Atomic diffusion investigation by XPCS

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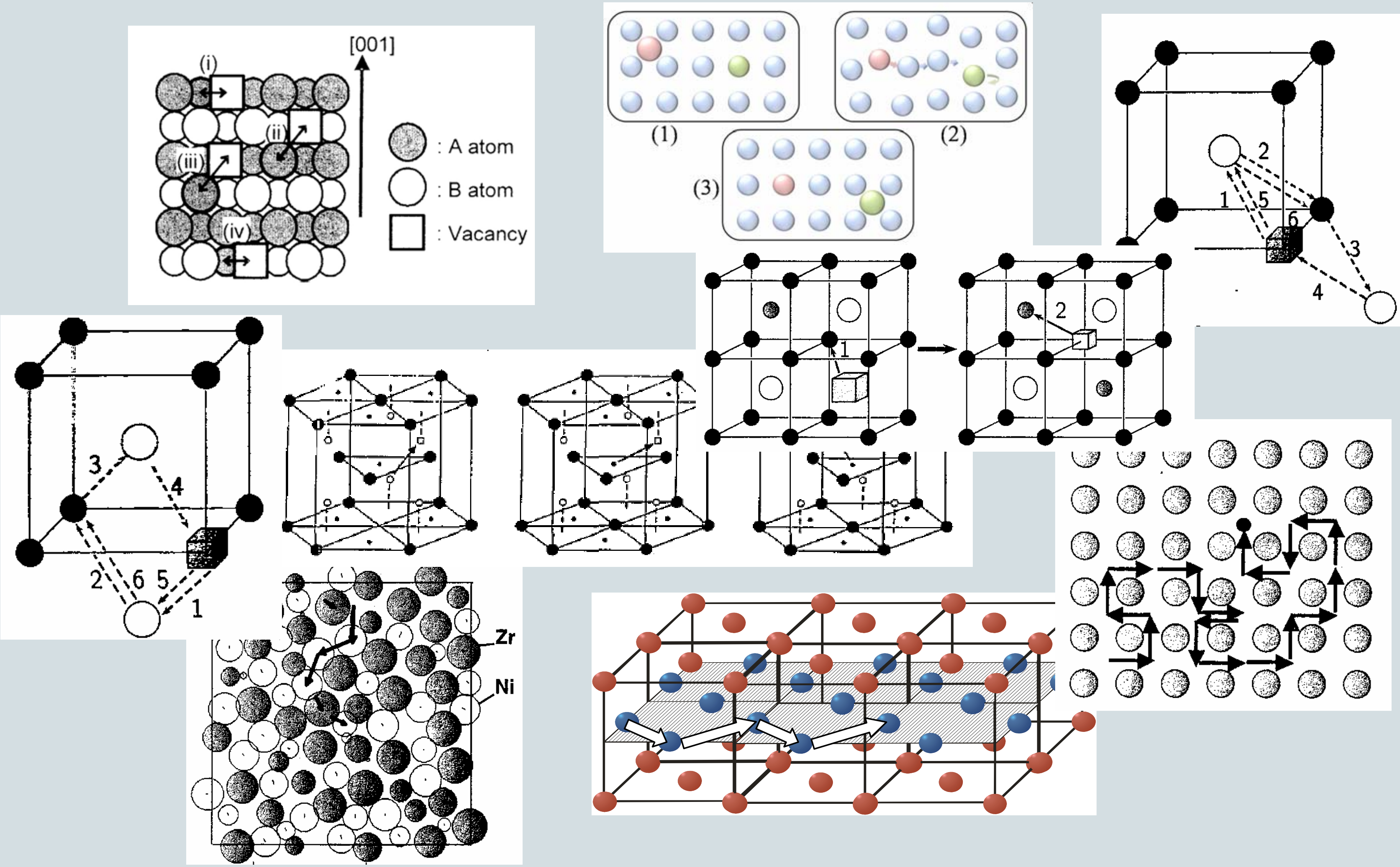
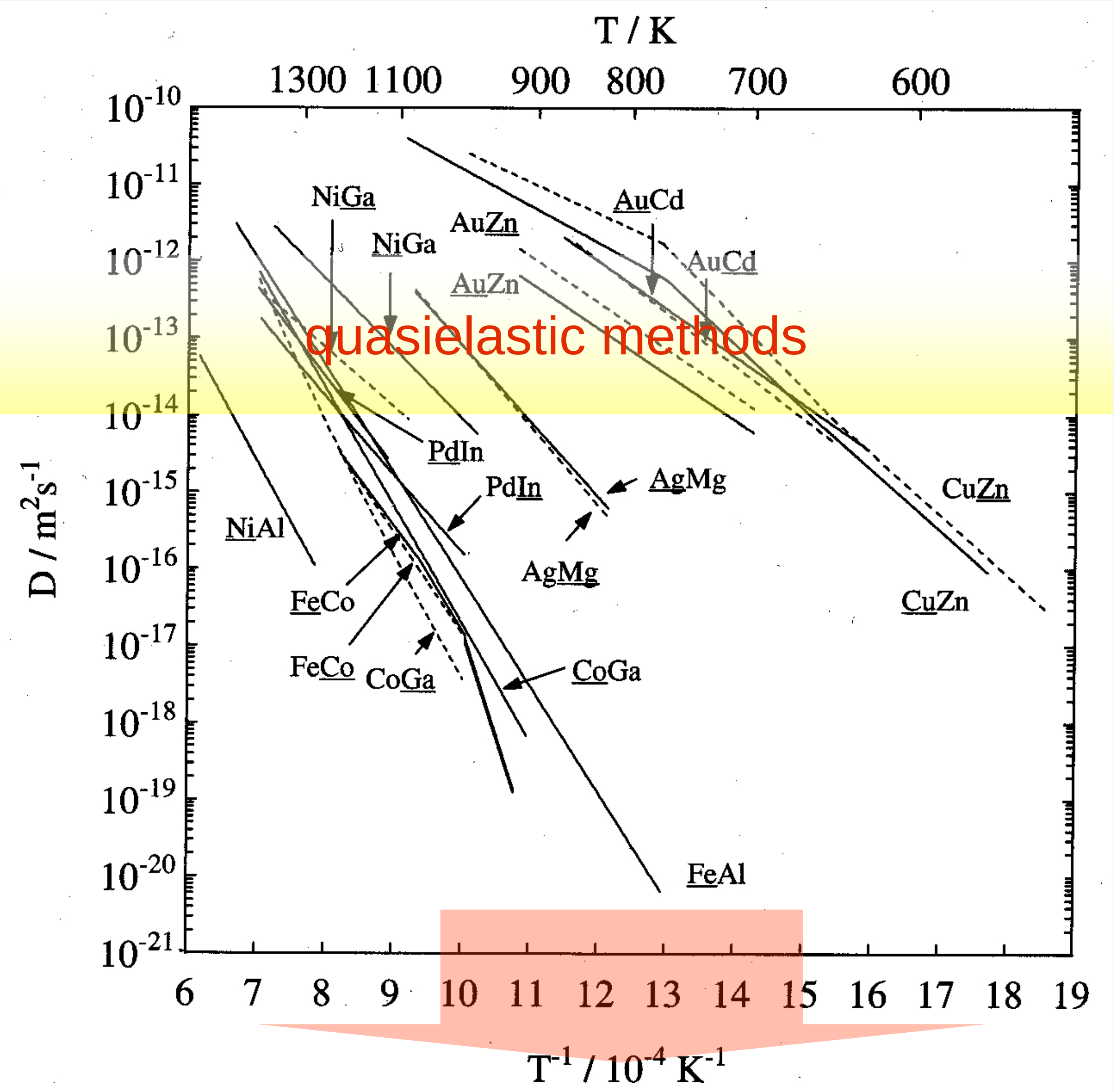
Atomic diffusion mechanisms





