Highlights and Summary

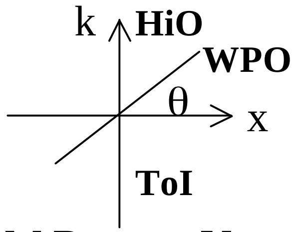
1. **Summary discussion**
2. **Next conference**
3. **Poster prize**
4. **Thanks.**

Summary

1. Nugent. Tutorial overview of phasing methods, as slices thro the Wigner fn. (FT of Mutual Coh. fn).

$dXdYdZ \quad dk_x dk_y \quad dk_z = 1$ *δ = 12 for ALS, δ <1 for electrons. $\delta = jA_c L_z/(2Ve)$

$A_c \quad L_z \quad \theta_x \theta_y \quad \Delta E$ *Use curved wavefront for unique inversion.



2. Fienup. 1. Get support of object from support of autocorrelation fn. JOSA 72, 610. M.Buerger Vector
2. HiO climbs out of local min. ER does not diverge. "oversampling" ?
3. Use gradient search methods instead of HiO. Minimize $E = \text{Sum } W(u)[\,|G(u)| - |F(u)|\,]^2$
4. Correlography (H-B Twiss).
5. Problems: Beam stop, Support for complex objects.

3. Van Dyck. 1. Best method - careful experimental design, model fitting with Max Likelihood metric CR
2. Resolution vs precision - σ_{CR} = resolution / sqrt(N) if N counts make a peak.
-example HREM of oxygen atoms at grain boundary in alloy.
3. P (No of params) < cell area/resolution^2. Rose criteria.
4. "A microscope is an information communication channel". Cramer-Rao.

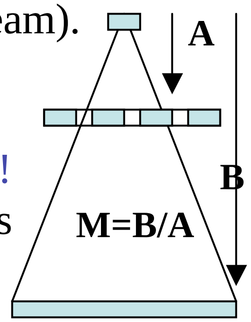
4. Weitkamp. 1. Hardware soln to phase problem - phase grating after object imposes Talbot fringes on an absorption grating.Grating interf. CCD measures transmission vs abs grating position.Moire.
Get differential phase contrast. M=1, contact print. Spider, lens. Shearing Interf.
2. Advantages: Large field of view, achromatic, quantitative, low resolution, no alignment

5. Bronnikov. 1. 3D reconstruction from projections - new algorithms. Lorenz and Radon transforms.
2. "2nd deriv of 3D Radon is propn to 2D Radon of phase contrast projection". $I = 1 - k\Delta^2 \phi$

6. Q. Shen. Nearfield HIO. M=1, resolution limited by detector pixels. cf Lindaas and Howells.

7. Wilkin. General formulation of in-line, near (or far)-field, partially coherent (X_c, ΔE) diffraction. Find optimum defocus, source size, deconvolution, "automatic" phase retrieval. (Fresnel fringes)

8. Mokso. Diverging beam point-projection method gives magnification. K-B mirrors for "point" source. Tomog. Results ! (Si at Al-Cu alloy gb ?). Need to characterise wavefield distortions. This is Gabor's original in-line holog. scheme (1949). Issues: 1. Res limited by source (smaller than CCD pixel ?. 2. At high mag, field of view small (number of res elements within beam).



9. Faulkner. Combine Ptychography ("Fold") with HIO. Get far-field patterns from a few overlapping areas illuminated by a probe. Escape the tyranny of the isolated sample ! Can be applied to previous speaker ! Fluctuation micros ? (variable coherence) Does atomistic imaging defeat the purpose of statistical characterisation ?

