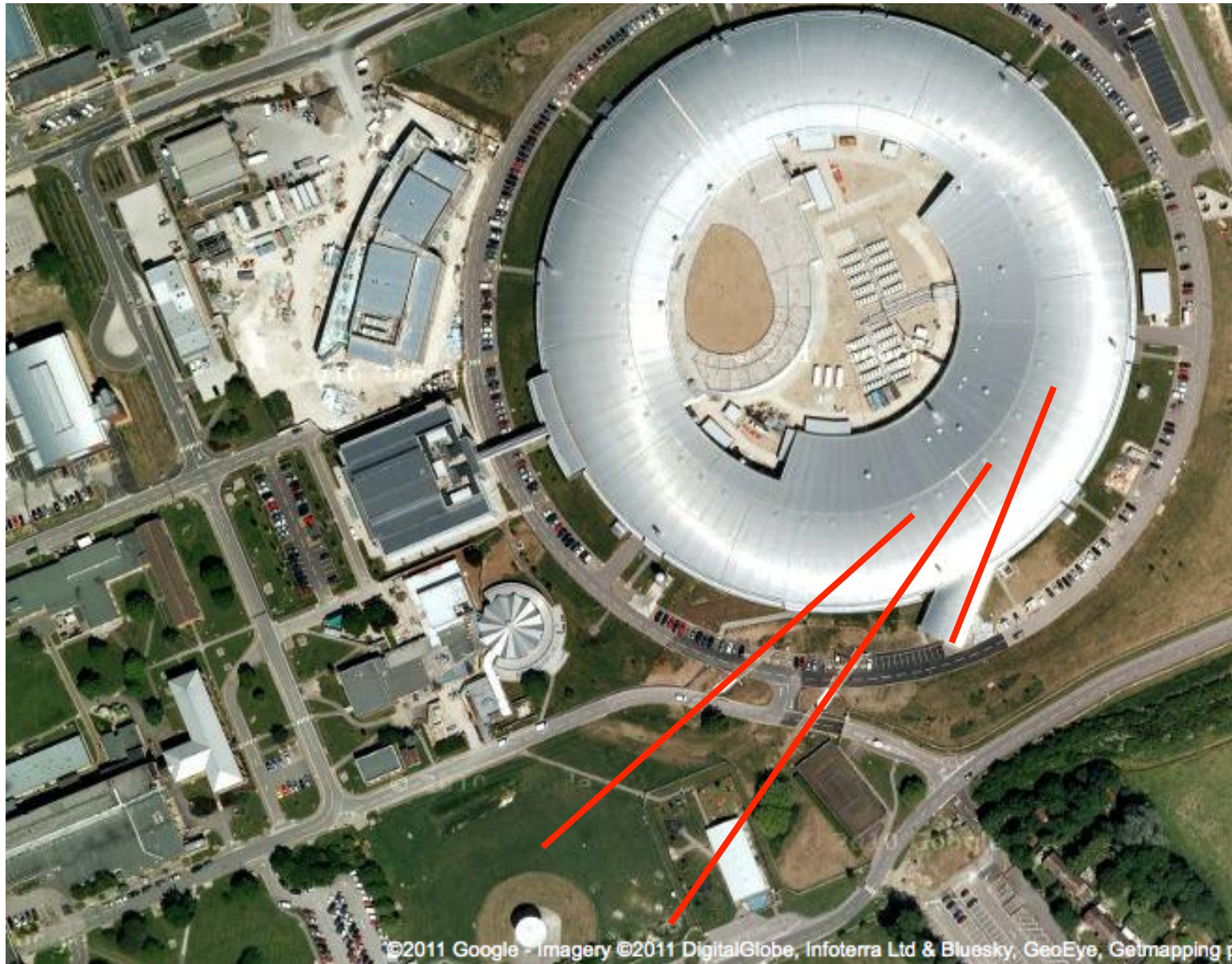
Growth of Source Brightness

H. Winick "SR Sources- a primer" (1995)

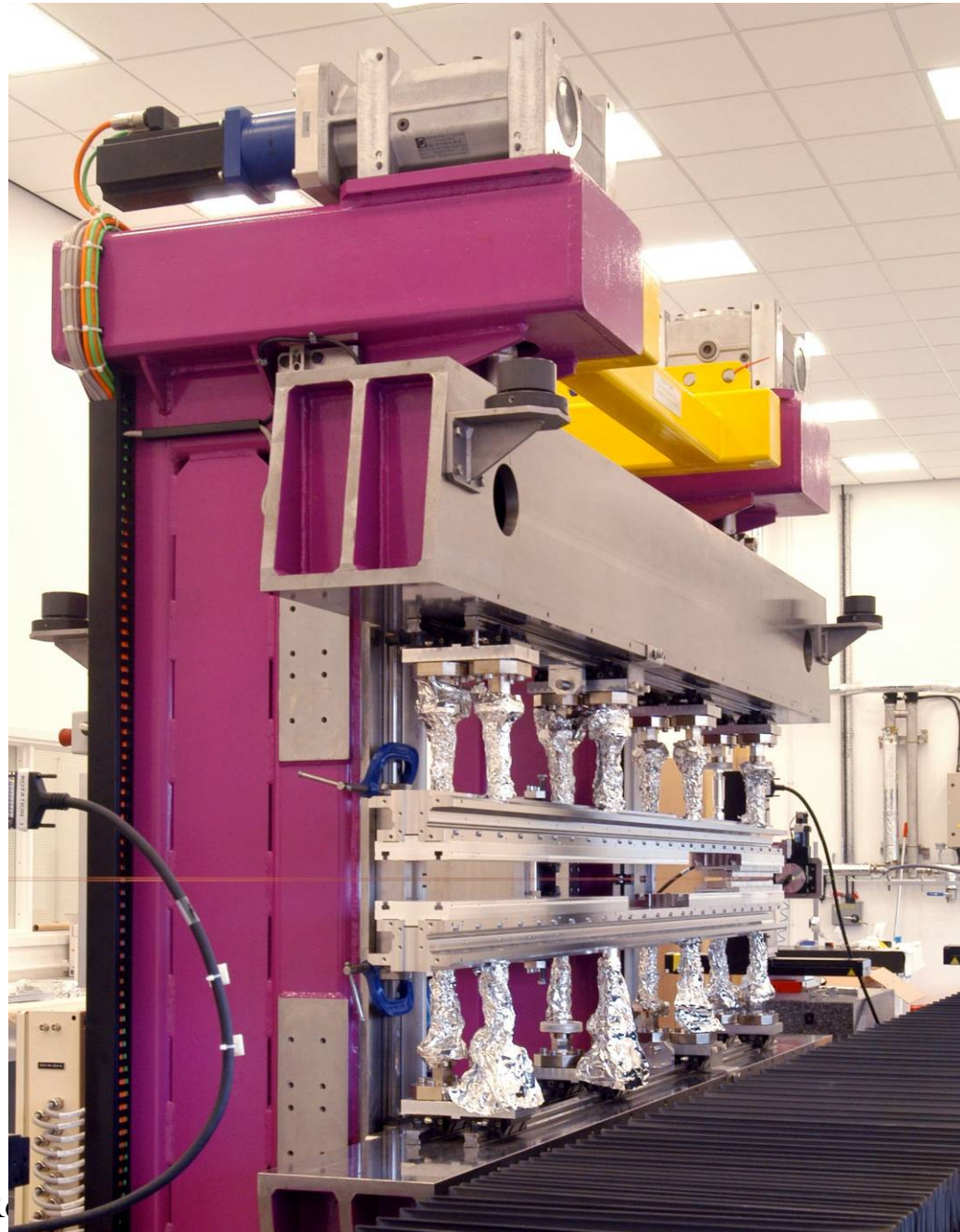
Henry Chapman, Bio-XFEL, Berkeley (2011)