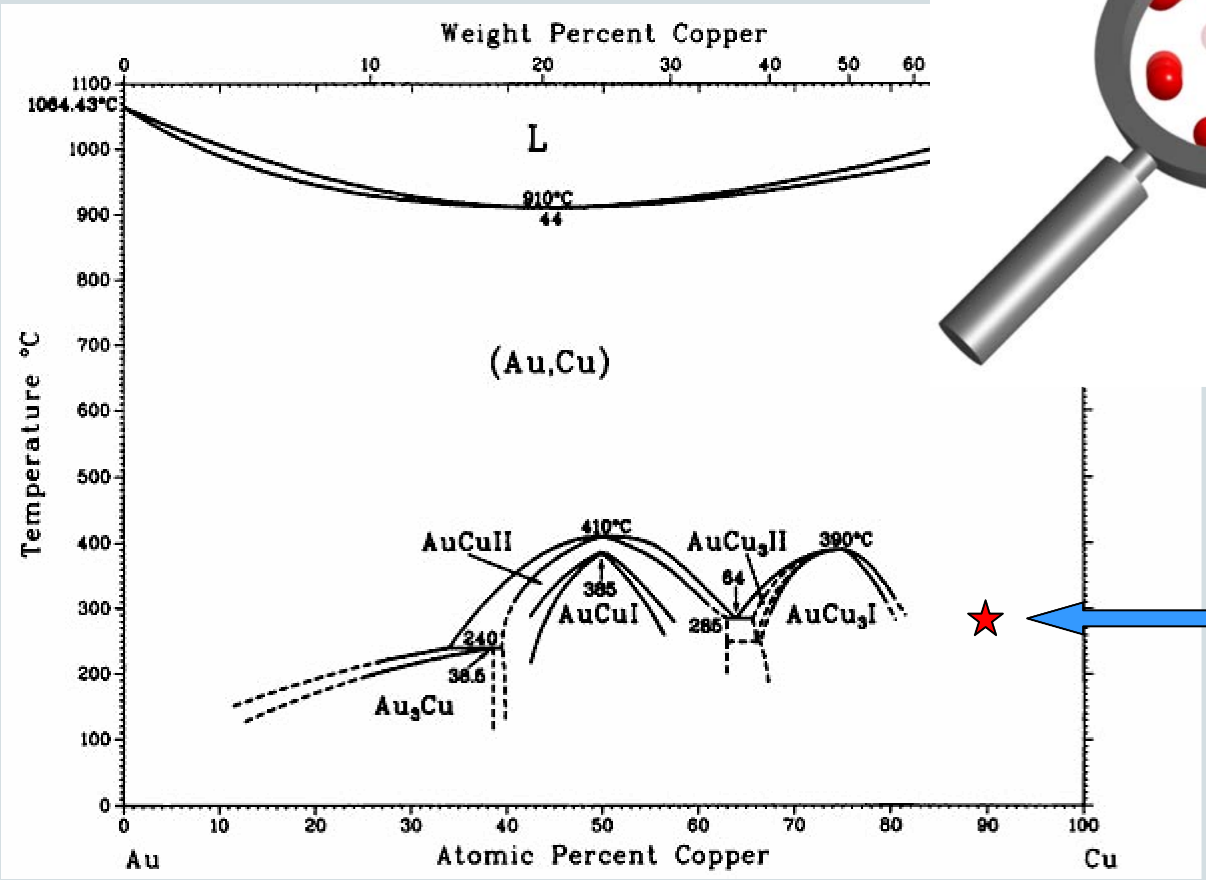
H. Mehrer, Diffusion in Solids, Springer 2007

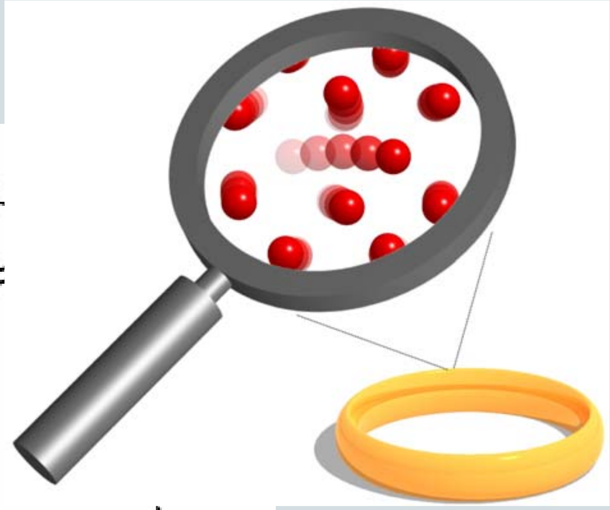
Our primary goal now and in future:

overcome limitations of atomistic methods (Mössbauer, QNS, NRS) to a few elements (^{57}Fe, H, Ni, Co,Ti) and fast diffusion using