10. Wu. Clinical phase contrast, eg breast cancer. Record in near-field, get phase constrast sharpness, deduce absorption constrast from theory. (cf Nugent et al). Need only one image. (less dose). Hard X-rays

11. Grubel. **Hard X-ray correlation spectroscopy.** Measure autocorreltn in time of I(q) in far-field. ($g_2(\omega,q)$)
XPCS fills a gap between lasers (smaller q), neutrons (higher freqs).
Examples: polymers, surface waves (glycerol/water), liquid xtals, non-eqbm dynamics.
The future: new faster detectors, XFEL - 10^9 more coherent flux. ns - ps pulses. SASE. (0.2-14kV)

12. Ludwig. Kinetics of phase transitions by XPCS. Cu-Pd coursening kinetics. Anti-phase domains. Uses two-time corn fn $C(t_1,t_2,q) = f(t)$, because non-equilibrium, Langevin theory.
(Use HREM , electron microdiffraction. JMC ?)

13. Gutt. XPCS at grazing incidence of liquid surfaces. Also metal-polymer systems and thin wetting films. water-ethanol. Confined liquids - 1 -60nm thick film of hexane. Homodyne to hetrodyne transition

14. Scheffold. XPCS (+SANS) of dense colloids. Photonic liquids, Sol-gel ceramics, Microrheology, Food. (Yoghurt, cheese). 3D-DLS to minimize multiple scattering. Diffuse Wave Scattering uses multiple scattering (cf Feynman) to extract $<r^2>$ RMS vs conc. with amplified sensitivity. Diffusion coeff., relaxation times vs q. Get elastic modulus of gel. aggregation (egg white). Slow relaxation exptl.

15. Robert. Slow dynamics in 2D-XPCS colloids. Also magnetic particles (ferrofluids) ageing, glass transition. nm lengthscales, eqlbrm, or non eqlbrm., need **faster area detectors,** anisotropic dynamics.

16 Falus. S/N of XPCS with area detectors. Better detectors ! **Optimizing design for better S/N.**RSI 71,3274 best pixel size, slit width, match pixel shape to source, use focussing. SMD camera. Use modified visible light camera. RSI 76, 43702. **GET THIS**. Test with block co-polymer layers.

17 Sutton. XPCS of Cu3Au at APS. Excellent overview of Langevin dynamics. Measures two-time corrn fn. (non-equilibrium). Incubation time. Cross-correlates I at different q and time. Ordering kinetics.

18. Livet. Hetrodyne measurements of XPCS from carbon black in rubber. Hetrodyning works. Find recovery after 100% elongation. Model for relaxation tested. Works for opaque materials.

19. Sikharulidze. XPCS in layered smectic liquid crystal membranes. Three modes of relaxation. Specular measurements. Mosaicity defines window of wave vectors.

20. Lurio. XPCS of polymer bilayer. Capilliary waves studied using diffuse streak from grazing beam. Form standing wave with maximum at buried interface and, later, at surface. Slow relaxation at buried layer, fast and slow at surface. Compare with theory.

21 Robinson. Phase contrast. Record shape-transform of small particles around g. If strain get complex object Use HiO to reconstruct 3D shape of particle. Use g to avoid central beam. 50nm resolution.

22 Chapman. CXDI . Shrinkwrap+Brookhaven chamber+16 mac cluster. 3D pyramid.Virtual focusing.Depth of field. Aerogel in 3D. Application to XFEL -"inertial imaging". Common line method with 2.

23 Stadler. Antiphase domains in B2 intermetallics. XPCS, detrended fluctuation analysis. (DFA). Phasing XPCS data. Measure diffuse around (001) in FeAl. No compact support ! Use G-S algorithm. Get dark line for APD. 3 micron beam. Use illumination function instead of support.

24 Eisebitt. CXDI of magnetic structures. Resonant magnetic scattering at Co L3. **FT Holog** with second small hole. Big hole filled with object. Nature 442, 835. For storage media- domain reversal.Stroke. patterned magnetic media - CoPd coated balls. Imaged with field applied, movie. Res 50nm.

25 Jacobsen. CDXI of biol cells. Why Xrays ? Thicker samples. Damage -Xanes vs dose. Zone plates 15nm Advantages of CXDI: Better NA, no aberations, hence less dose. Chapman Corner. Cryo holder. Use zone plate for low res image ? No. Use PPM, or STXM. Yeast cell, freeze dried. 750 eV. Compare results from different random starting phases. Resolution-from FT of image. Dose Fractn

26 Vartaniants. CXDI on quantum dots (Ge on Si) in periodic array. Diffuse around 202 Bragg. Also grazing incidence. Multiple scattering in reflection.

