International Work Shop on Phase Retrival
and Coherent Diffraction

X-ray Intensity Fluctuation Spectroscopy of the Ordering in Cu_3Au

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Collaborators

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Outline

Why Coherence?

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

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

where the coherence function is defined as:

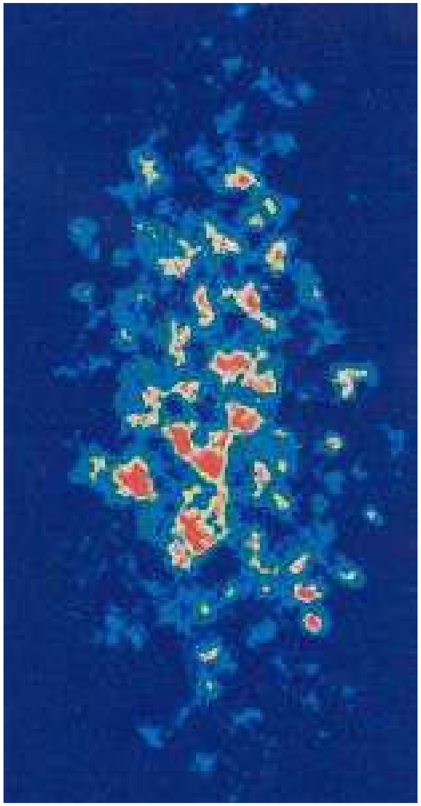
$$\beta(\vec{\kappa}) = \frac{1}{V^2 I_0^2} \int_V \int_V e^{i\vec{\kappa}\cdot(\vec{r}_2-\vec{r}_1)} \left| \Gamma(\vec{0}, \vec{r}_2^{\perp} - \vec{r}_1^{\perp}, \frac{\vec{Q}\cdot(\vec{r}_2-\vec{r}_1)}{\omega_0}) \right|^2 d\vec{r}_1 d\vec{r}_2$$

A good estimate for β is: $\beta(\vec{0}) \approx \frac{V_{coherence}}{V_{scattering}}$

Reference: M. Sutton, Coherent X-ray Diffraction, 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).

Coherent diffraction

(001) Cu_3Au peak



Sutton et al., The Observation of Speckle by Diffraction with Coherent X-rays, Nature, **352**, 608-610 (1991).

Langevin Dynamics

$$\frac{\partial \Psi(\vec{x},t)}{\partial t} = M\nabla^2 \frac{\partial F}{\partial \Psi} + \eta(\vec{x},t)$$

$$\langle \eta(\vec{x},t) \rangle = 0$$

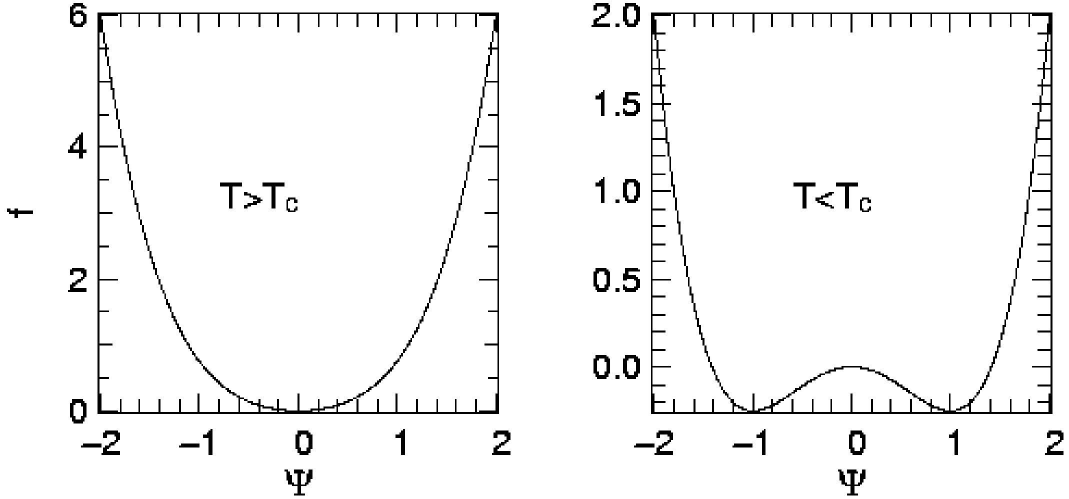
generalized Einstein-Stokes

$$\langle \eta(\vec{x},t)\eta(\vec{x}',t') \rangle = -2M\nabla^2 k_b T \delta(\vec{x}-\vec{x}')\delta(t-t')$$

Which is linear using the free energy: $F = \int \left(\frac{\kappa|\nabla\psi(\vec{x},t)|^2}{2} + \frac{r\psi^2}{2} \right) d\vec{x}$

Phase transitions kinetics

$$F = \int \left(\frac{\kappa |\nabla \psi(\vec{x},t)|^2}{2} + \frac{r\psi^2}{2} + \frac{u\psi^4}{4} \right) d\vec{x}$$