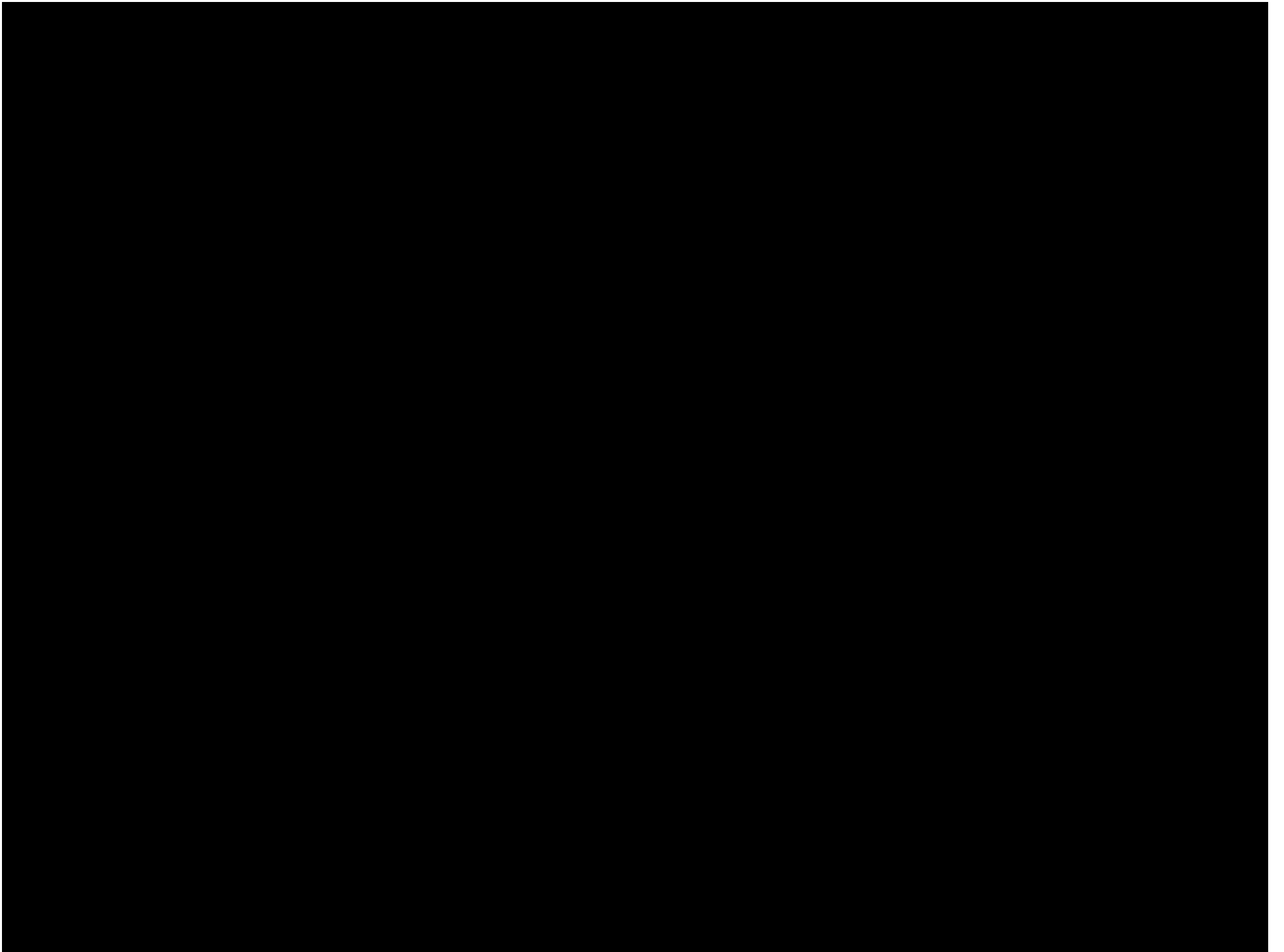
Diamond Light Source, 2009



Diamond in-vacuum X-ray Undulator

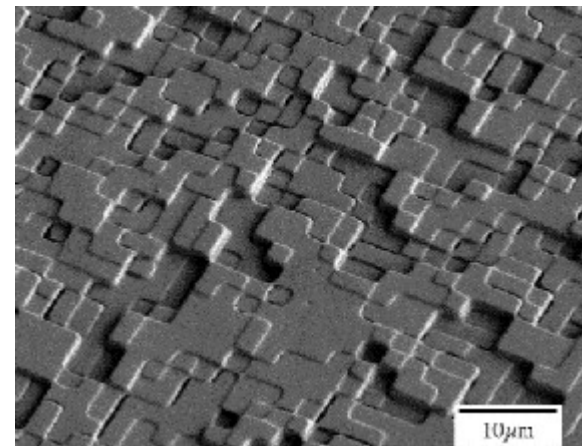
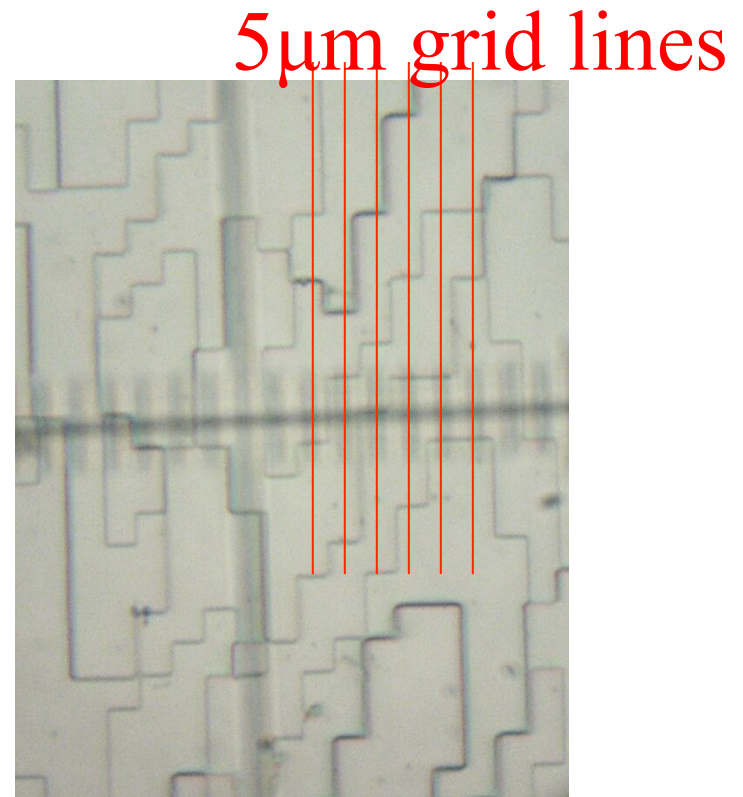
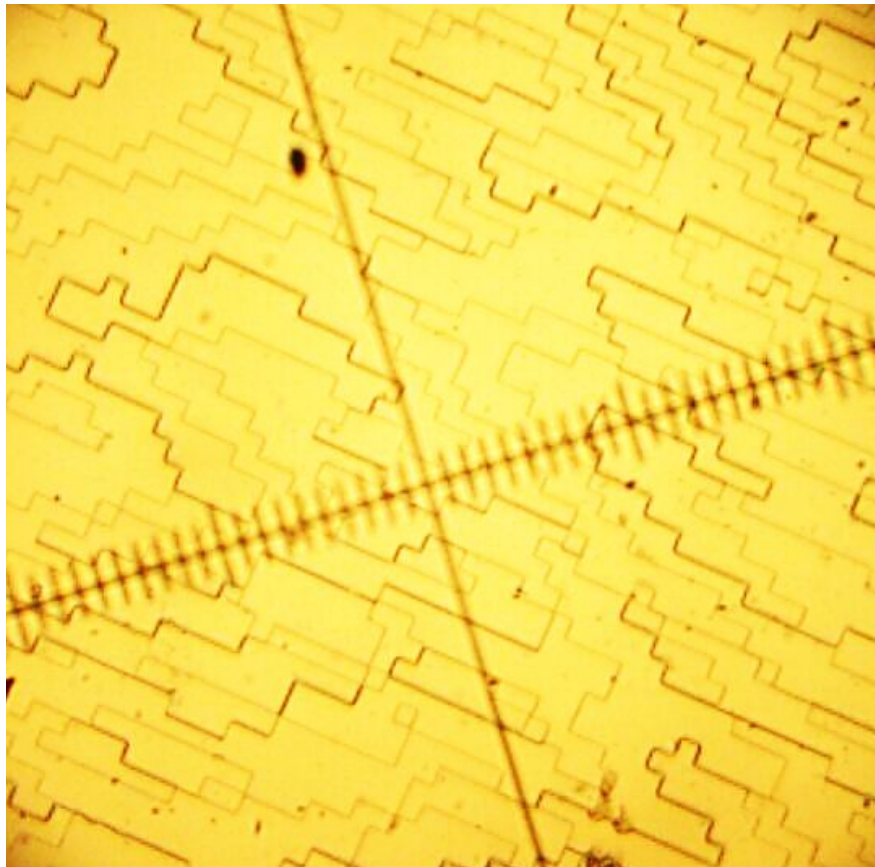


I. K. R



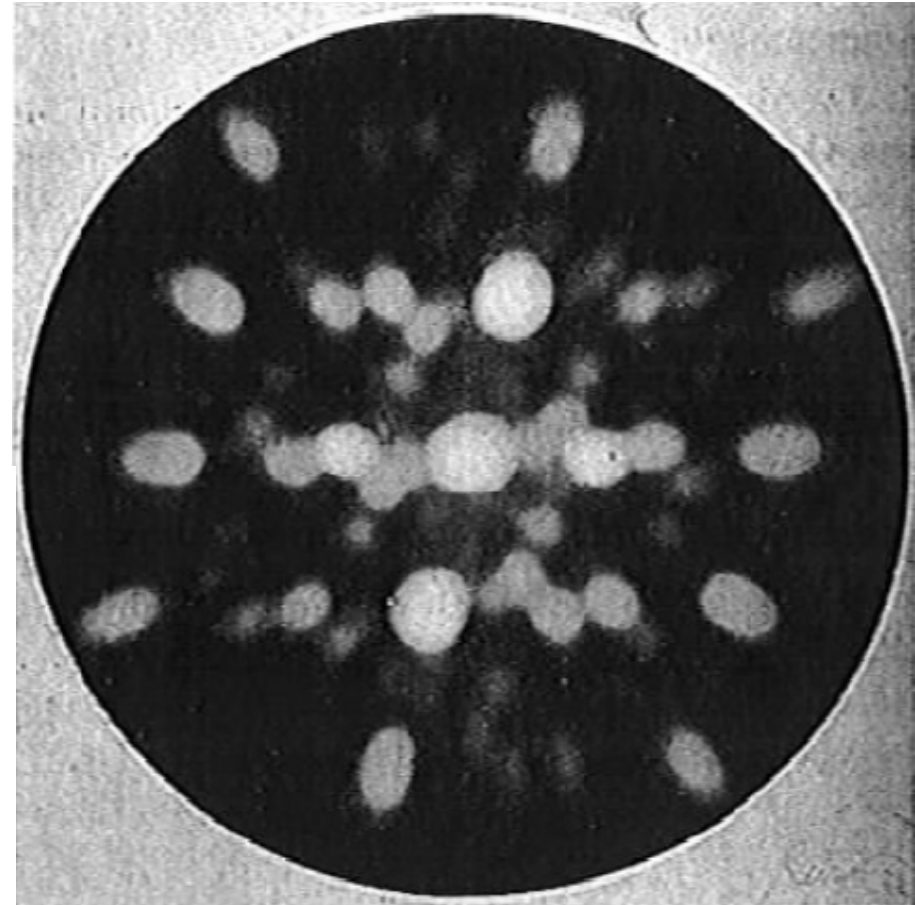
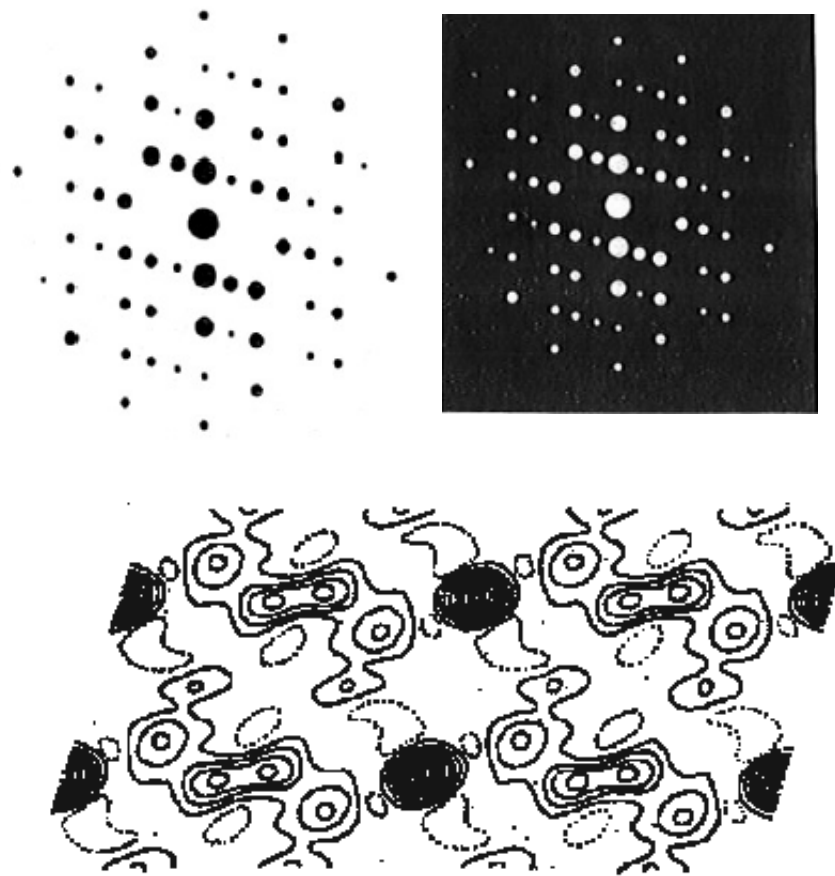
Microscope Images of Gratings