X-ray Photon Correlation Spectroscopy

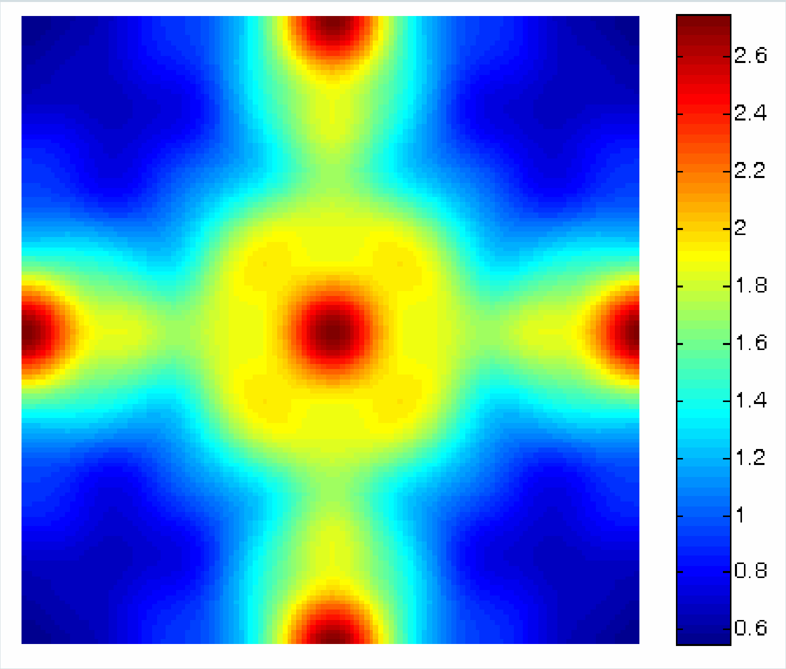
Single atom diffusion



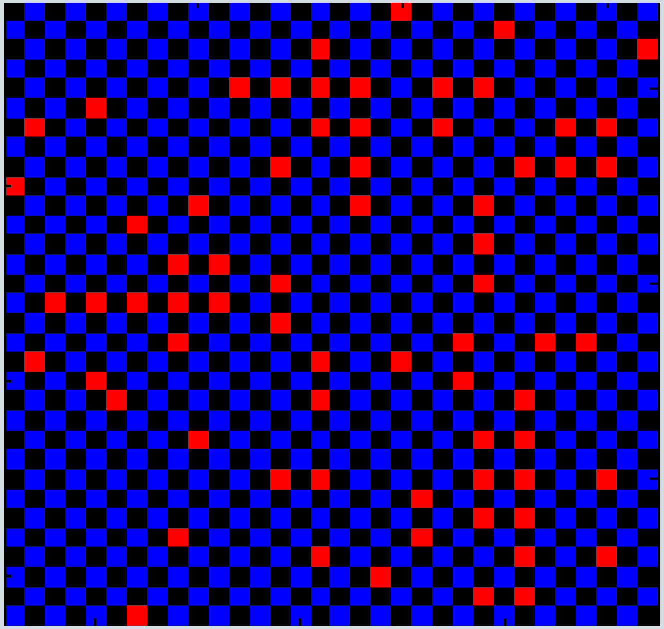


$Cu_{90}Au_{10}$

M. Leitner et al., *Nature Mater.* **8,** 717 (2009) reciprocal (001) plane



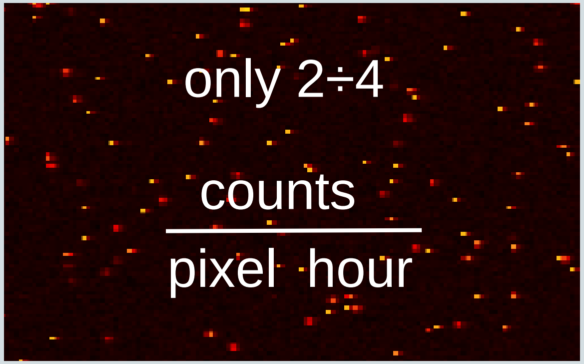
slice through (100) MC-cell:



B. Schönfeld, M.J. Portmann, S.Y. Yu, G. Kostorz, Acta Mat. **47**, 1413 (1999)

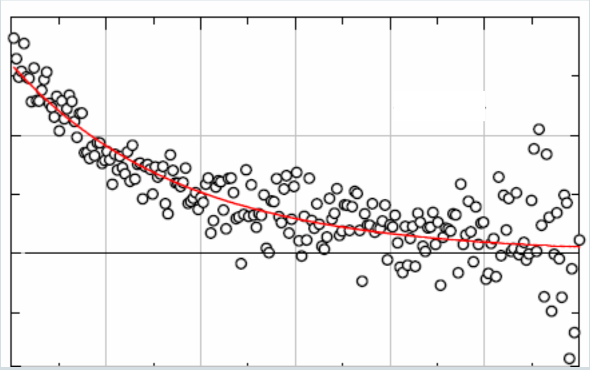
1) calculating

$$g^{(2)}(\mathbf{q},\Delta t)=\frac{\langle I(\mathbf{q},.)\,I(\mathbf{q},.+\Delta t)\rangle}{\langle I(\mathbf{q},.)\rangle^{2}}$$



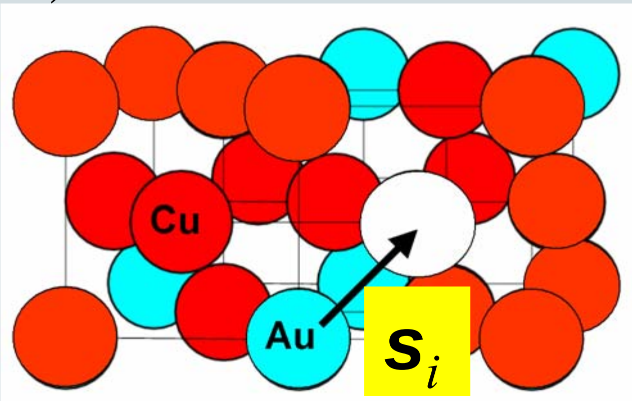
2) fitting

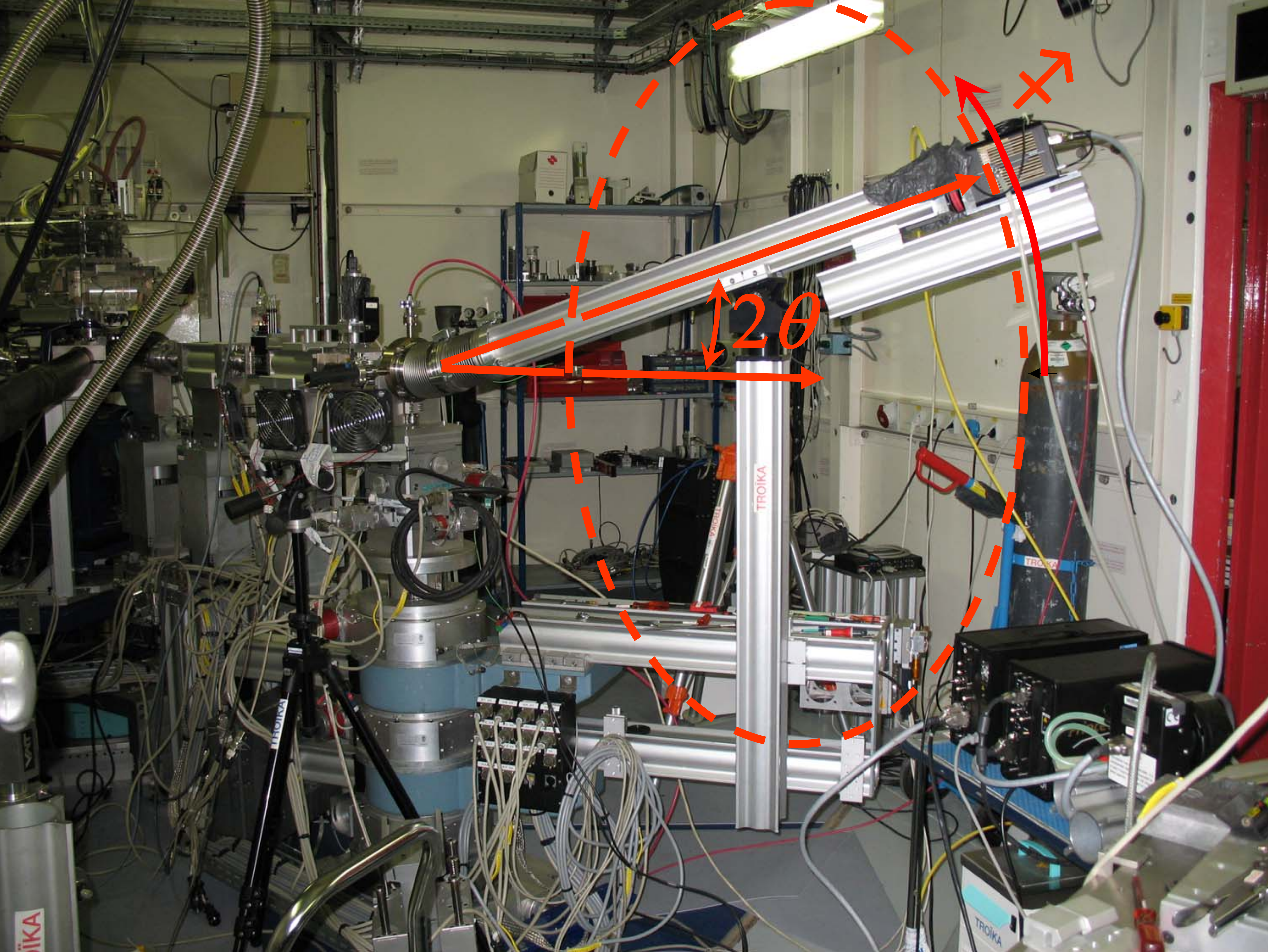
$$g^{(2)}(\mathbf{q},\Delta t)=1+\beta\, e^{-2\Delta t/\tau(\mathbf{q})}$$