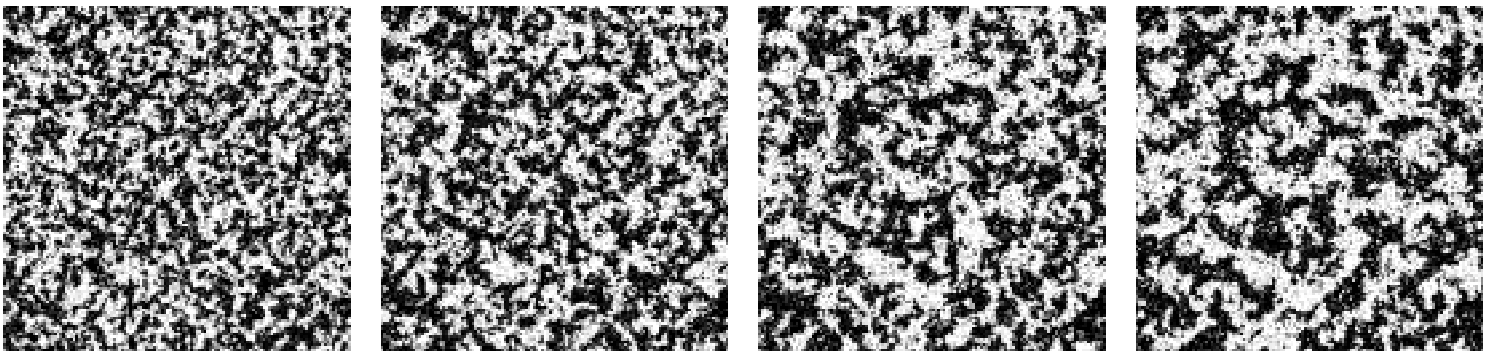


Non-Conserved (model A): $L \sim t^{1/2}$

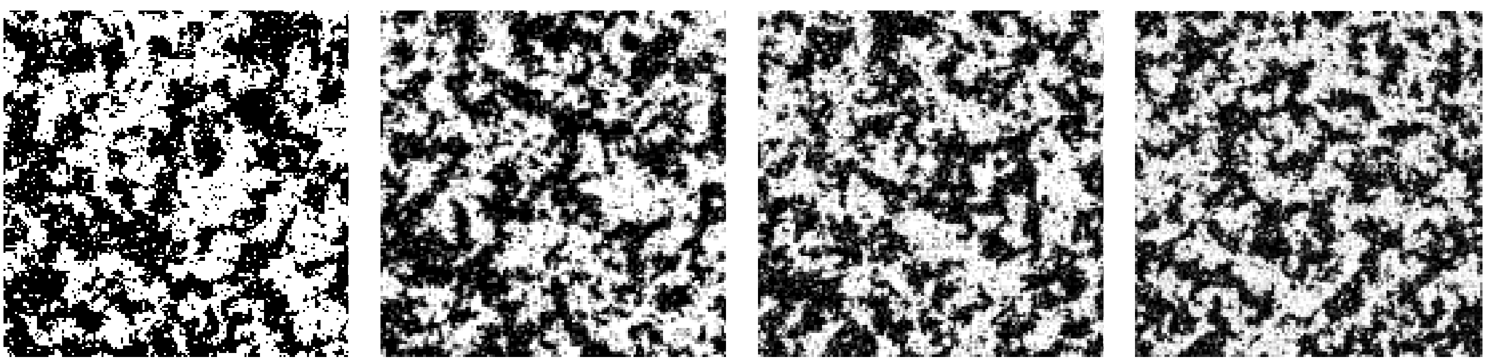
Conserved (model B): $L \sim t^{1/3}$

Scaling of Ising model

time=50 t=100 t=200 t=400



$2\sqrt{2}L$ $2L$ $\sqrt{2}L$ L



Scaling

$$S(q,t,T) = \langle \Psi^*(\vec{q},t)\Psi(\vec{q},t)\rangle_T$$

$$\varepsilon = |T - T_c|/T_c$$

$$\xi \simeq \alpha_0 \varepsilon^{-\nu}$$

$$\tau \simeq \alpha_1 \varepsilon^{-z\nu}.$$

Scaling implies:

$$S(q,\varepsilon,t) = b^{\gamma/\nu} S(qb, \varepsilon b^{1/\nu}, tb^{-z}).$$

Power Laws Galore

temperature dependence, $b=\varepsilon^{-\nu}$, $q=0$ or $q \ll \xi^{-1}$

$$S(0,\varepsilon,t)=\varepsilon^{-\gamma}S(0,1,t\varepsilon^{\nu z})$$

susceptibility, infinite t $(t \gg \tau)$

$$S(0,\varepsilon,\infty)=\varepsilon^{-\gamma}S(0,1,\infty)$$

wavevector dependence, $b=q^{-1}$, $(\varepsilon \ll (q\alpha_0)^{1/\nu})$ and $(t \gg \alpha_1(\alpha_0 q)^z)$

$$S(q,0,\infty)=q^{-\frac{\gamma}{\nu}}S(1,0,\infty)$$

time dependence, $b=t^{1/z}$

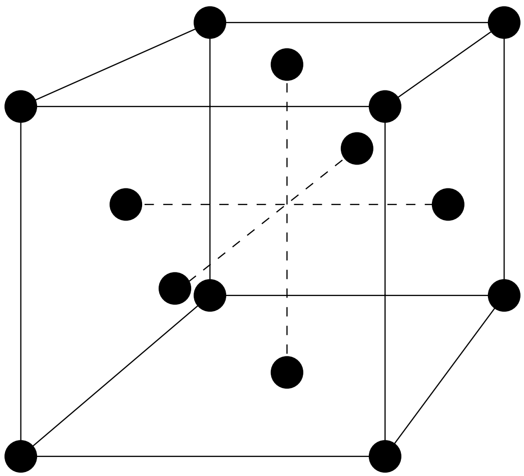
$$S(q,\varepsilon,t)=t^{\gamma/\nu z}S(qt^{1/z,},\varepsilon t^{1/\nu z},1)$$

$t \ll \alpha_1/(\alpha_0 q)^z$ and $t \ll \alpha_1\varepsilon^{-z\nu}$

$$S(q,\varepsilon,t)\simeq t^{\gamma/\nu z}S(0,0,1)$$

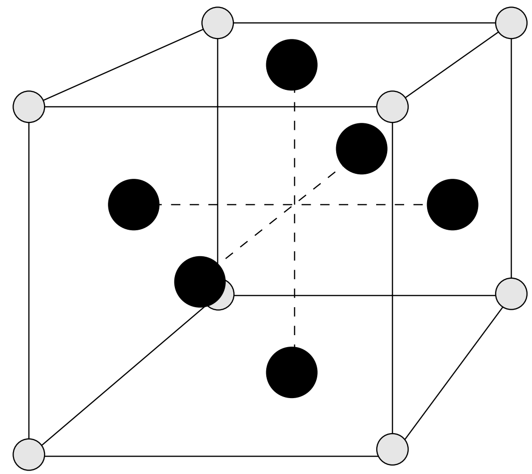
Order-disorder phase transitions in Cu_3Au

Disorder:



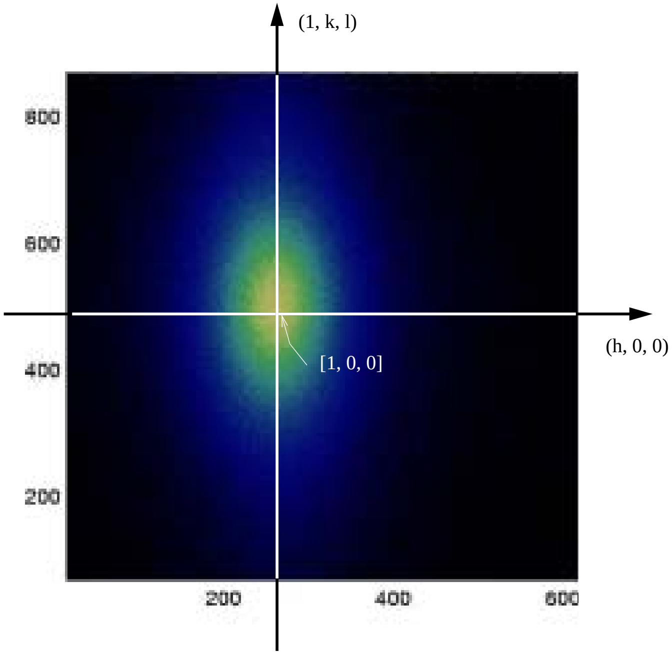
f=0.75 f_{Cu}+0.25 f_{Au}

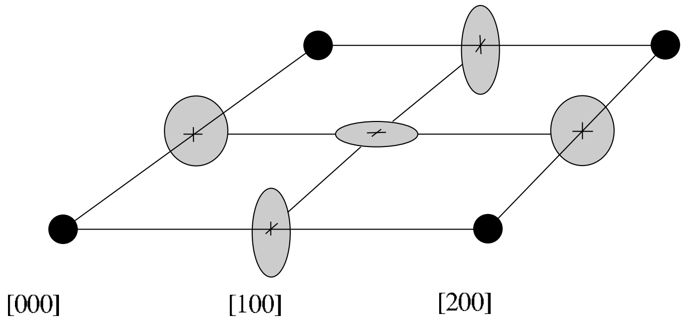
Order:



f_{Cu}, f_{Au}

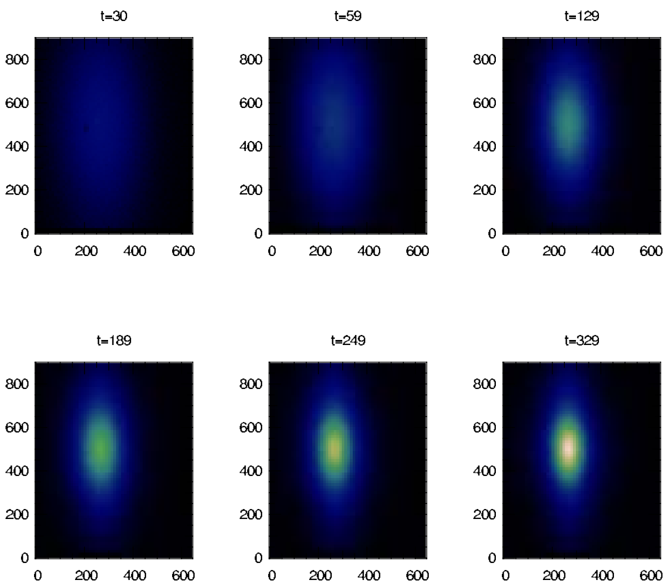
Scattering from Cu_3Au

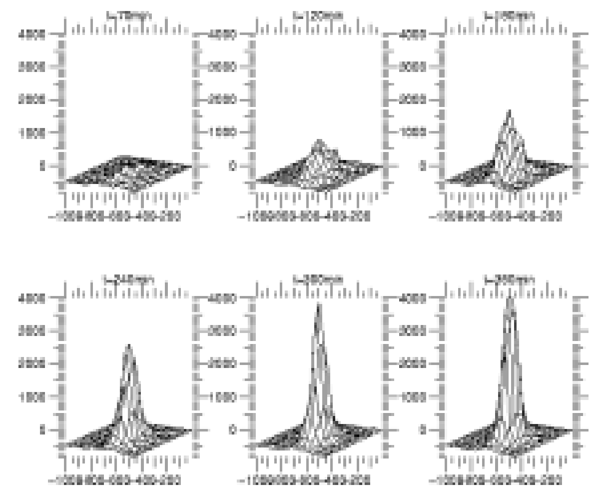




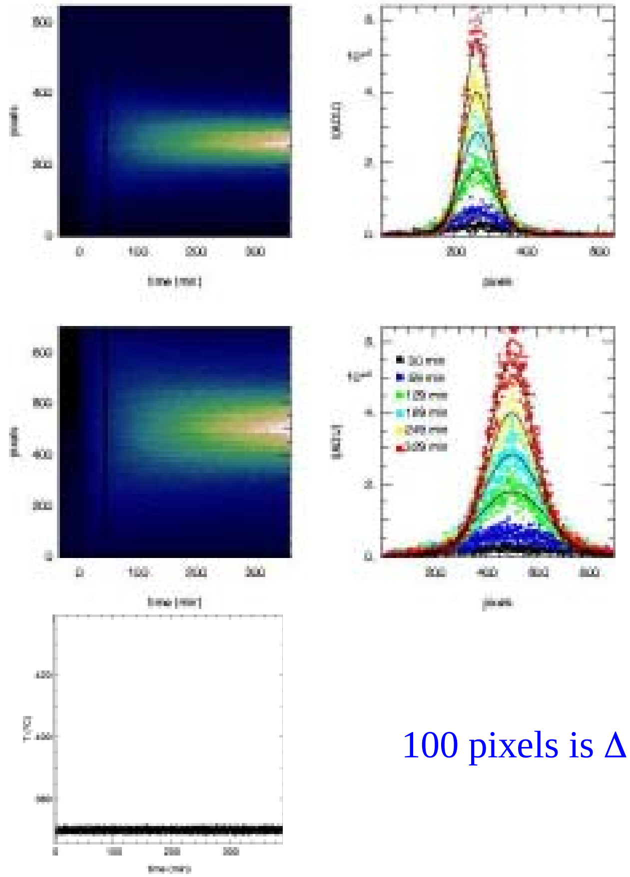
B.E.Warren, *X-ray Diffraction*, Dover, NY, 1969,1990