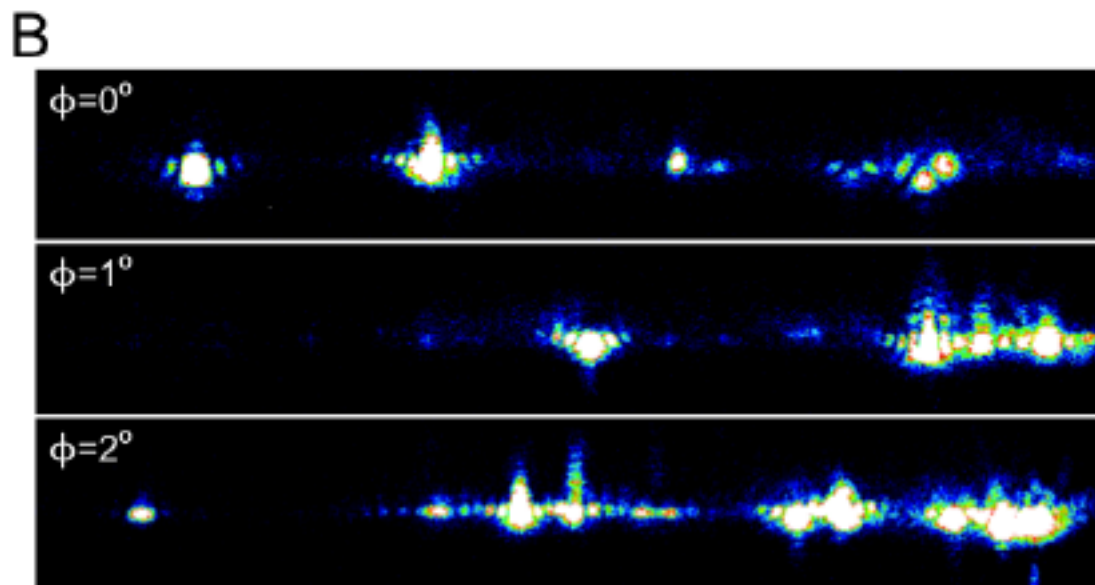
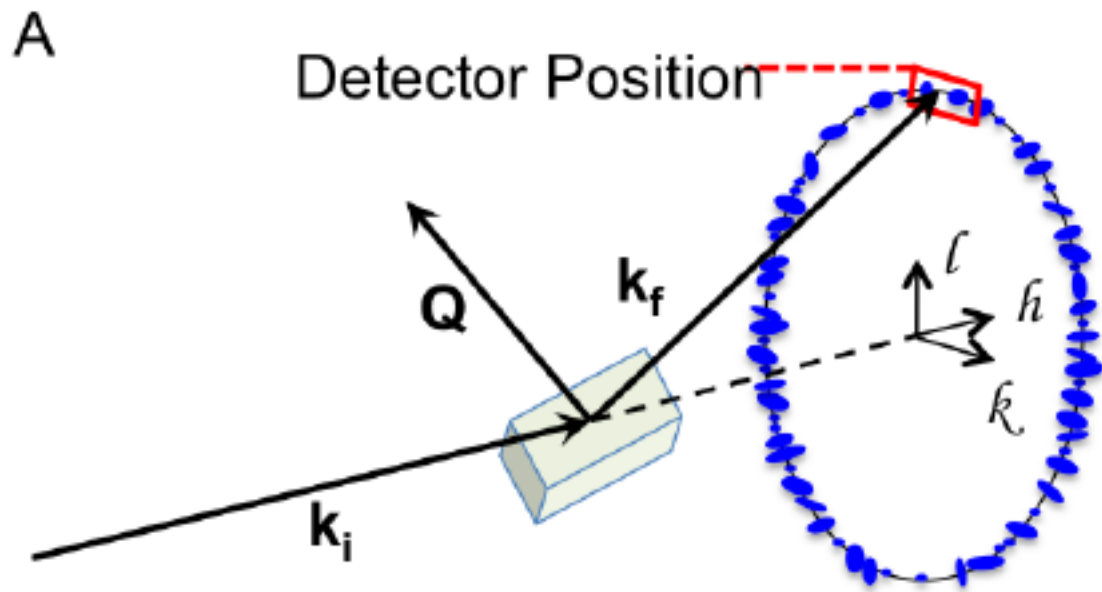
Digital Optics Corp: phase grating



Bragg's "X-ray Microscope"

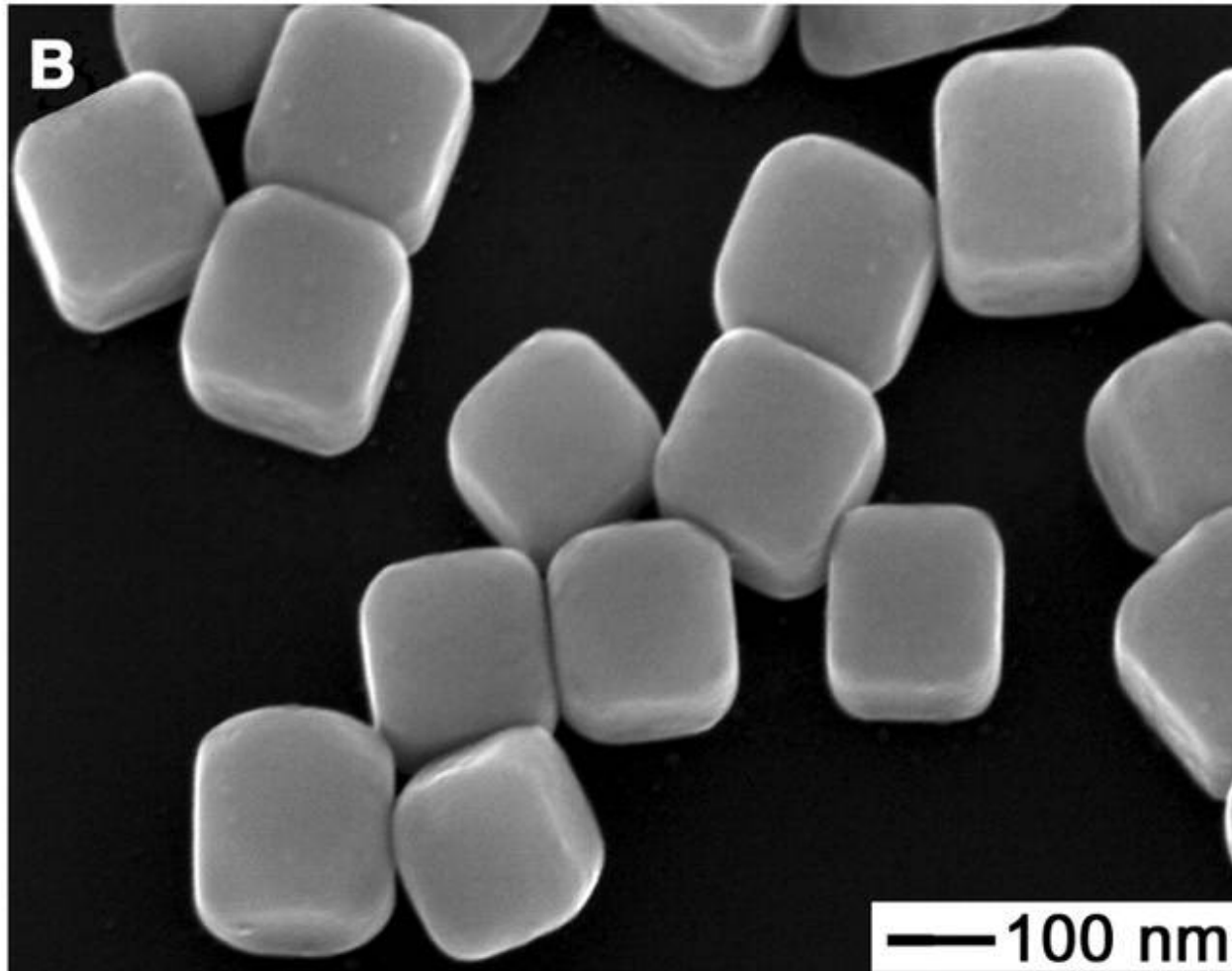
WLBragg Nature, 143, 678 (1939): diopside, $\text{CaMg}(\text{SiO}_3)_2$

