Coherent Diffraction
APS Undulator Workshop

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Mark Sutton
Centre for the Physics of Materials
McGill University

Why Coherence?

Coherence allows one to measure the dynamics of a material (X-ray Intensity Fluctuation Spectroscopy, XIFS).

$$\langle I(\vec{R},t)I(\vec{R}+\delta\vec{R},t+\tau)\rangle =$$
$$\langle I(R)\rangle^2 + \beta(\vec{\kappa})\ \frac{k^8}{(4\pi R)^4} V^2 I_0^2 \left|S(\vec{Q},t)\right|^2$$

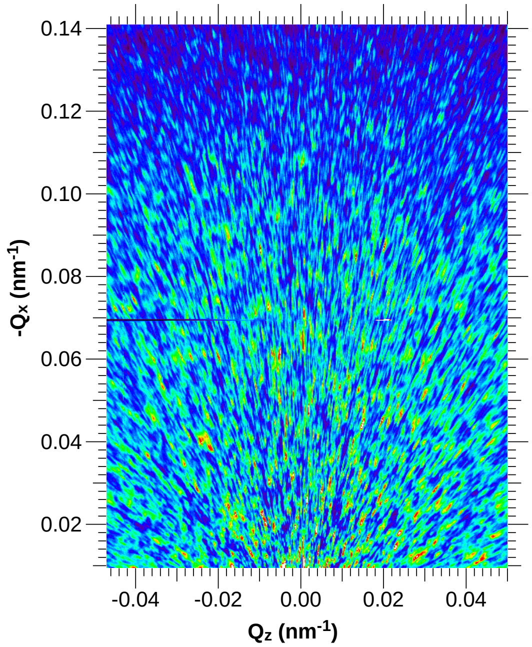
where the coherence factor is defined as:

$$\beta(\vec{\kappa}) =$$
$$\frac{1}{V^2 I_0^2}\int_V\int_V e^{i\vec{\kappa}\cdot(\vec{r}_2-\vec{r}_1)} \left|\Gamma(\vec{0},\vec{r}_2^{\perp}-\vec{r}_1^{\perp},\frac{\vec{Q}\cdot(\vec{r}_2-\vec{r}_1)}{\omega_0})\right|^2 d\vec{r}_1 d\vec{r}_2$$

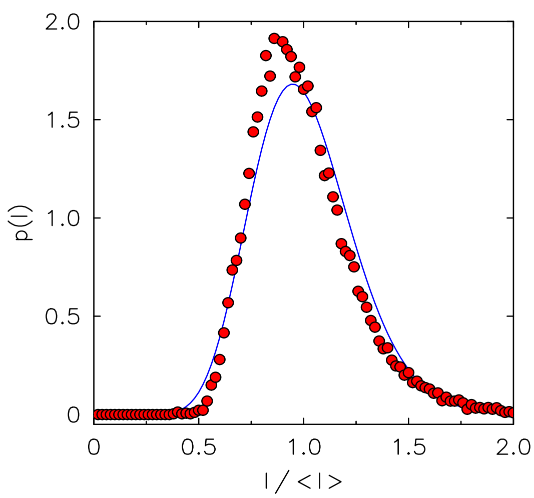
A good estimate for β is:

$$\beta(\vec{0}) \approx \frac{V_{coherence}}{V_{scattering}}$$

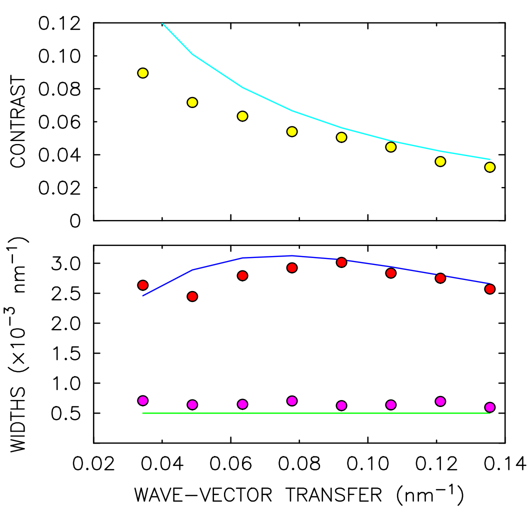
Coherent X-Rays and X-Ray Speckle



Scattering from an aerogel under partially-coherent x-ray illumination at 8-ID-E. The intensity fluctuations constitute x-ray speckle.