Scattering from Cu_3Au





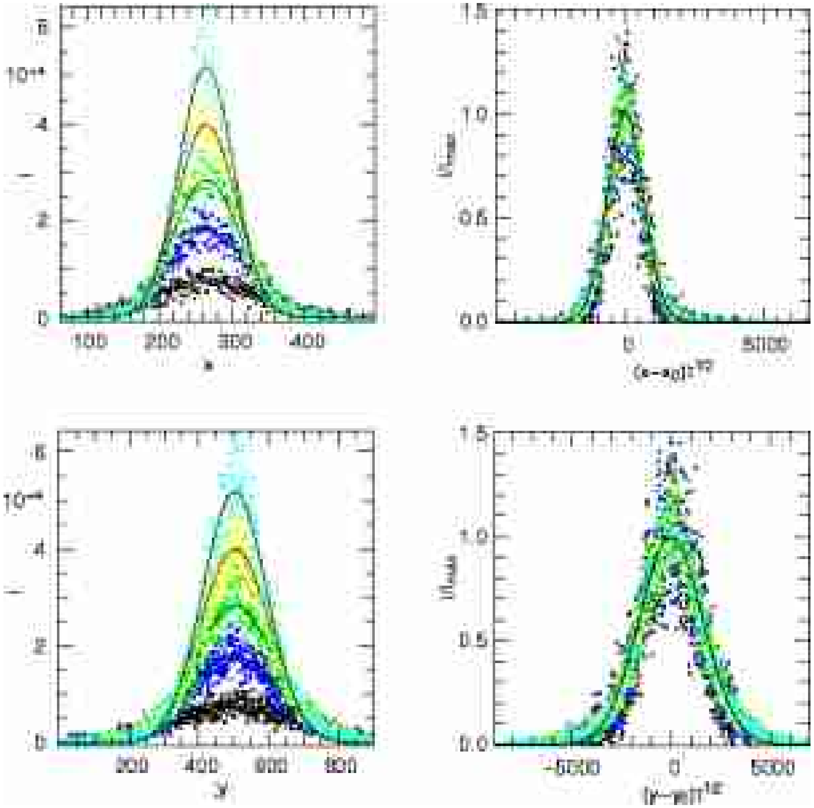
Time resolved scattering of Cu_3Au



100 pixels is $\Delta|\vec{Q}| = .0009$ Å^{-1}.

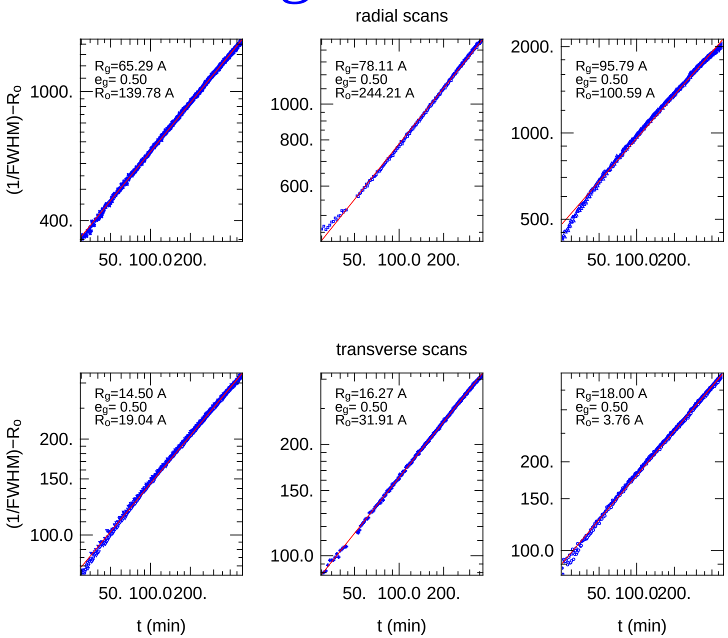
Scaling

Scaling $\quad I/I_{max} = f\left(qt^{1/2}\right)$



Power Law

Domain growth $L \sim t^{1/2}$



(a) 360°C (b) 370°C (c) 375°C

Gaussian Decoupling

$$\langle I(\vec{q},t_1)I(\vec{q},t_2)\rangle_T = \langle \Psi^*(\vec{q},t_1)\Psi(\vec{q},t_1)\Psi^*(\vec{q},t_2)\Psi(\vec{q},t_2)\rangle_T$$

$$= \langle \Psi^*(\vec{q},t_1)\Psi(\vec{q},t_1)\rangle_T \langle \Psi^*(\vec{q},t_2)\Psi(\vec{q},t_2)\rangle_T$$

$$+\langle \Psi^*(\vec{q},t_1)\Psi(\vec{q},t_2)\rangle_T \langle \Psi^*(\vec{q},t_2)\Psi(\vec{q},t_1)\rangle_T$$

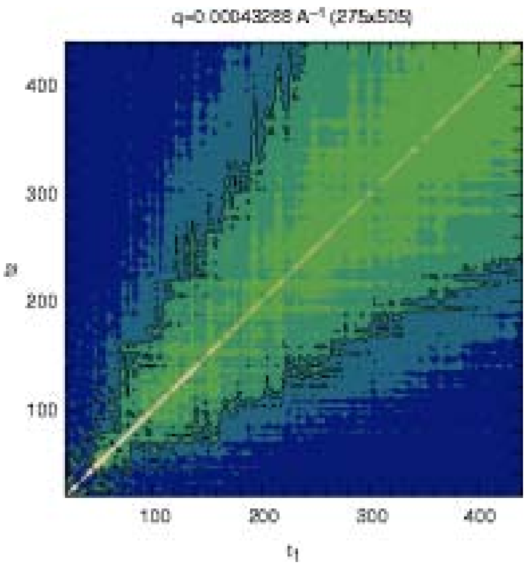
$$+\langle \Psi^*(\vec{q},t_1)\Psi^*(\vec{q},t_2)\rangle_T \langle \Psi(\vec{q},t_1)\Psi(\vec{q},t_2)\rangle_T$$

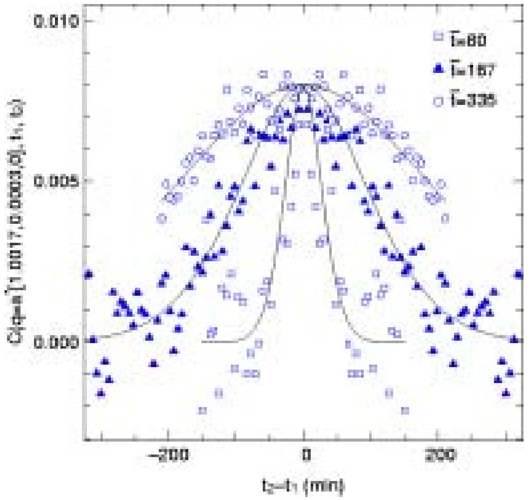
$$= [1+\delta(\vec{q})]S^2(\vec{q},t_1,t_2) + \langle I(\vec{q},t_1)\rangle_T \langle I(\vec{q},t_2)\rangle_T$$