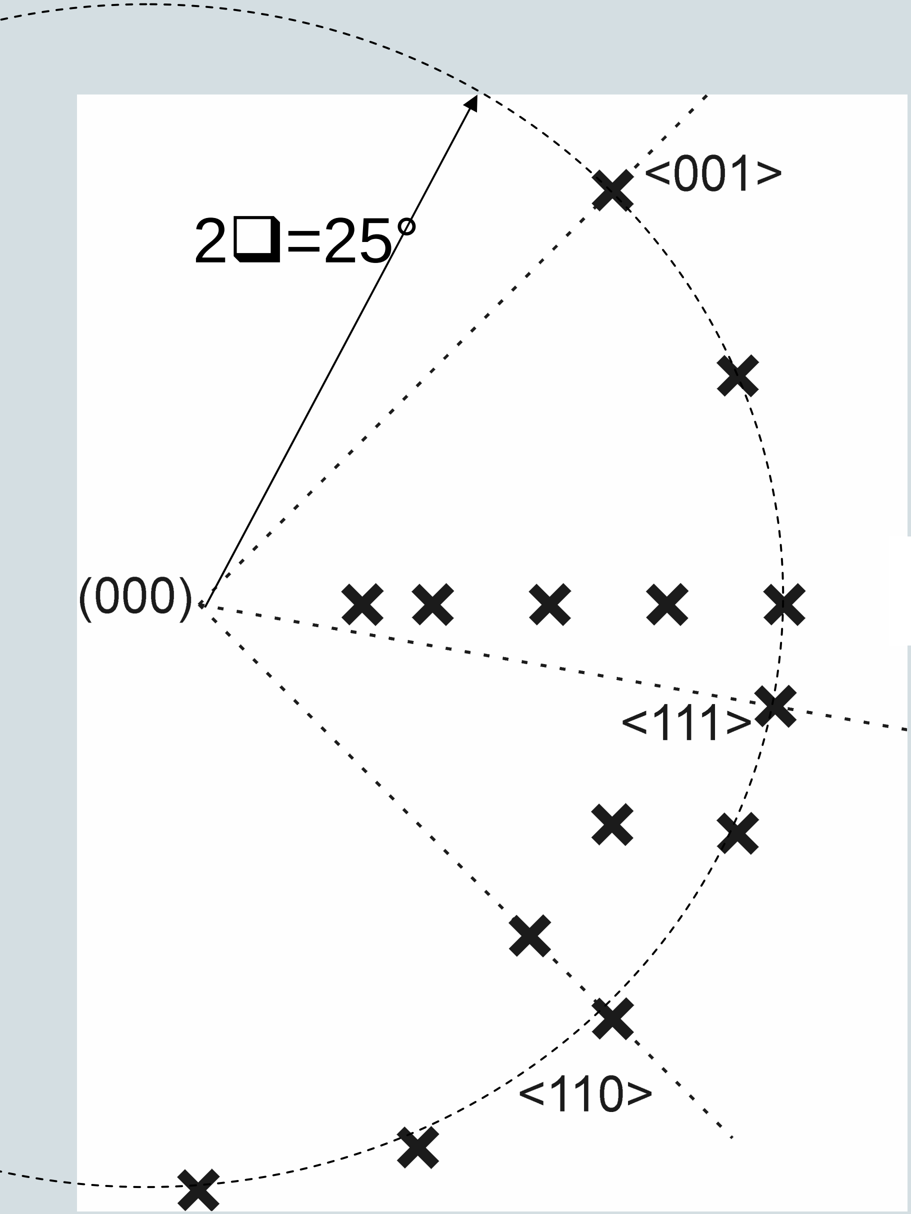


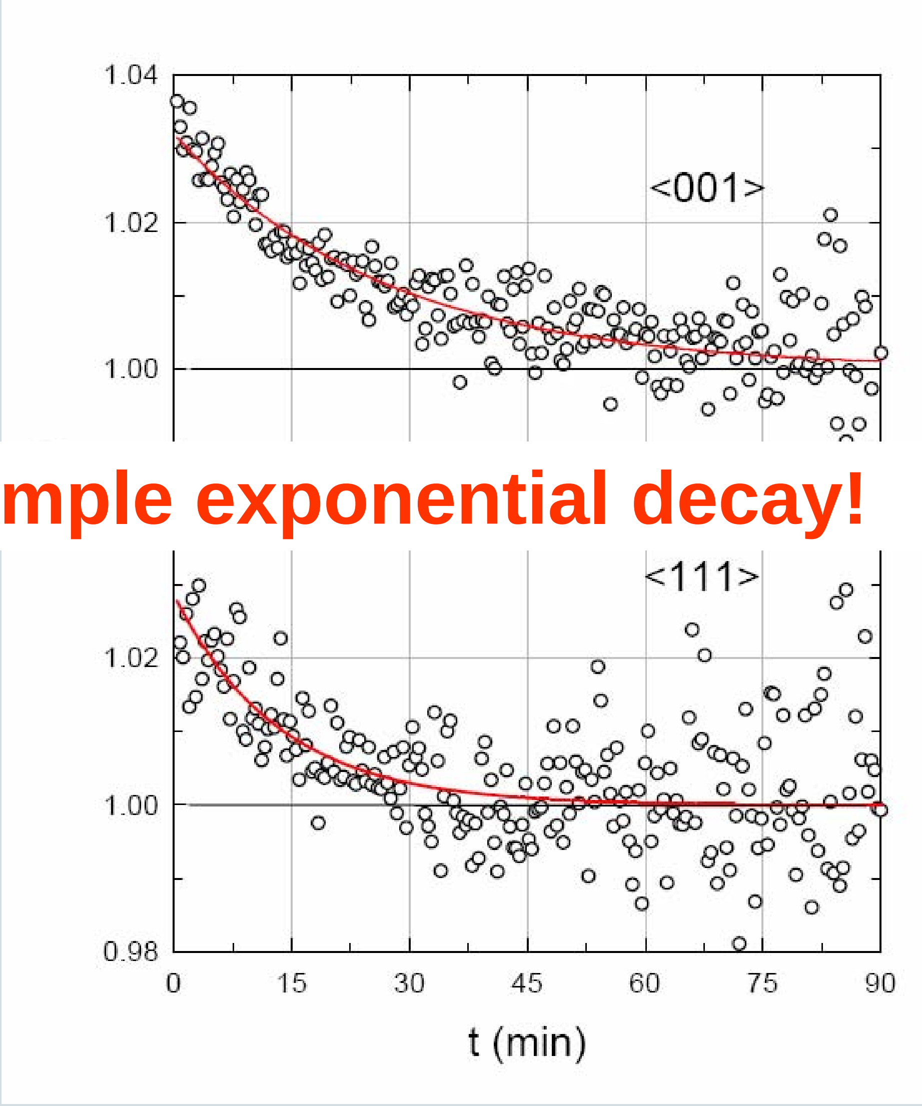
3) verifying hypotheses

$$\tau(\mathbf{q})=\tau_0\,\frac{I_{\mathrm{SRO}}(\mathbf{q})}{1-\sum_i p_i\cos(\mathbf{s}_i\cdot\mathbf{q})}$$