27 Nishino. CXDI applications. e-coli, Au lithog in 3D, porous silicon. Iterative normalisation solution to beamstop problem. Faster on-beamline data analysis. IP Flex. 87 sec for 1000 itns of 1K^2. Image plate - 5K^2, 25 micron pixels. Rigaku.

29. Zuo Electron CXDI at atomic resolution. Long range order demands excellent angular resolution. Use of probe and aberrations as support for reconstruction of double-walled nanotube.

30 Chesnel Resonant Magnetic Scattering at ALS. Memory effect in CoPt - XRM and Speckle(t) patterns, new BL 12.0.2 Manganite orbital ordering -time dep of speckle. Perpendicular exchange bias thin film.

Quick comments, for discussion.

1. Resolution. Should be a property of the instrument, not the sample.
   Use test object, quote diffraction pattern limit, use spectrum of reconstruction
   Note - for phase contrast, res depends on phase diff thro' Au and C ball, or...

2. Do we want phased XPCS data ? Statistical characterisation in time vs atomistic for predicting properties. Use both into electronic str calculation.

2. Can CXDI ever achieve atomic resolution ? Next PP says no. 2K CCD, 2 samples per atom gives < 500 atom cube. Not enough signal.
   Can CXDI achieve atomic resolution with FEL ? LCLS (Henry) gives same number of photons in 1/10 of a 200ns pulse as entire pyramid 3D data had.
   But, nanoparticle would explode !. For XPCS, use second pulse-cross correlate.

3. Beam-stop problem. Solns. 1. Nishino's normalisation. 2. Small windows 3. Eisebitt's masking. 4. Fast readout. 5. Hole in detector, tiled detector.

4. M. Howells. Dose goes as resolution^{-4}. Coherence width should be twice object width. Antiphase domains Zhu/Cowley **Acta A38, 718.** TEM movies of interfaces at atomic resolution at high temp.... **Ultramic 56, 225**

5. Reliability of algorithms. Prepared substrates, Fragment completion URA, FTH.

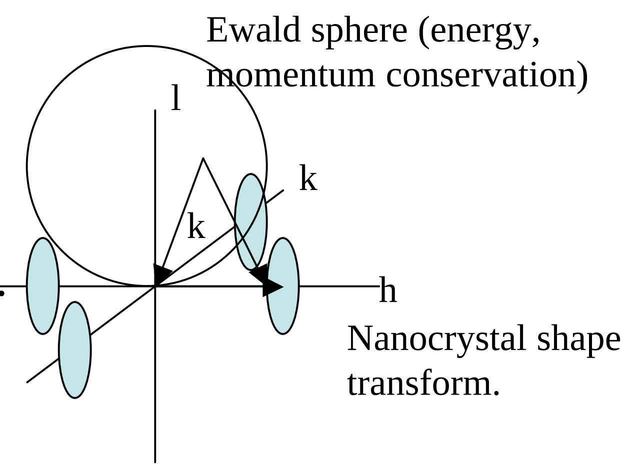
6. Find Killer Application ! (Cloetens, Wilkens)

Is atomic-resolution diffractive imaging possible with X-rays ?

Consider 10nm nanoparticle, HAP. Spring-8. **5 kV** Undulator, λ = 2 Ang, Si mono, zone-plate.

* After Si mono, flux is 10^{13} photons/sec.
*Rocking curve width for InSb nanodot is **12 millirads** for 10nm thickness.
*Cannot fill this with zoneplate, which limits divergence to 2mrad for 100nm outer zone.
*Horizontal divergence FWHM is 40 microradians, allowing X50 demag.
* Source size is 25 X 500 microns FWHM, becomes 0.5 X 10 microns.
*Flux into 10nm square is $10^{13} * 0.01^2 / (0.5*10) = 2X10^4$ photons/sec.
*Diffraction efficiency for 10nm thickness is 3.4×10^{-4},
* This gives **7 X 10^4 photons/sec into (111) at 2 mRad** (more with worse mono).
*Spatial coherence needed for HiO is $X_c = 20\text{nm} = \lambda/\Delta\Theta$, so need $\Delta\theta < 10$ mRad (we have 2mR)
*Damage ? Cooling ? Better with TEM tomog ?