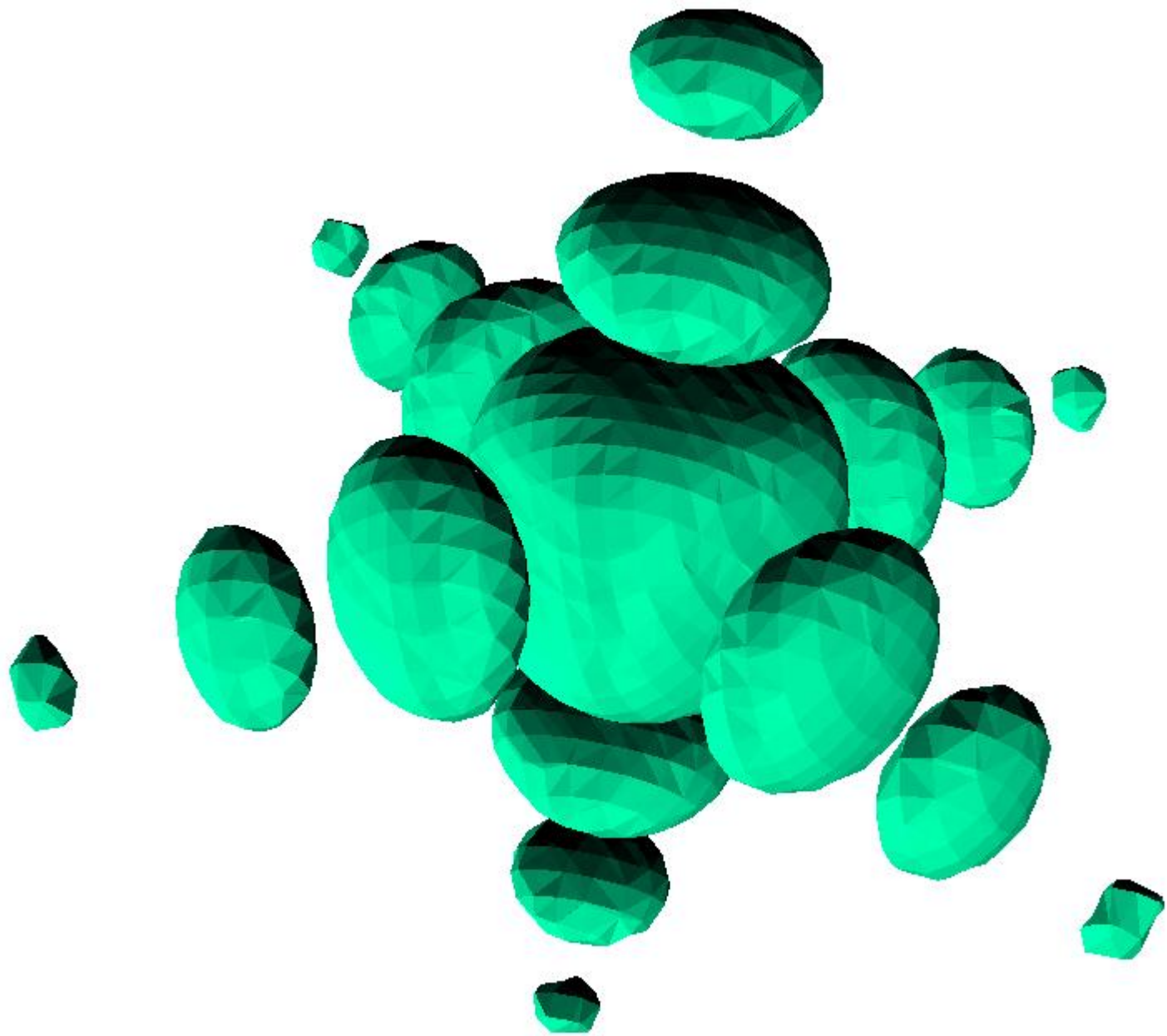




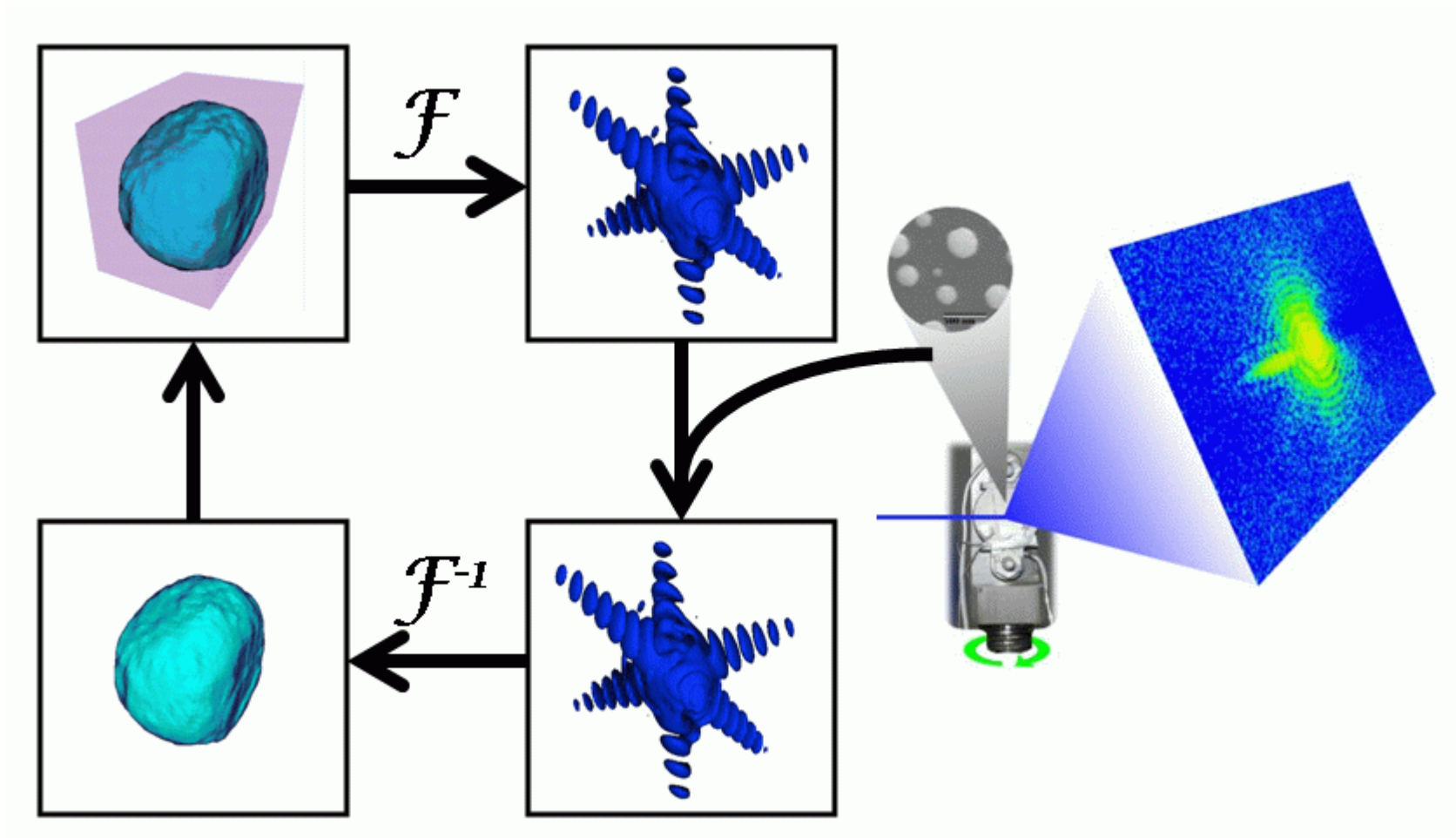
Chemically synthesized Ag Nanocubes

Y. Sun and Y. Xia, *Science* 298 2177 (2003)





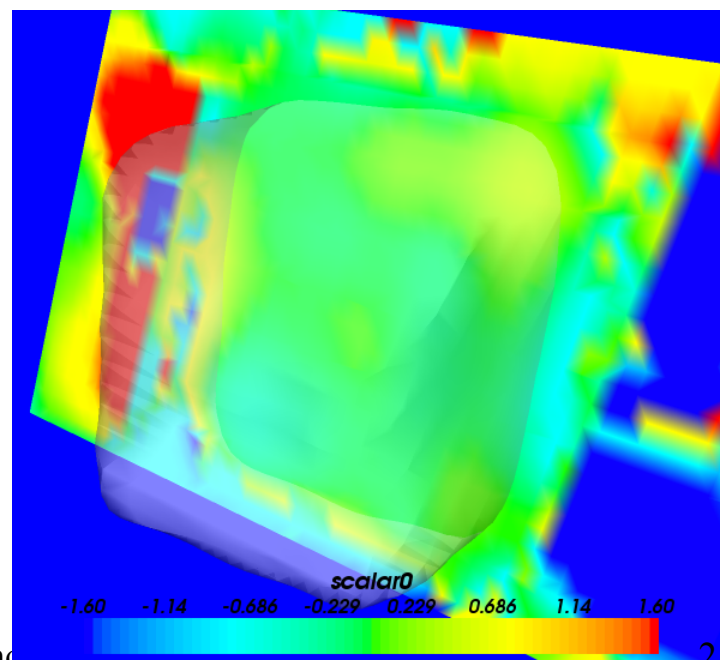
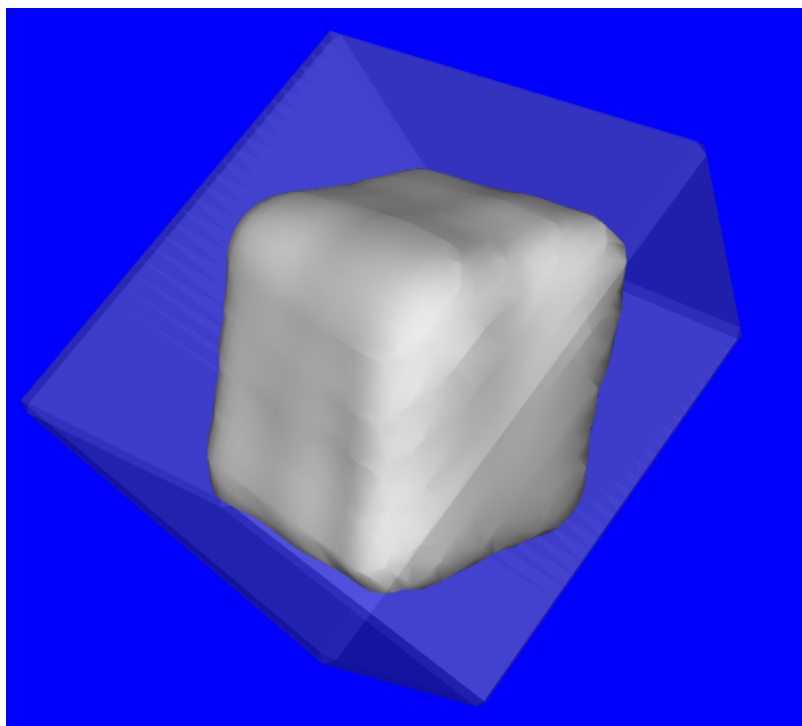
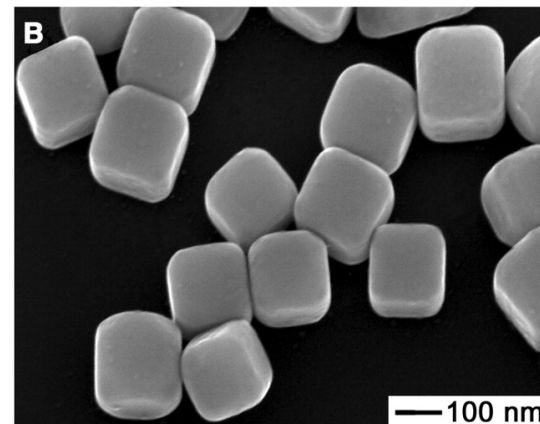