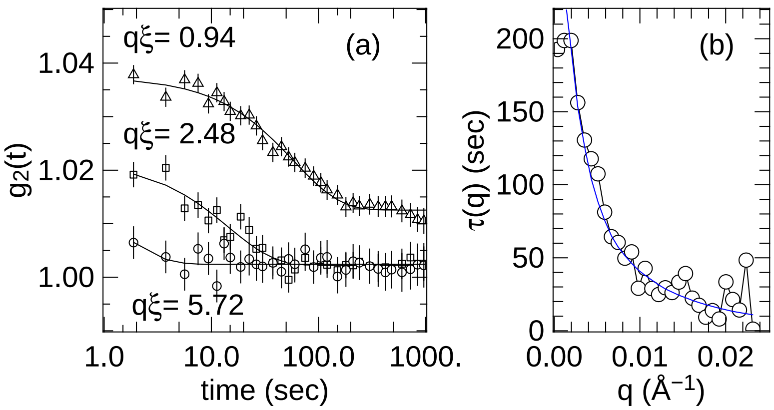


Speckle intensity distribution in a ring of scattering at $Q = 0.08$ nm^{-1} ($\circ$ = data, — = theory). The speckle contrast is $\mathrm{var}(I)/\langle I \rangle$.



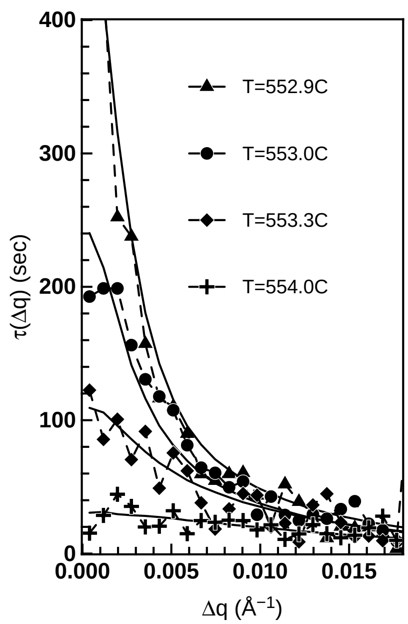
Comparison between data obtained at 8-ID ($\circ$) and theory (—) for the speckle contrast and speckle widths, as measured by the spatial autocorrelation of the speckle pattern.

Time Correlations in Fe_3Al



(a) Measured autocorrelation functions versus time delays for various Q's for sample at T=553.3C. The solid line corresponds to a single exponential fit. (b) Fitted time constants versus Q.

Measured autocorrelation functions versus Q for several temperature near T_c. The solid line is a scaled S(Q) and shows S(Q) is proportional to the measured time constants in this system.



Signal to Noise

One can show that the signal to noise in an X-ray intensity fluctuation spectroscopy measurement is:

$$\frac{s}{n} \approx \beta(\vec{0}) \sqrt{N_{speckles}}\, B_0\, \lambda^2 \,\frac{\Delta E}{E}\, \frac{d\sigma}{d\Omega} L$$

Reference: Area detector based photon correlation in the regime of short data batches: data reduction for dynamic x-ray scattering, D. Lumma, L.B. Lurio, S.G.J. Mochrie, and M. Sutton, Rev. Sci. Instr. **71**, 3274-3289 (2000).