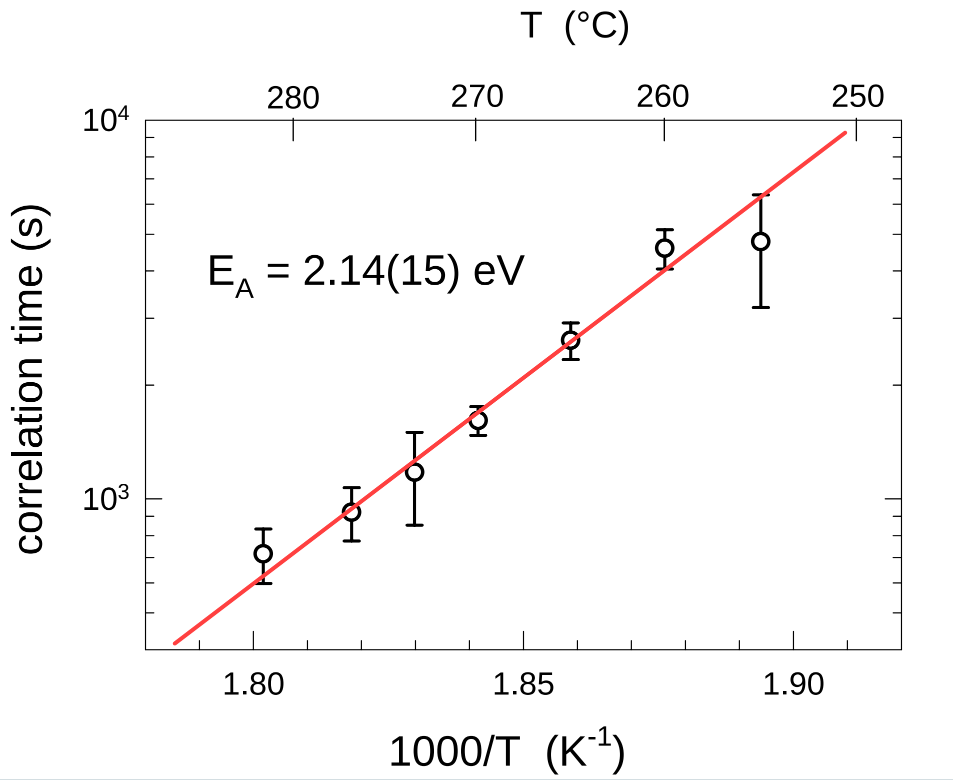



2θ
TROIKA

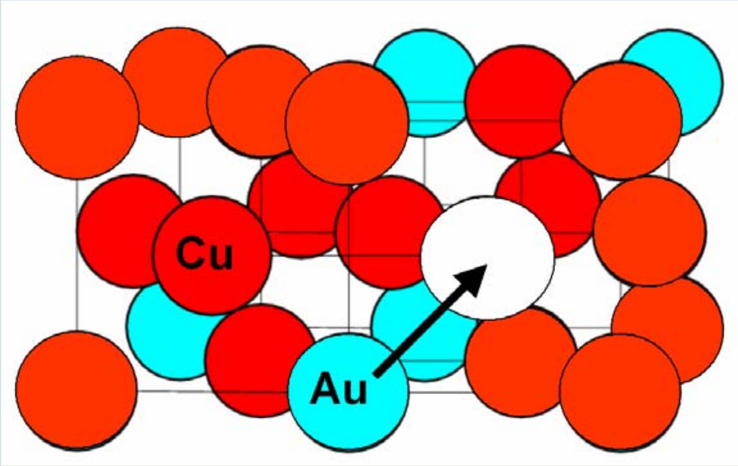


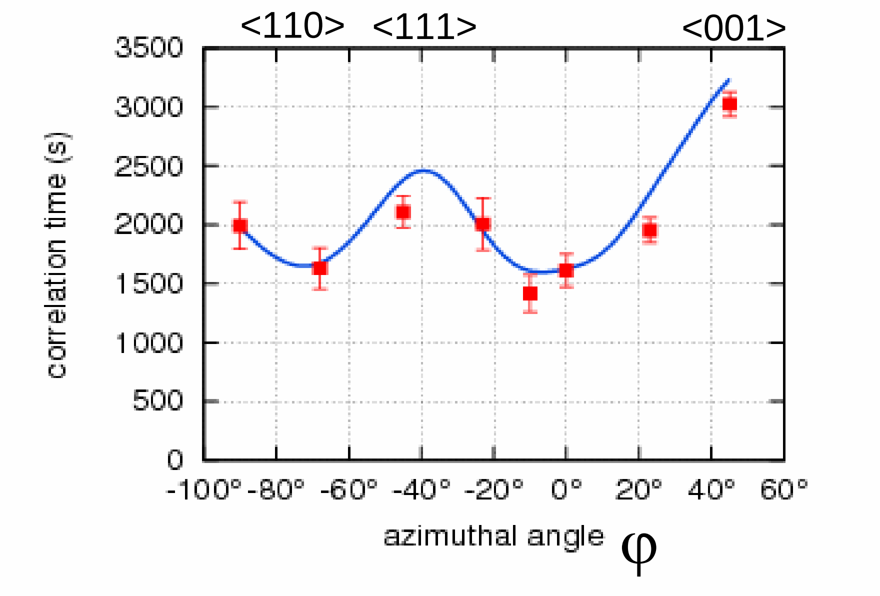


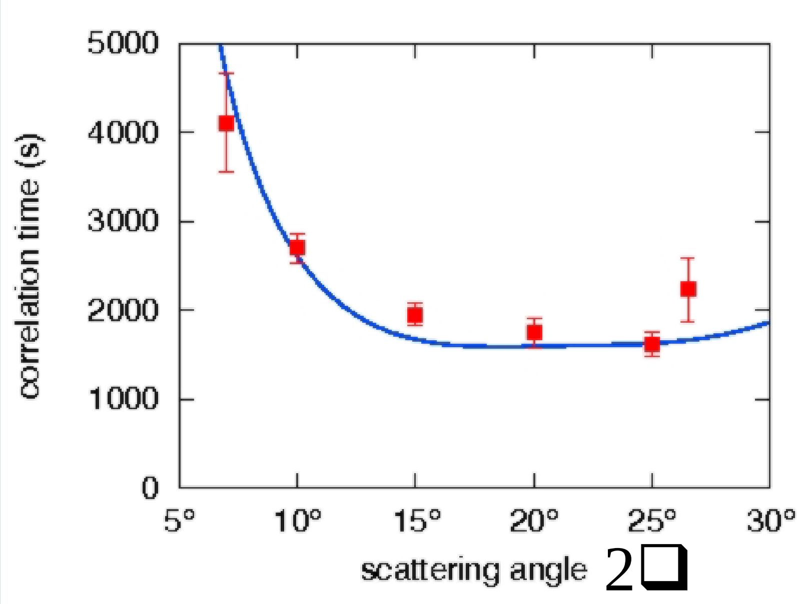
simple exponential decay!