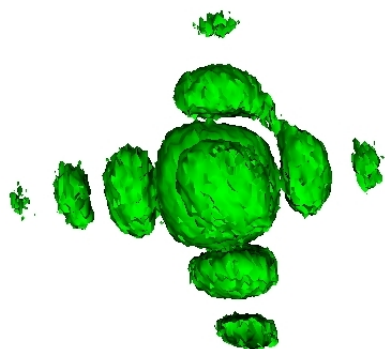
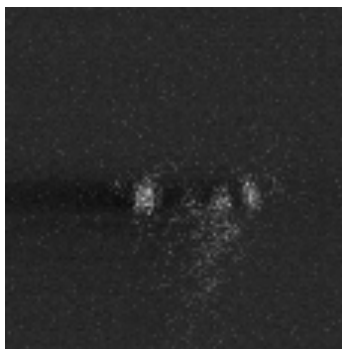
Generic “Error Reduction” method



J. R. Fienup *Appl. Opt.* 21 2758 (1982)

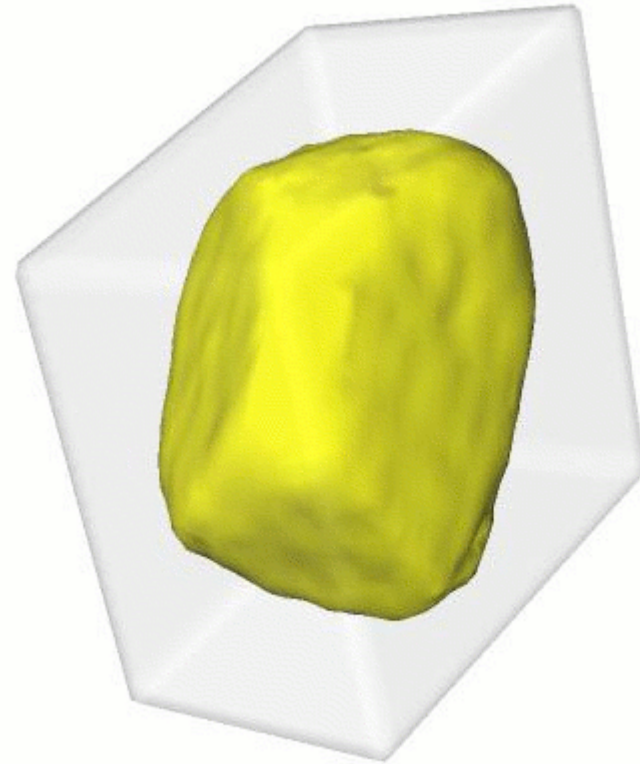
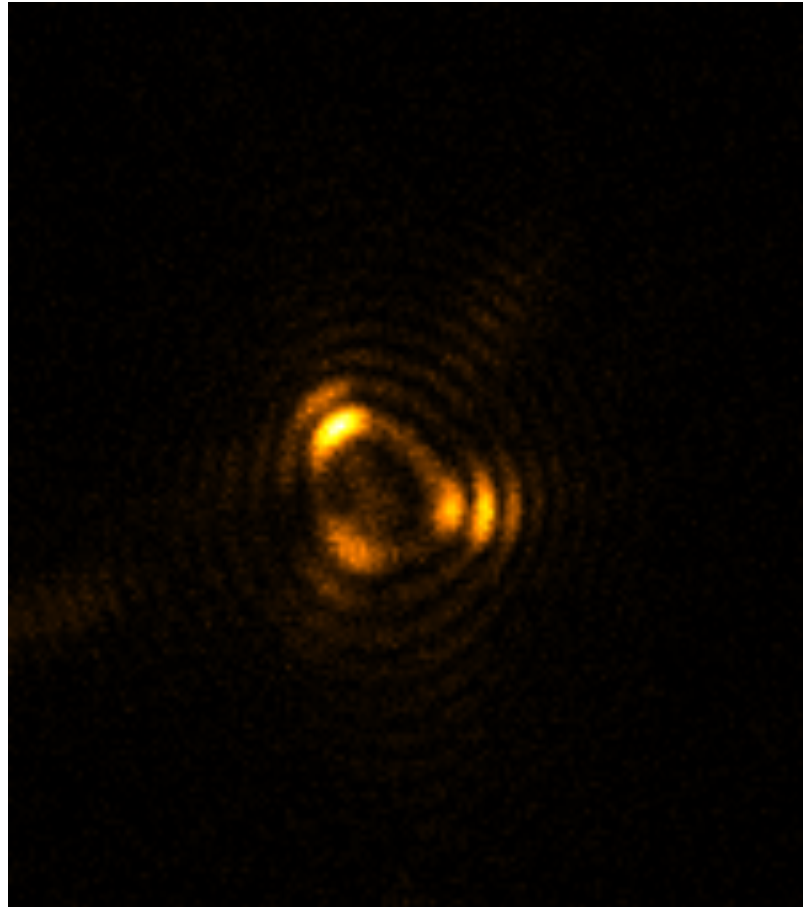
R. W. Gerchberg and W. O. Saxton *Optik* 35 237 (1972)