Mutual Coherence Function

Define

$$\Gamma(\vec{r}_1, \vec{r}_2, t_1, t_2) = \langle E^*(\vec{r}_1, t_1) E(\vec{r}_2, t_2) \rangle.$$

where $\vec{E}(\vec{r}, t)$ is the electric field. Also define

$$W(\vec{r}_1, \vec{r}_2, \nu) = \int_{-\infty}^{\infty} \Gamma(\vec{r}_1, \vec{r}_2, \tau) e^{2\pi i \nu \tau} d\tau$$

and it's normalized form:

$$\mu(\vec{r}_1, \vec{r}_2, \nu) = \frac{W(\vec{r}_1, \vec{r}_2, \nu)}{W(\vec{r}_1, \vec{r}_1, \nu)^{1/2} W(\vec{r}_2, \vec{r}_2, \nu)^{1/2}}.$$

Finally, it is easy to see the relationship of $W(\vec{r}_1, \vec{r}_2, \nu)$ to correlations in the frequency dependent electric fields:

$$\langle E^*(\vec{r}_1, \nu_1) E(\vec{r}_2, \nu_2) \rangle = W(\vec{r}_1, \vec{r}_2, \nu_1) \delta(\nu_1 - \nu_2).$$

Reference: Coherent X-ray Diffraction, Mark Sutton Chapter in **Third-Generation Hard X-ray Synchrotron Radiation Sources: Source Properties, Optics, and Experimental Techniques**, edited by. Dennis M. Mills, John Wiley and Sons, Inc, New York, (2002).

Relationship to Brightness

The conventional brightness has the form:

$$B(\vec{r},\hat{s},\nu) = \frac{1}{4\pi^2}\,\frac{I_0 H(\nu)}{\sigma_{s_h}\sigma_{s_v}\sigma_h\sigma_v} e^{-(\frac{x^2}{2\sigma_h^2}+\frac{y^2}{2\sigma_v^2})} e^{-(\frac{s_x^2}{2\sigma_{s_h}}+\frac{s_y^2}{2\sigma_{s_v}})}$$

where $\hat{s} = (s_x, s_y, 1) = (x/z, y/z, 1)$, the σ's are the beam sizes and angular spreads and $H(\nu)$ is frequency spectrum.

Brightness is related to coherence

$$B(\vec{r},\hat{s},\nu) = k^2\; I(\vec{r})H(\nu)\frac{1}{(2\pi)^2}\int \mu(\vec{v})e^{ik\hat{s}_\perp\cdot\vec{v}}d\vec{v}$$

and we can show that

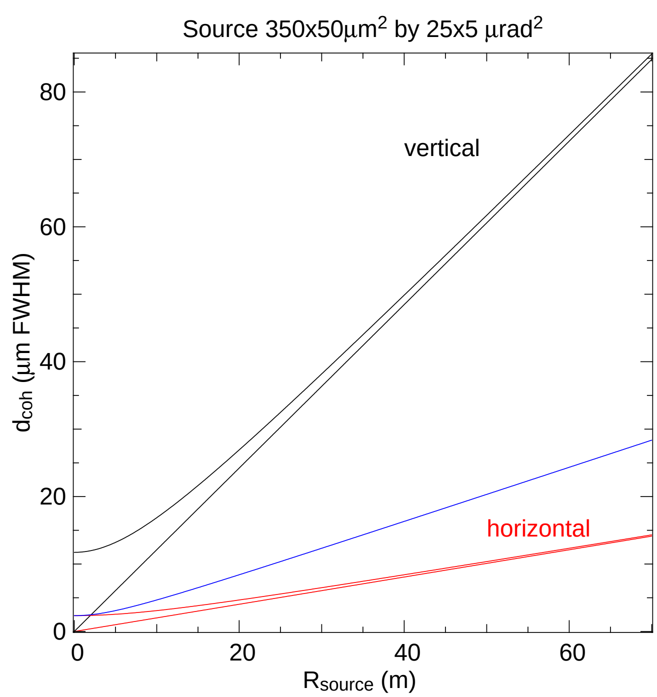
$$W(\vec{r}_1,\vec{r}_2,\nu) = \frac{I_0 H(\nu)}{2\pi\sigma_h\sigma_v} e^{-(\frac{(x_1+x_2)^2}{8\sigma_h^2}+\frac{(y_1+y_2)^2}{8\sigma_v^2})} e^{-(\frac{(x_2-x_1)^2}{2\rho_h^2}+\frac{(y_2-y_1)^2}{2\rho_v^2})}$$

where ρ_i are coherence lengths and $\rho_i \;=\; 1/(k\sigma_{s_i})$.