How to fake atomic resolution now….
(place experimental diffuse around every recip lattice point).



Eg **Robinson, Vartanyants et al PRL 87, 195505 (2001).**

Homometric structures.

One family of homometric structures (**Acta Cryst 7, p. 237**; Pauling's Bixbyite) may be generated using the result that…..

$$\rho_1(r) = l(r) * m(r)$$

and

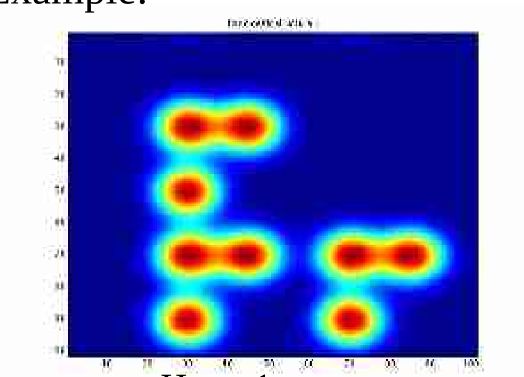
$$\rho_2(r) = l(r) * m^*(-r)$$

$$\textit{have same Fourier modulus } |R(u)|, \textit{ since}$$

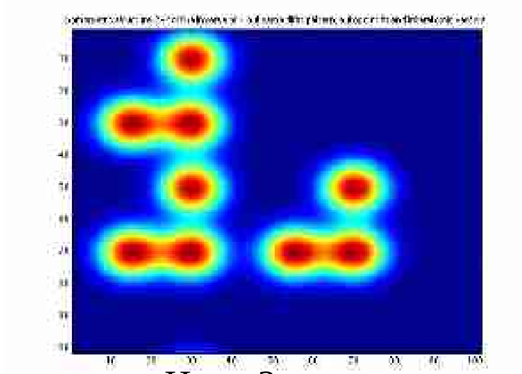
$$R_1(u) = L(u)M(u) \quad and \quad R_2(u) = L(u)M^*(u)$$

If l(r) is a lattice and m(r) a molecule, then m, m* are enants, but ρ_1, ρ_2 are not enants.

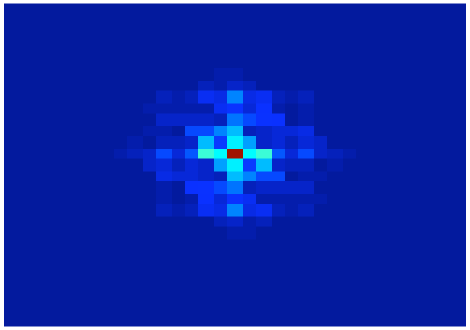
Example:



Homo1



Homo2



Fourier Mod of either

Note: Homo1 is not the inverse (enantiomorph) of Homo2.

Conclusion: HiO could not distinguish these unless tight support provided.

Distinguished by Multiple scattering ELNES!

Next conference ? - 2007.

*M.Howells Asiloma.80 miles south of SFO.Wild pacific coast.BookNow !
*G. Van der Veen et al . Return to Pork Rolls !
*R. Millane New Zealand (Lord of the Rings)
*Gerhard Grubel. Hamburg. (Rostock ?)
*I. Robinson,Diamond,Gerrit Van der Laan UK. LakeDistrict,Cowes
*C. Jacobsen. Skiing in Colorado
*Nugent/Wilkens. Tasmania.
*Suny Sinha San Diego.
*Saldin (Wisc) , L. Marks. Chicago.

Require: Cheap for students, direct flights, local organiser with budget. ($30K ?)

Nice places: Greek islands, Tuscany (Volterra), Lake Como(Bellagio),Sicily,Crete,Hawaii
Result: Try Asiloma first.

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Poster prizes. Till Metzger