3D Ag Nano Cube

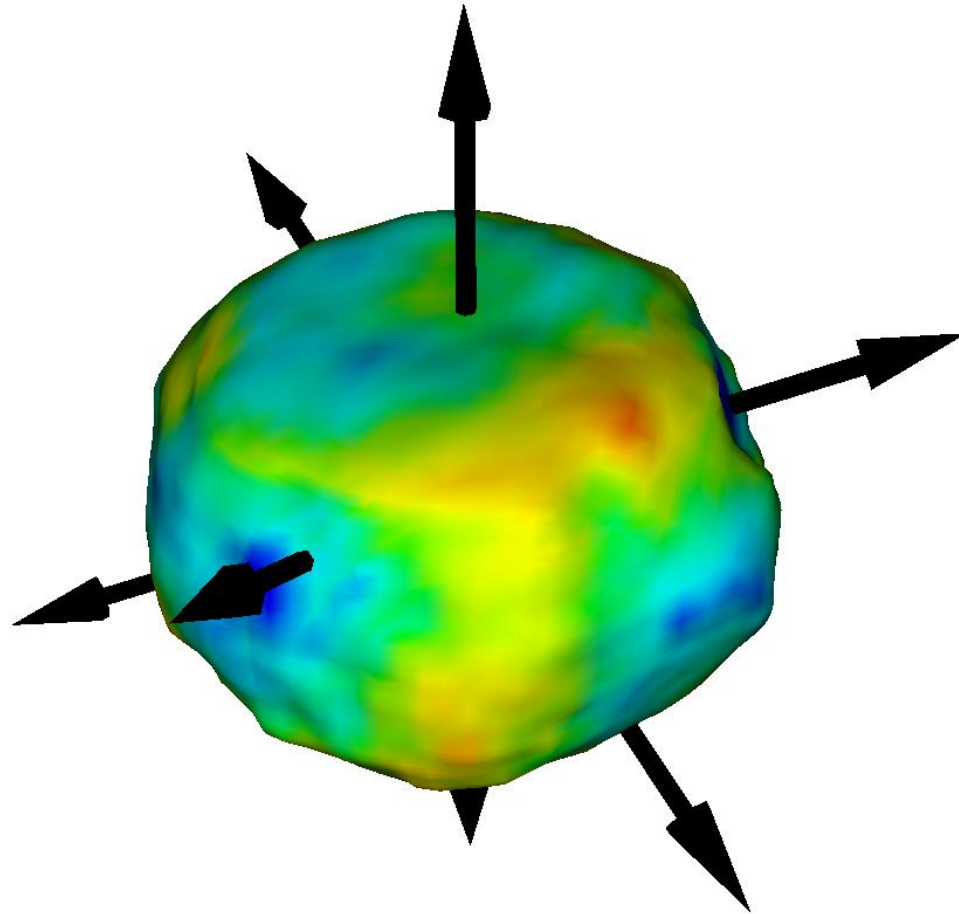


Gold nanocrystal reconstruction

showing support used for 20 HIO followed by 10 ER

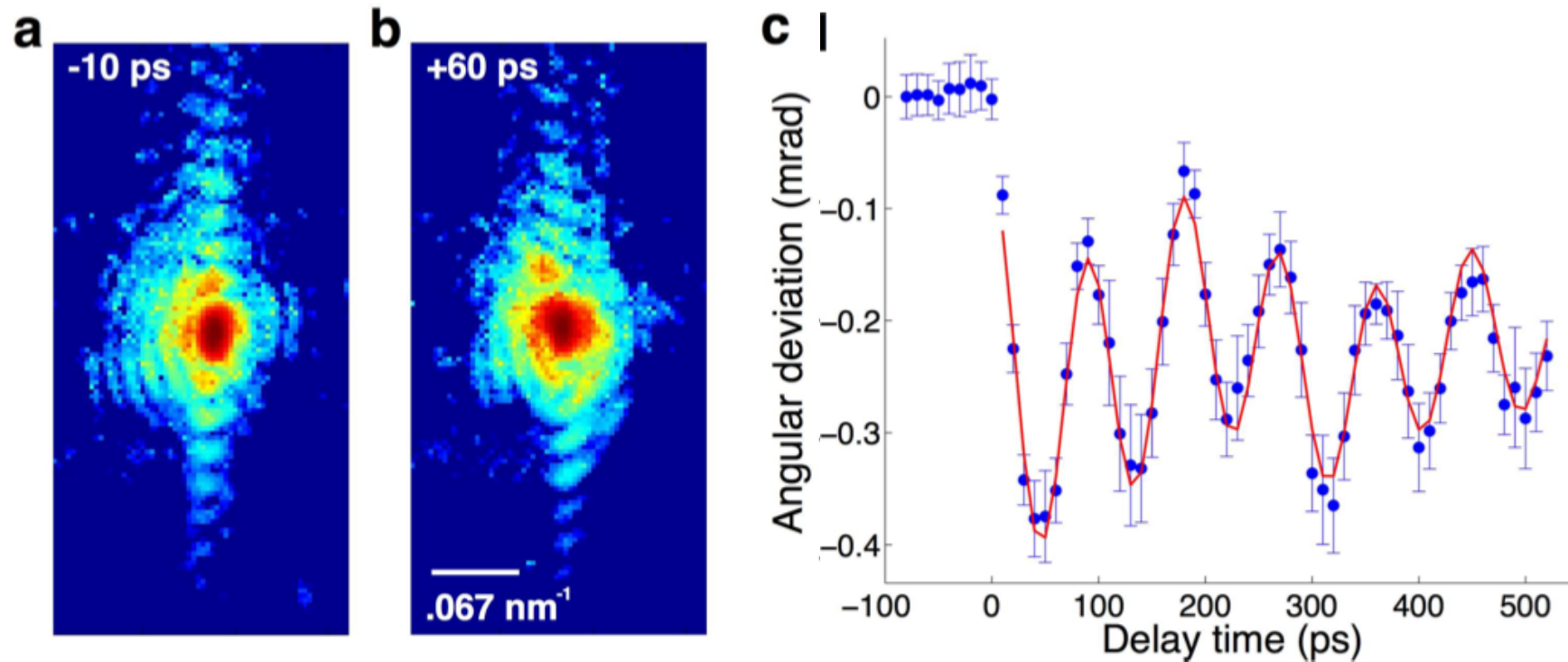


Phase isosurface of residual strain



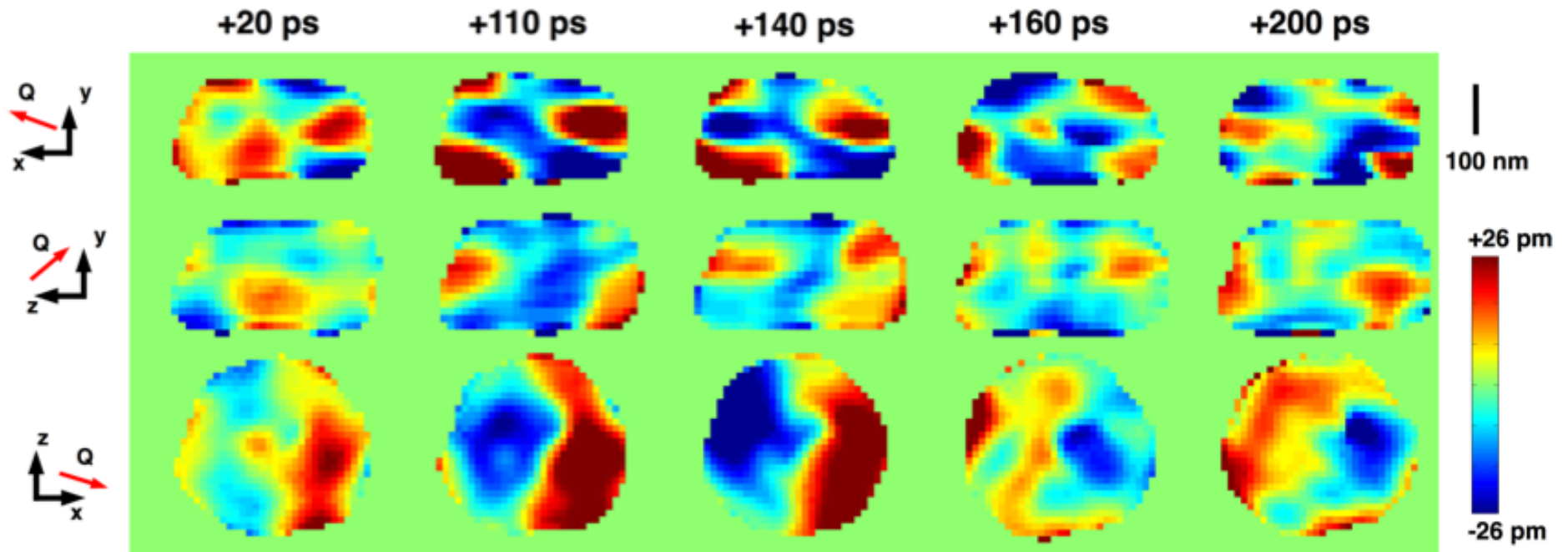
Ultrafast Imaging after Laser Heating

Jesse Clark et al (to be published)