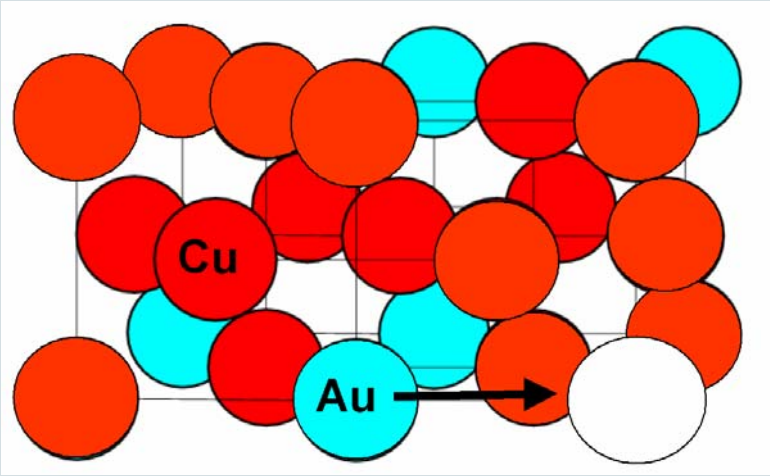
T (°C)
280
270
260
250
10^4
10^3
correlation time (s)
E_A = 2.14(15) eV
1.80
1.85
1.90
1000/T (K^-1)

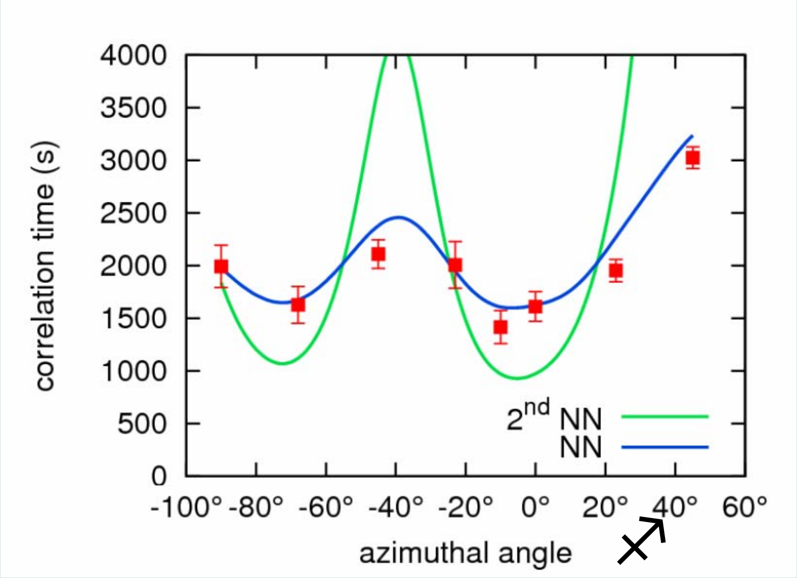


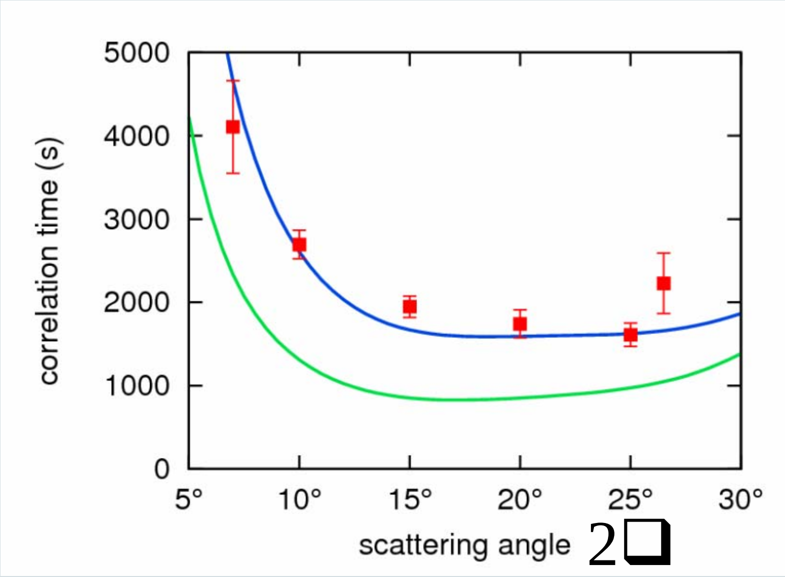




only one parameter fited !!


Cu
Au


correlation time (s)
4000
3500
3000
2500
2000
1500
1000
500
0
-100° -80° -60° -40° -20° 0° 20° 40° 60°
azimuthal angle
2^{nd} NN
NN


correlation time (s)
5000
4000
3000
2000
1000
0
5° 10° 15° 20° 25° 30°
scattering angle

Local dynamics in metallic glass

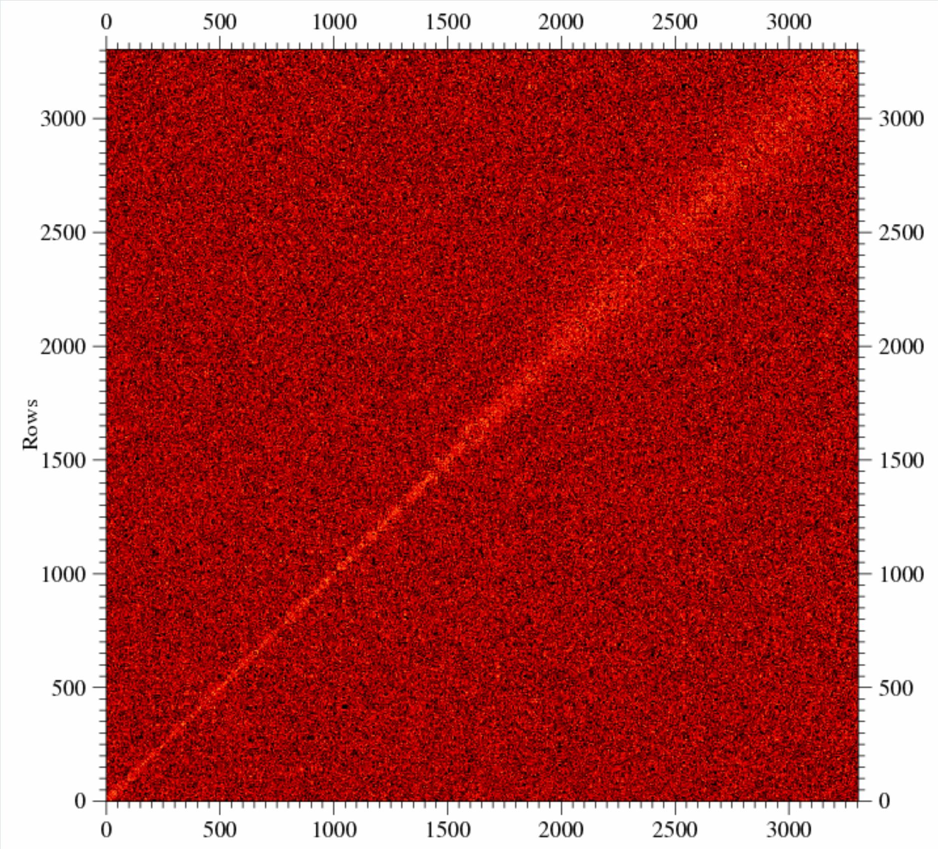
Systems far from equilibrium characterized by spatial and/or temporal heterogeneity
e.g. dilute colloidal gels