Where: $S(\vec{q},t_1,t_2) = \langle \Psi^*(\vec{q},t_1)\Psi(\vec{q},t_2)\rangle_T$ and $S(\vec{q},t) = S(\vec{q},t,t)$

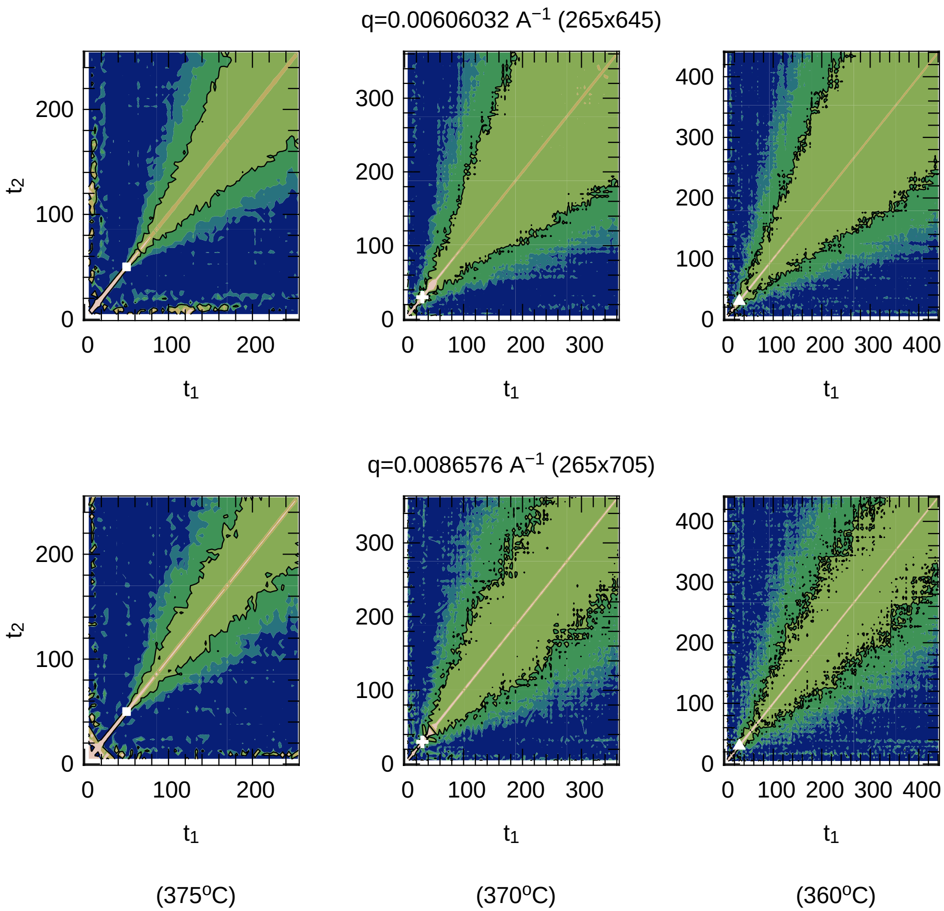
Two-Time Correlation Functions

Non-stationary so autocorrelate $\frac{I(q,t_1)-\langle I(q,t_1)\rangle}{\langle I(q,t_1)\rangle}$