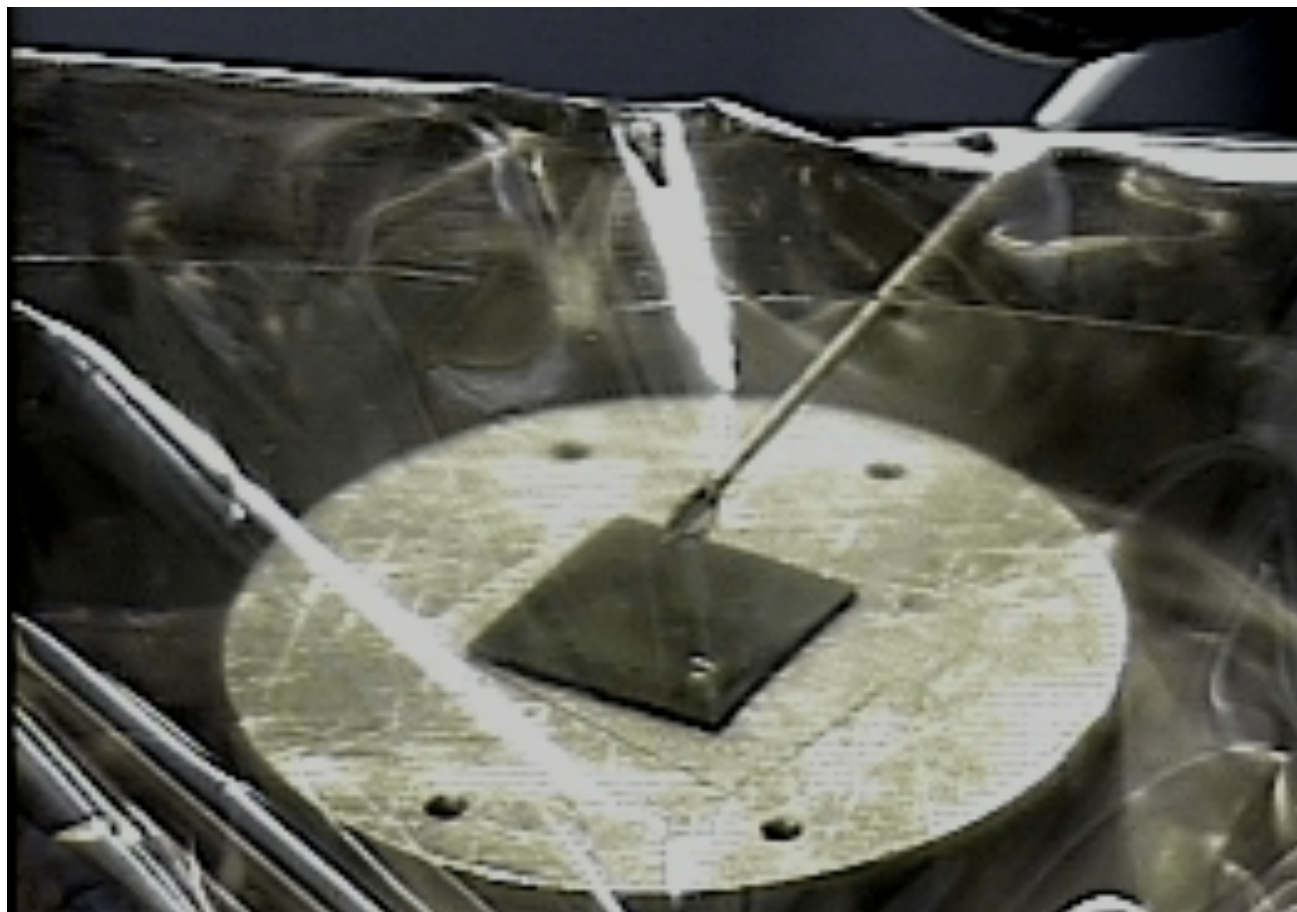


Ultrafast Imaging after Laser Heating

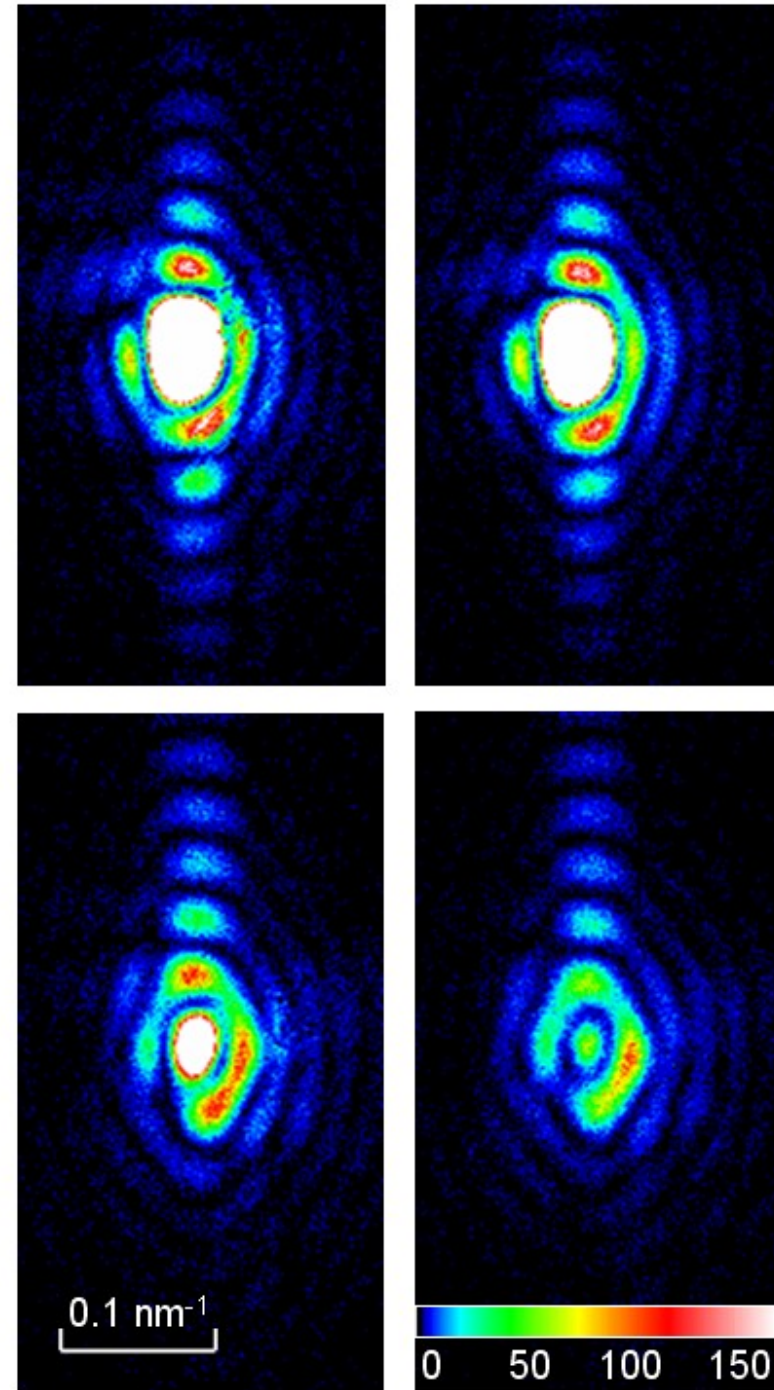
Jesse Clark et al (to be published)



Dosing with C_3H_7SH in ethanol



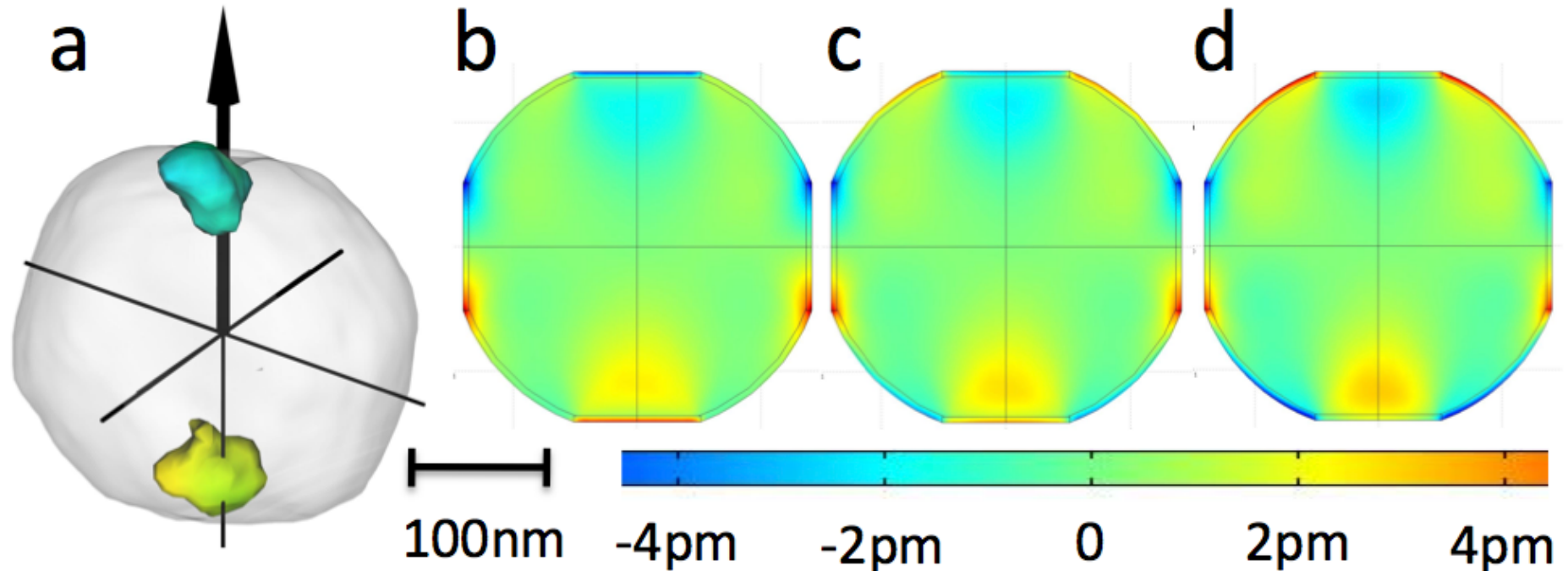
Diffraction pattern before and after dosing thiol on Au nanocrystal