Undulator A Coherence Lengths

Can propagate the partial coherence to experimental station and the coherence lengths are:

$$d_{coh} = \rho_i \sqrt{1 + \left(\frac{z}{k \sigma_i \rho_i} \right)^2}$$



Coherence lengths of an undulator source versus distance. The coherence lengths for an incoherent sources are plotted for comparison. Blue line is shrinking horizontal size half.

Detector Resolution

Speckle size (width of $\beta(\vec{\kappa})$) is given by diffraction limit of beam:

$$\Delta\theta \approx \frac{\lambda}{d_{coh}}$$

Need to resolve this on detector, so want detector size to be close to d_{coh} i.e.

$$\frac{\lambda}{d_{coh}} \approx \frac{d_{coh}}{R_{det}}$$

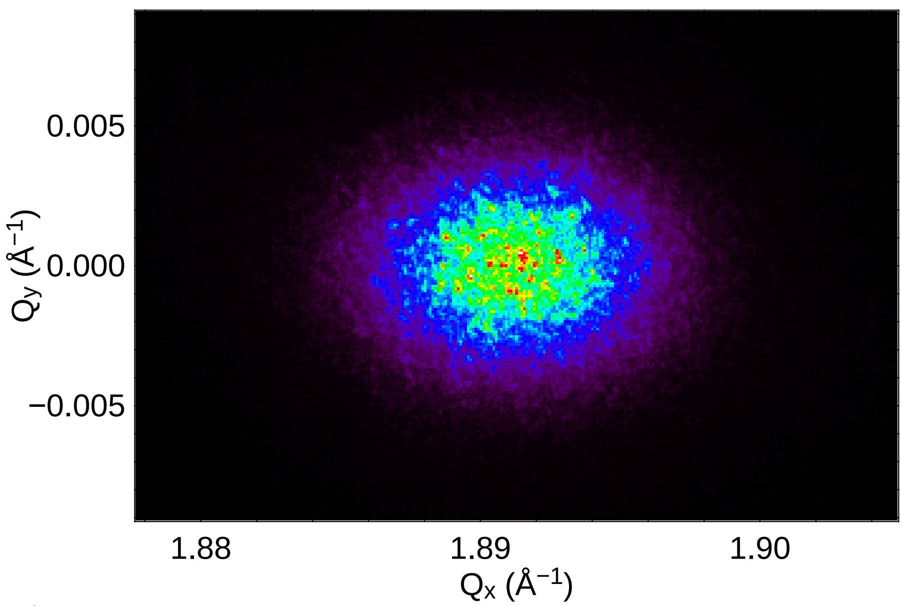
or

$$R_{det} = \frac{d_{coh}^2}{\lambda}$$

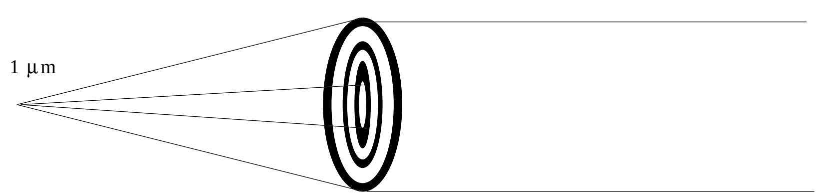
Problem if horizontal and vertical lengths are too different. Also, we don't want the coherence length to be too large as this would not match detector size or it will be too far away for optimum. Similarly, don't want too large a mismatch between speckle size and the diffraction width of the scattering under study.

Optics

With perfect optics, one can trade coherence length for angular spread. Thus one could demagnify the vertical (by .25) and magnify the horizontal (by 2) to get 20 μmx20 μm coherence lengths as this matches the typical CCD pixel size. But optics need not be 100% transmissive and tends to add aberrations. Need to consider which undulator output best matches required optics. (Note: We also need better optics.)



(100) peak of disordered Fe_3Al taken using a zone plate with 1 μm focal spot.



Fresnel Zone Plate