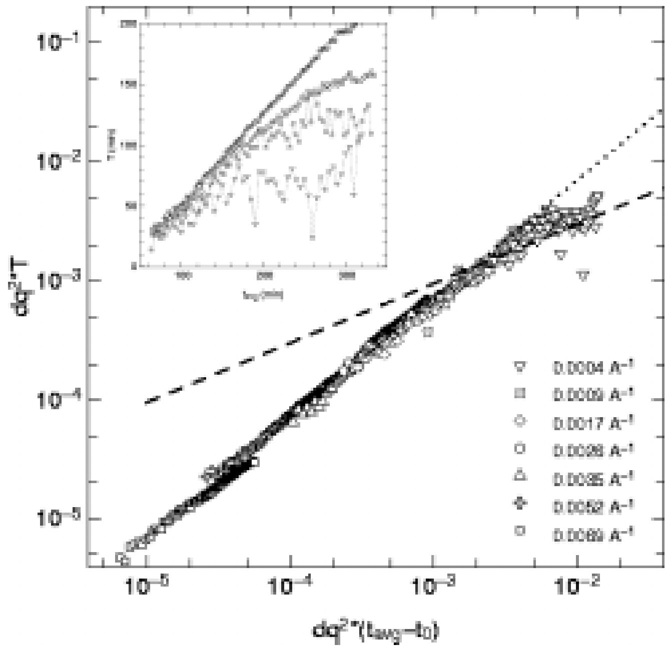
Two-Time Correlation Functions



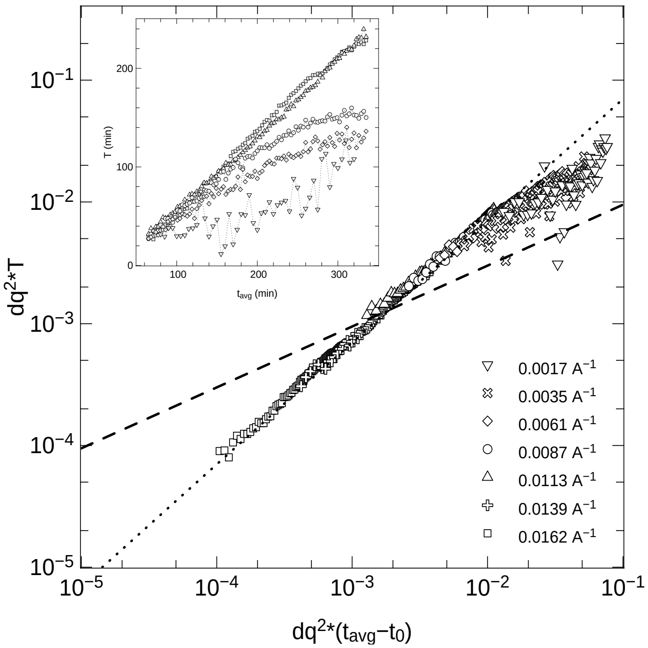
Tranverse direction

“two-time” scaling analysis

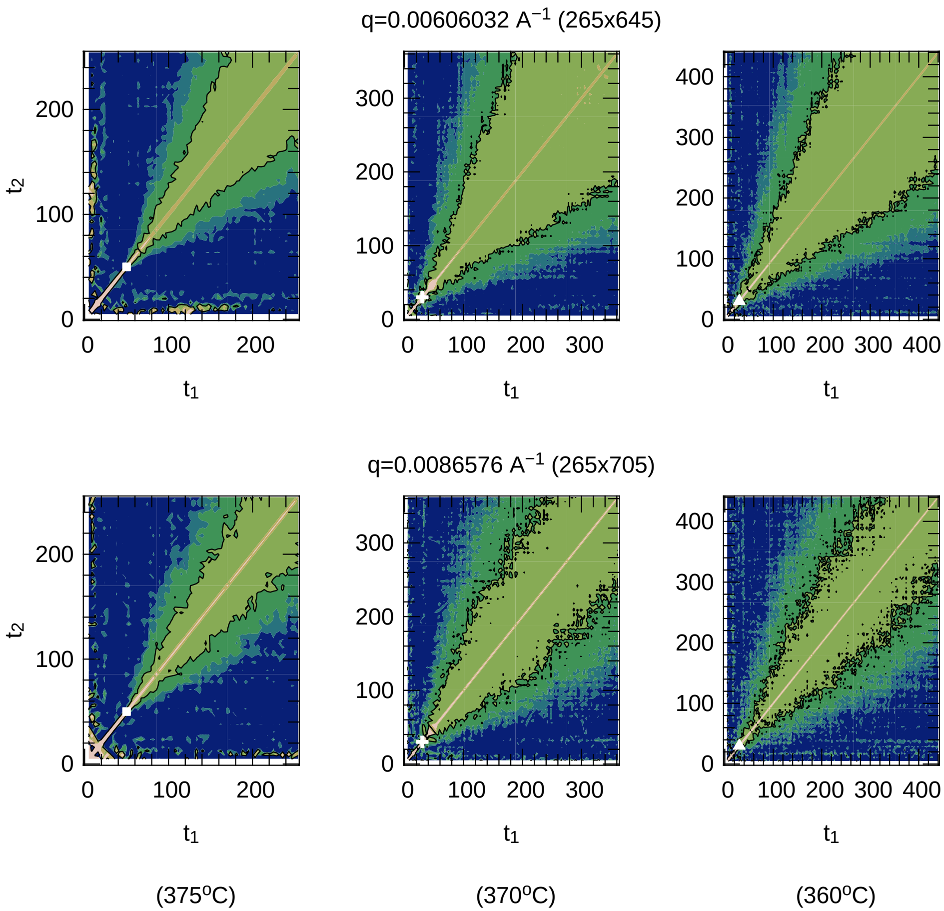
Radial:



Transverse:



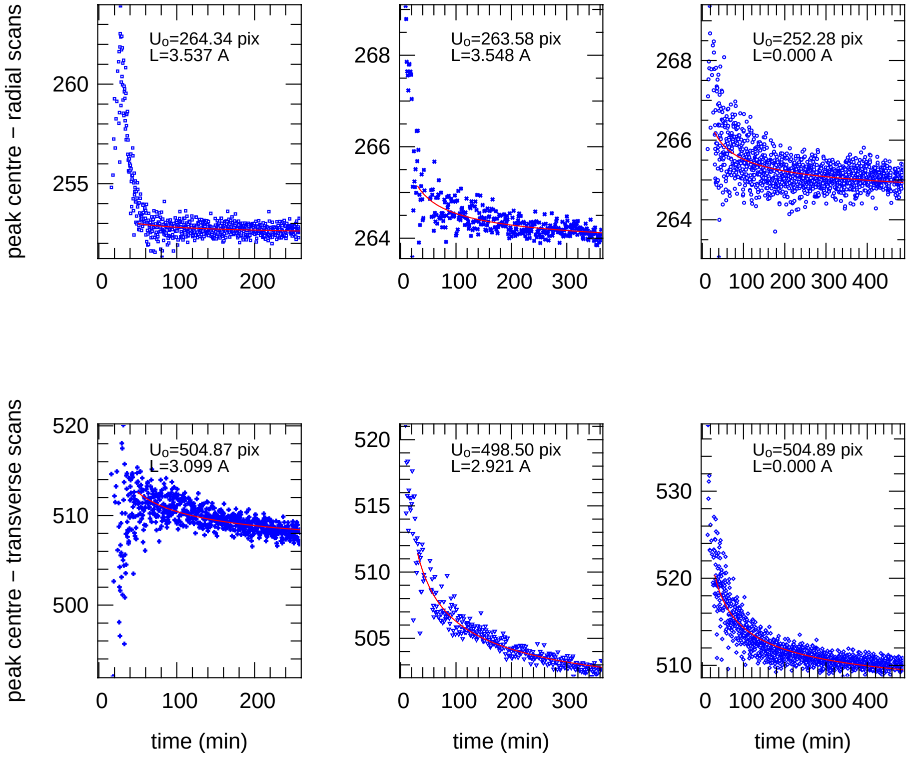
Two-Time Correlation Functions



Tranverse direction

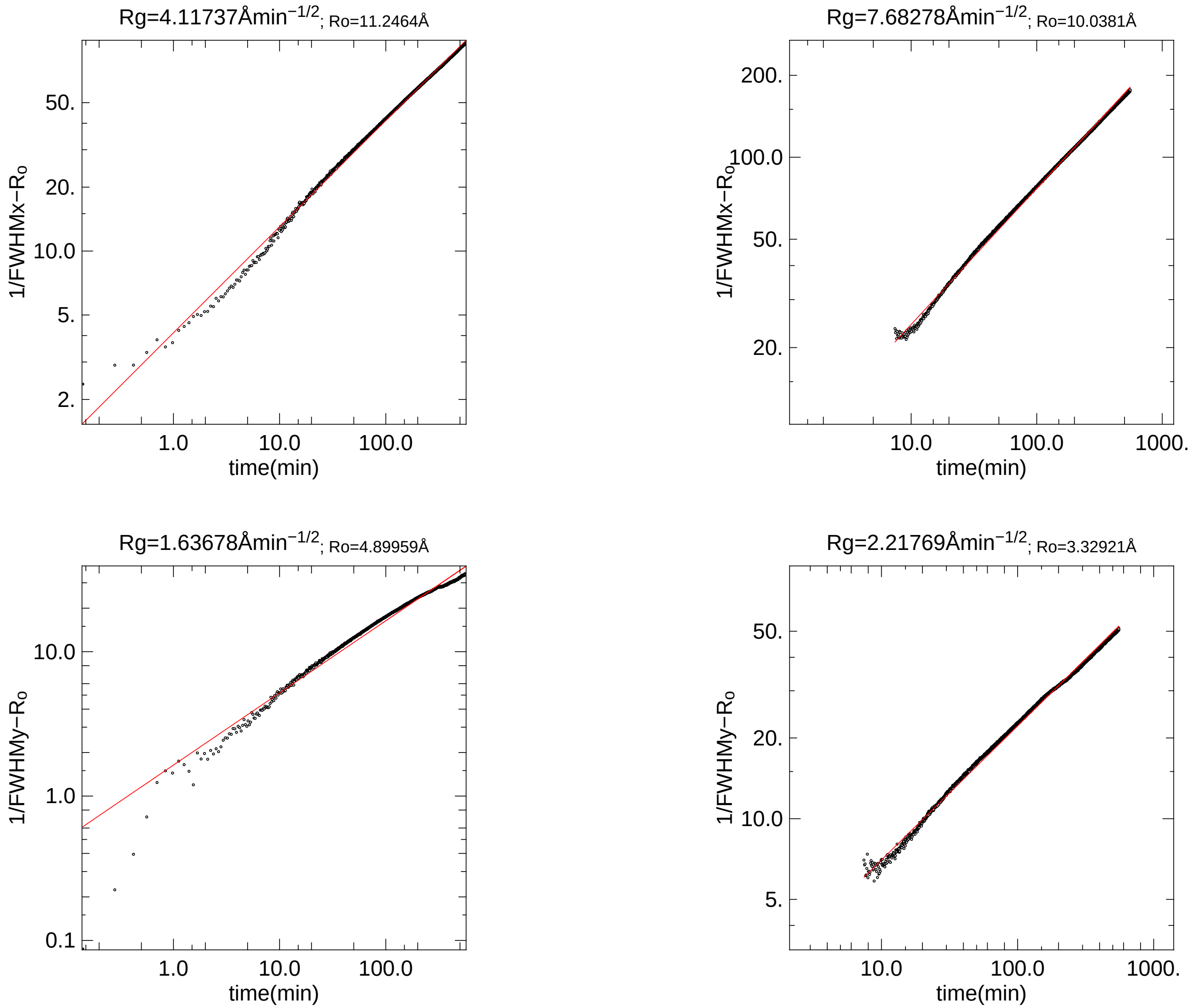
Peak Shift

Peak shift versus time. (1 pixel = $0.88 \times 10^{-5} \text{Å}^{-1}$)

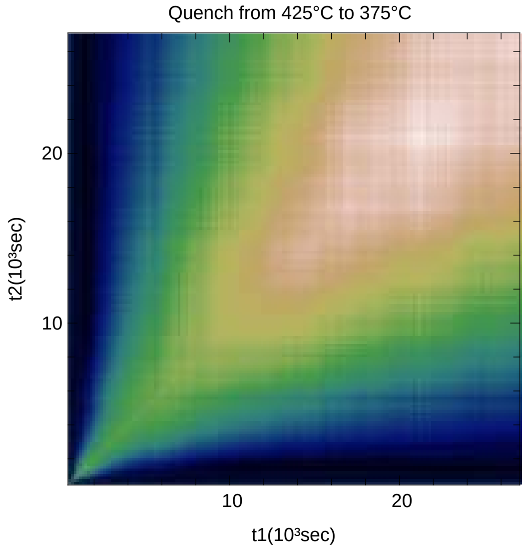


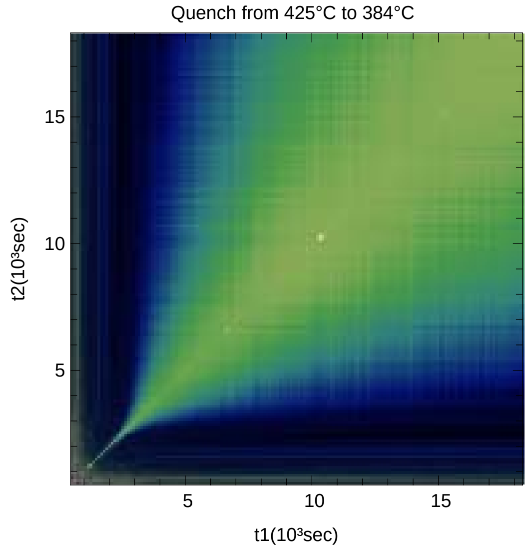
(a) 375°C (b) 370°C (c) 360°C

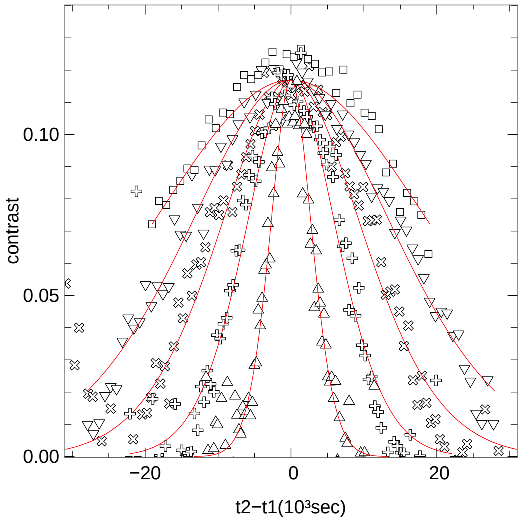
Time scaling



Upgrades to the beamline allow us to obtain better data, especially important for the early time region.