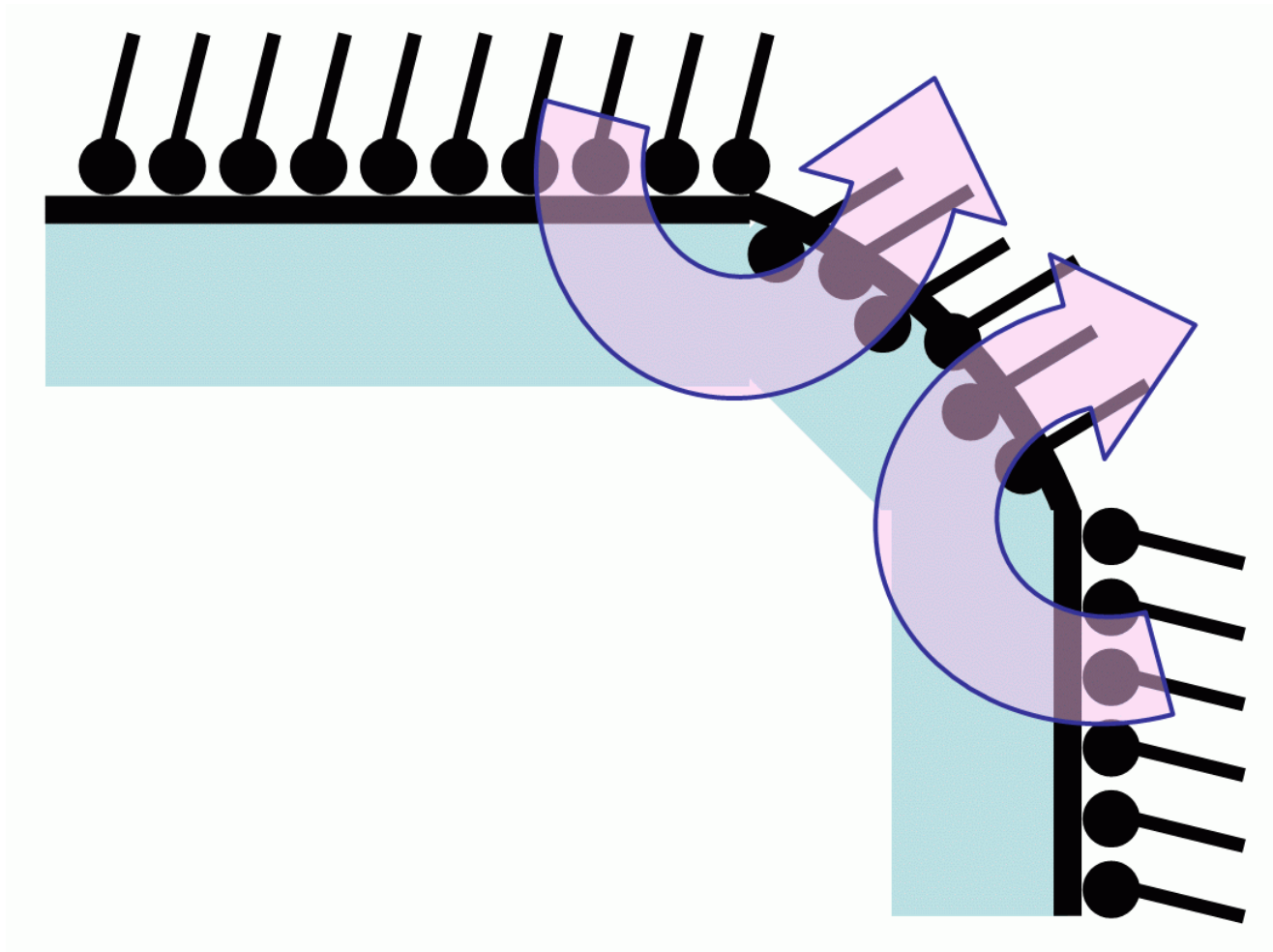
I. K. Robinson, UCL Scien

Finite-element Analysis

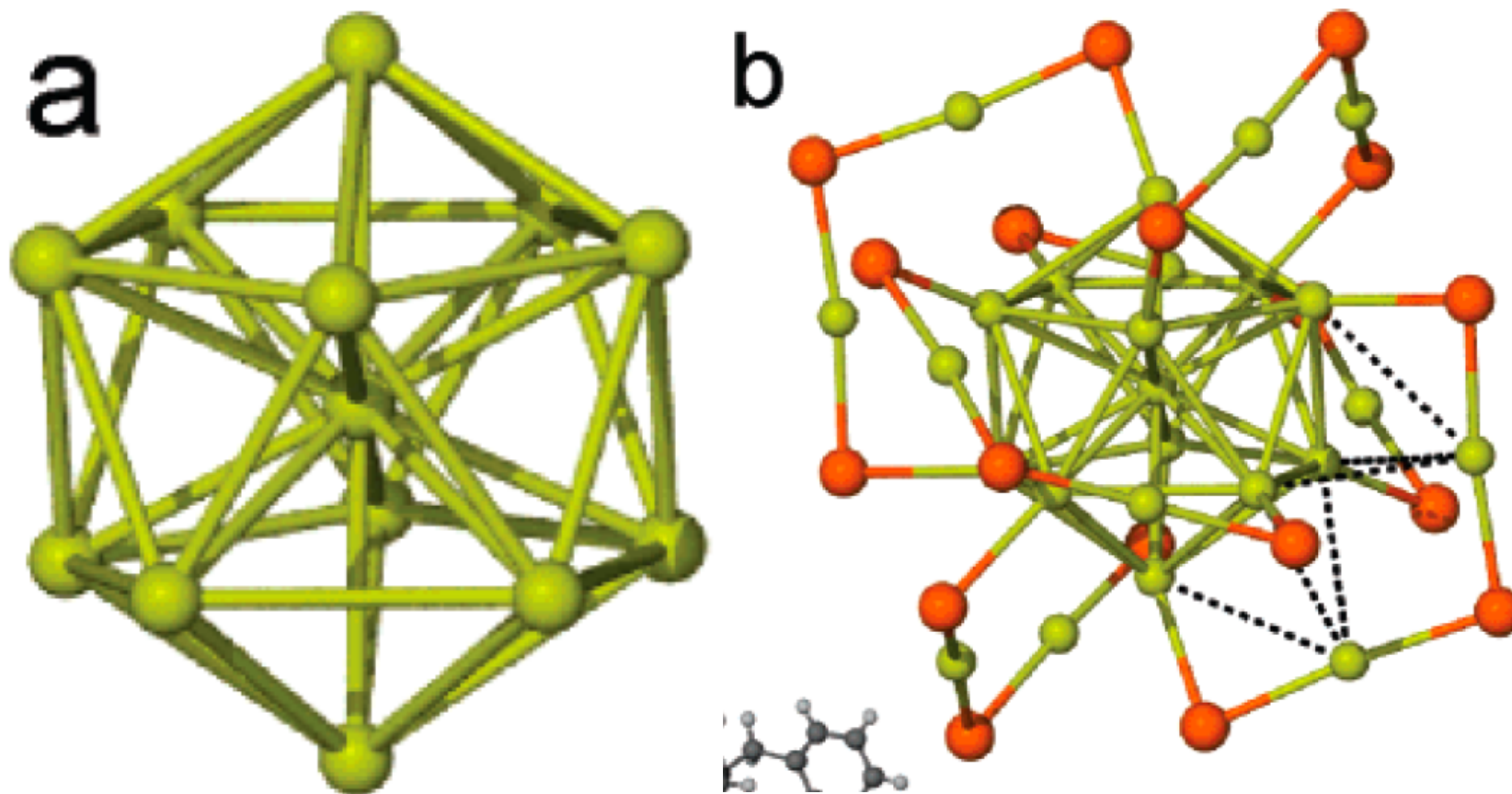
Differential stress introduced in “skin”
 $\pm 3 \times 10^8 \text{ Pa}$ in 5nm thickness = 1.5N/m



Differential adsorption, thiol/Au

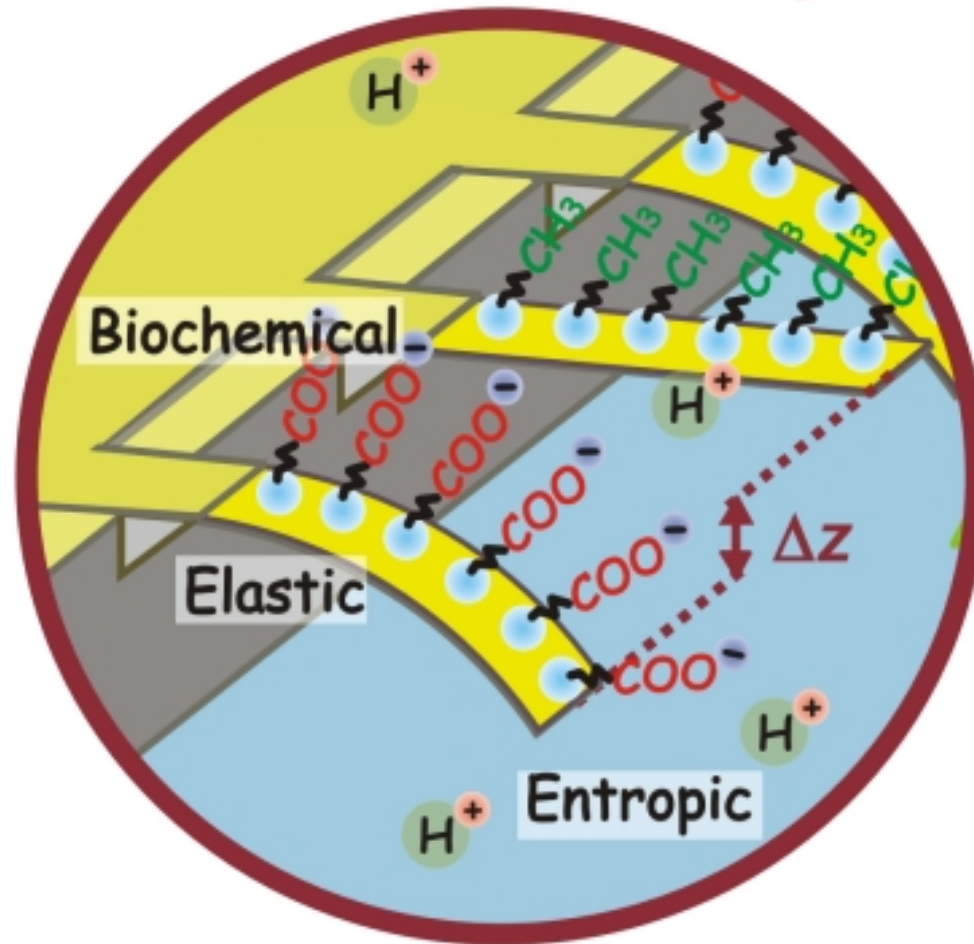


Gold-sulphur structure $\text{Au}_{13}(\text{Au}_2\text{RS}_3)_6$ $=\text{Au}_{25}\text{RS}_{18}$ Heaven et al, JACS 130 3755 (2008)



Nanocantilevers

Dr Rachel McKendrie, LCN



Conclusions

- 100 years of Bragg Diffraction
- Coherent Diffraction Imaging
- Nanocrystal shapes and strains
- Ultrafast imaging
- Strain changes upon coating
- Sensor activated by strain