Zr-based amorphous alloy $Zr_{65}Al_{7.5}Ni_{10}Cu_{17.5}$

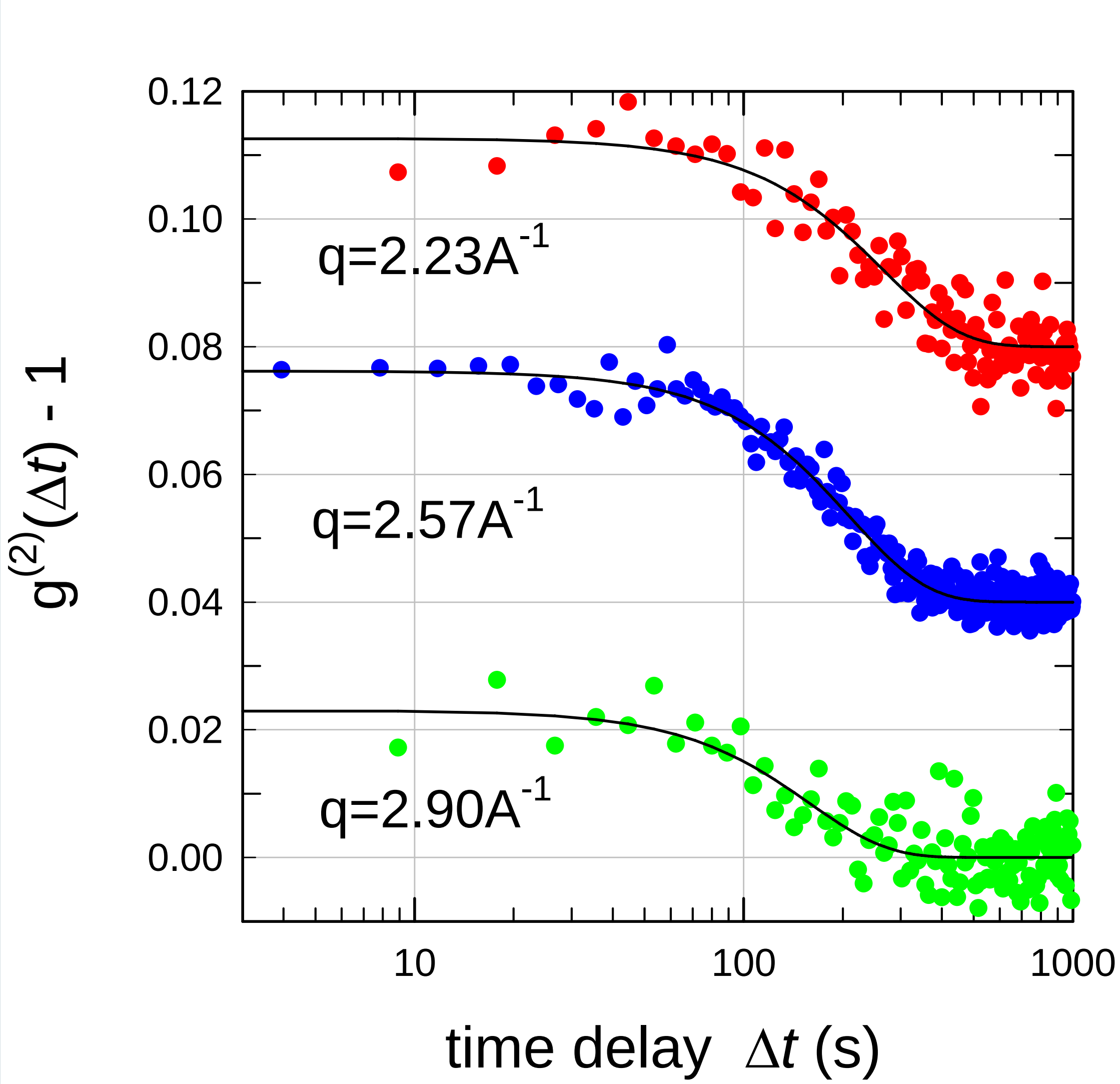
metallic glasses - the paradigm of dense random packing of spheres

Calorimetric glass transition   Tg=624K at 2K/min
Extrapolated quasi-stationary Tg=605K
T. Zhang, A. Inoue and T. Masumoto, Mater. Trans. JIM **32** (1991) 1005