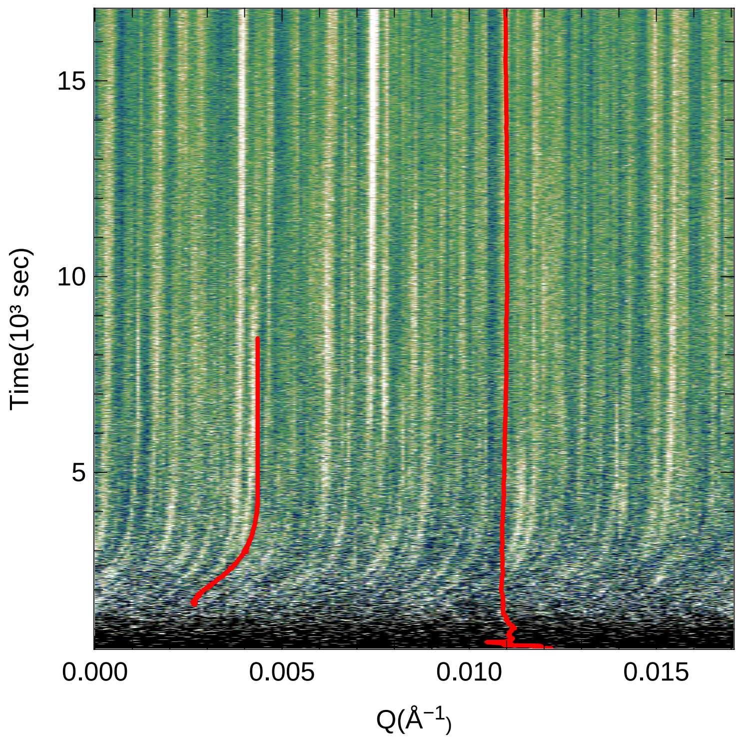


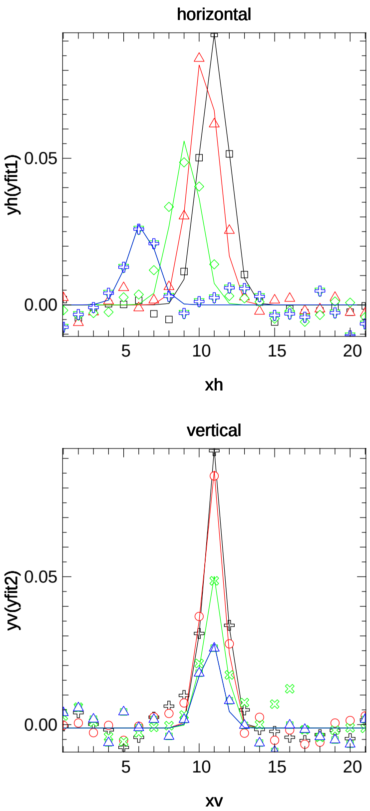




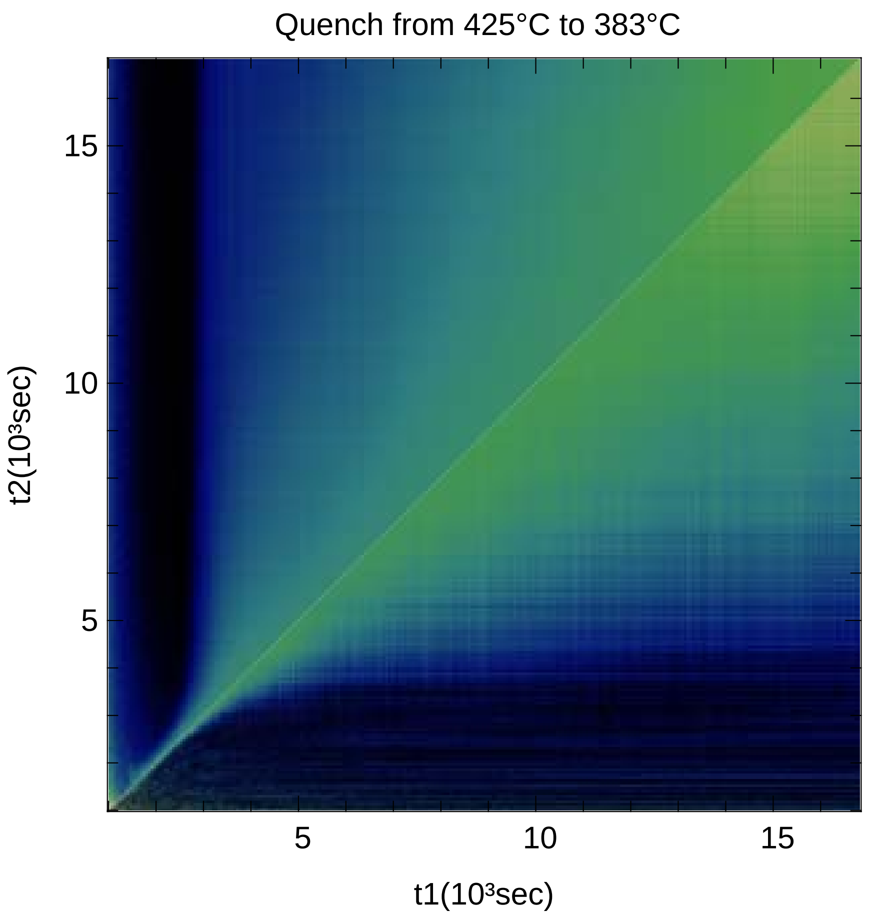
Cross-section of several slices

New Data


15
10
5
Time(10³ sec)
0.000
0.005
0.010
0.015
Q(Å⁻¹)


horizontal
yh(yfit1)
0.05
0.00
5
10
15
20
xh
vertical
yv(yfit2)
0.05
0.00
5
10
15
20
xv

Two-$\vec{Q}$ two-time



References

Experiments:

1. (Borosilicate glass) A. Malik, A. R. Sandy, L. B. Lurio, G. B. Stephenson, S. G. J. Mochrie, I. McNulty, and M. Sutton,
   Phys. Rev. Lett. **81**, 5832 (1998).
2. (AlLi) F. Livet, F. Bley, R. Caudron, D. Abernathy, C. Detlefs, G. Grübel and M. Sutton,
   Phys. Rev. E **63**, 036108-1 (2001).
3. (Cu_3Au) A. Fluerasu, M. Sutton, and E.M. Dufresne,
   Phys. Rev. Lett. **94**, 055501 (2005).
4. (Cu-Pd) K. Ludwig, F. Livet, F. Bley, J-P. Simon, R. Caudron, D. Le Bolloćh and A. Moussaid,
   Phys. Rev. E (B?) (2005).

Theory:

1. (Model A) G. Brown, P. A. Rikvold, M. Sutton and M. Grant,
   Phys. Rev. E **56**, 6601 (1997).
2. (Model B) G. Brown, P. A. Rikvold, M. Sutton and M. Grant,
   Phys. Rev. E **60**, 5501 (1999).