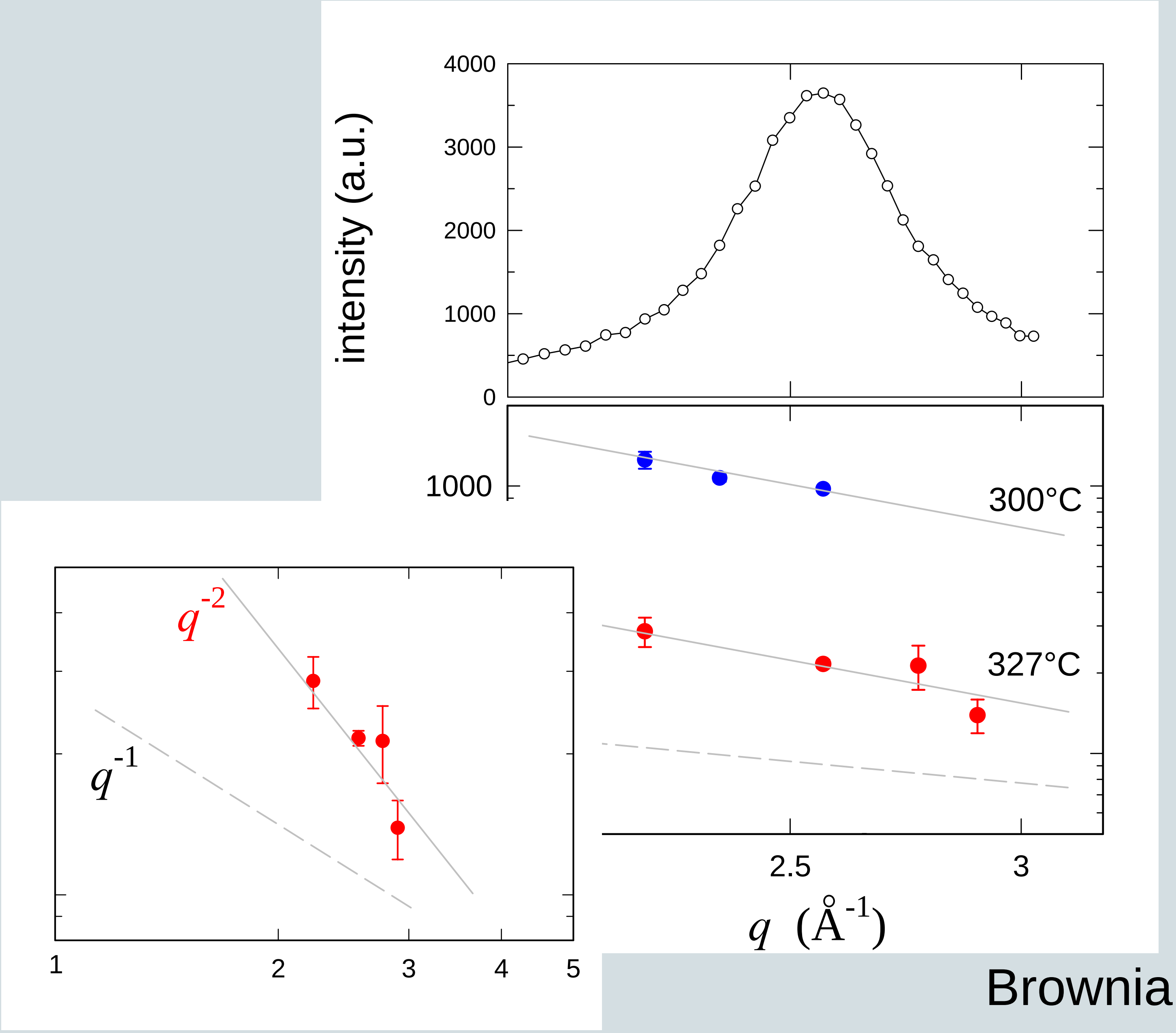
Very long relaxation times



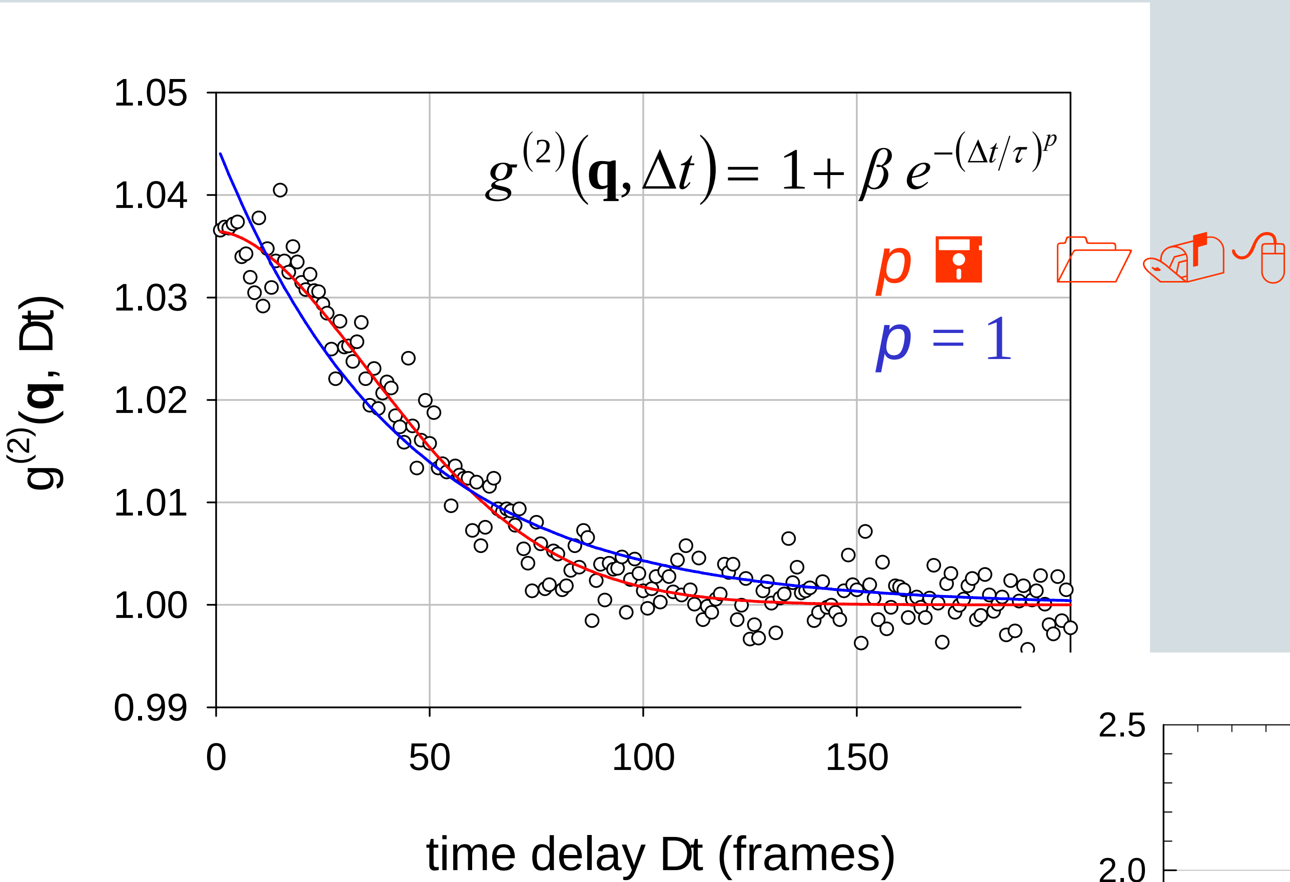
600K (327°C)



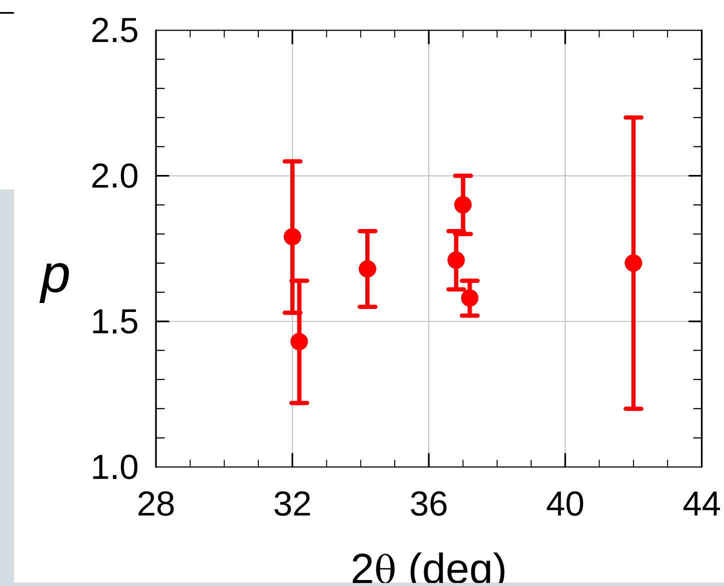
0.12
0.10
0.08
0.06
0.04
0.02
0.00
q=2.23A-1
q=2.57A-1
q=2.90A-1
g(2)(Δt) - 1
10
100
1000
time delay Δt (s)



Brownian dynamics ?



$g^{(2)}(\mathbf{q}, \Delta t) = 1 + \beta\, e^{-(\Delta t/\tau)^p}$
p
p = 1
1.05
1.04
1.03
1.02
1.01
1.00
0.99
0
50
100
150
g(2)(q, Dt)
time delay Dt (frames)



2.5
2.0
1.5
1.0
28
32
36
40
44
p
2θ (deg)

Key parameters from your point of view the instrument should have like:

Source parameters:	
- energy	tunable energy
- pulse pattern	uniform distribution preferable
- pulse length	as long as possible
- polarization	irrelevant
Beamline optics:	
- monochromatizity	as high as possible (preferred 10^{-6}) due to the increased pulse length and the lower peak intensity
- spot size	about 10 μm
- degree of coherence	as high as possible (lead to lower peak intensity)
- diagnostics	not relevant
Detector:	
- pixel size	10-20 μm
- number of pixels	at least 10^6, the more the better
- framerate	10 Hz
- accessible q-range	40° scattering angle (about 3 A^{-1})
Sample environment:	self-made furnaces
- temperature	
- external fields	

Thanks to:

Lorenz M. Stadler
Bastian Pfau
Friedrich Gröstlinger
Gero Vogl

Faculty of Physics
Universität Wien

A. Fluerasu, A. Madsen at ESRF