

UED Investigation of Thin Film Melting

Ian Robinson

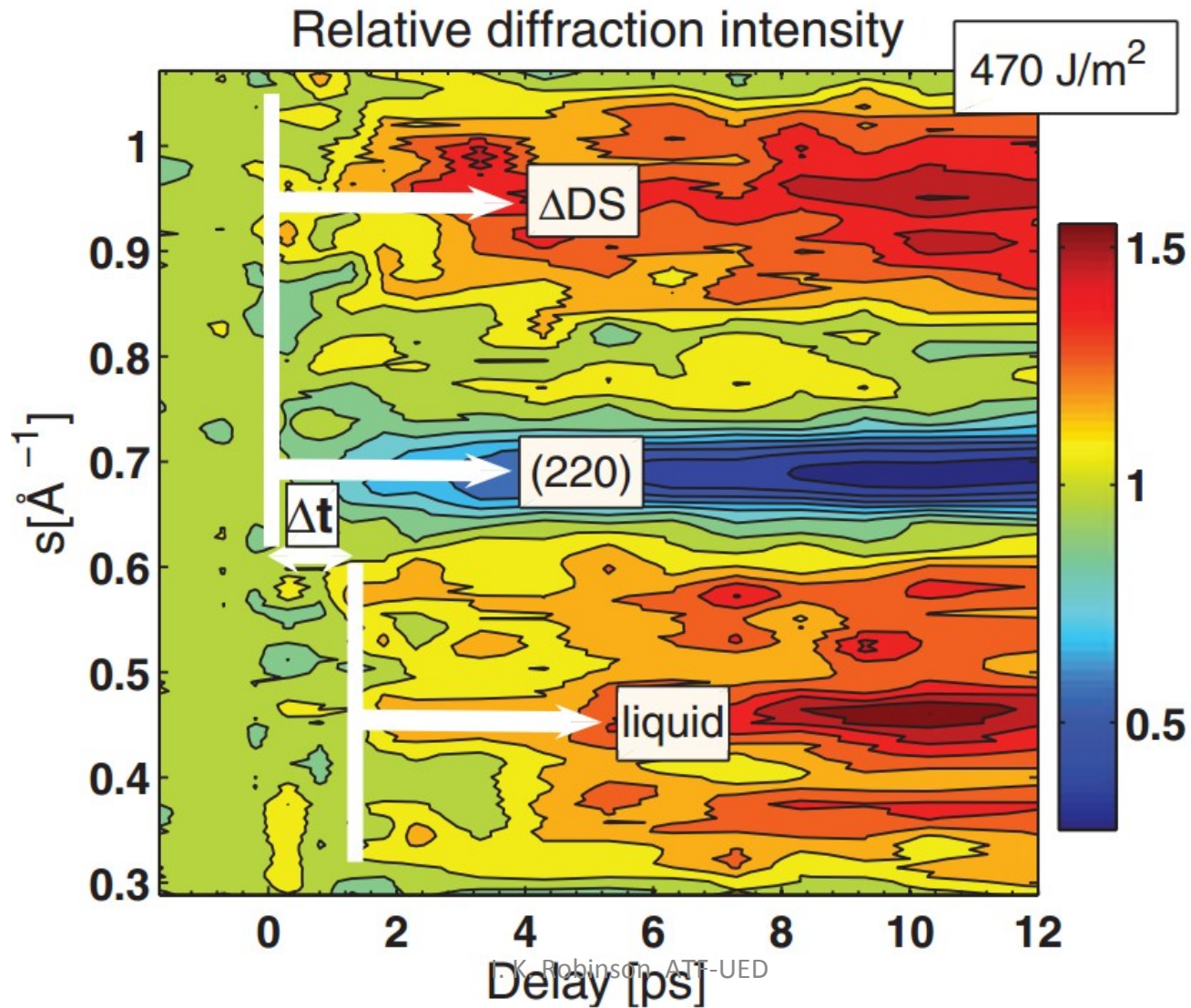
X-ray Scattering Group, CMPMSD

XFELs in Materials Science

- Pump-probe access to time scales of phase transitions
- Search for new “hidden” phases of matter
- LCLS (Stanford) already delivering, but little available time
- EU-XFEL in Hamburg will come on line in 2017
 - 3x greater capacity
 - Higher energy X-rays
- Some systems can be explored now with UED

Transient Melting of Au (by UED)

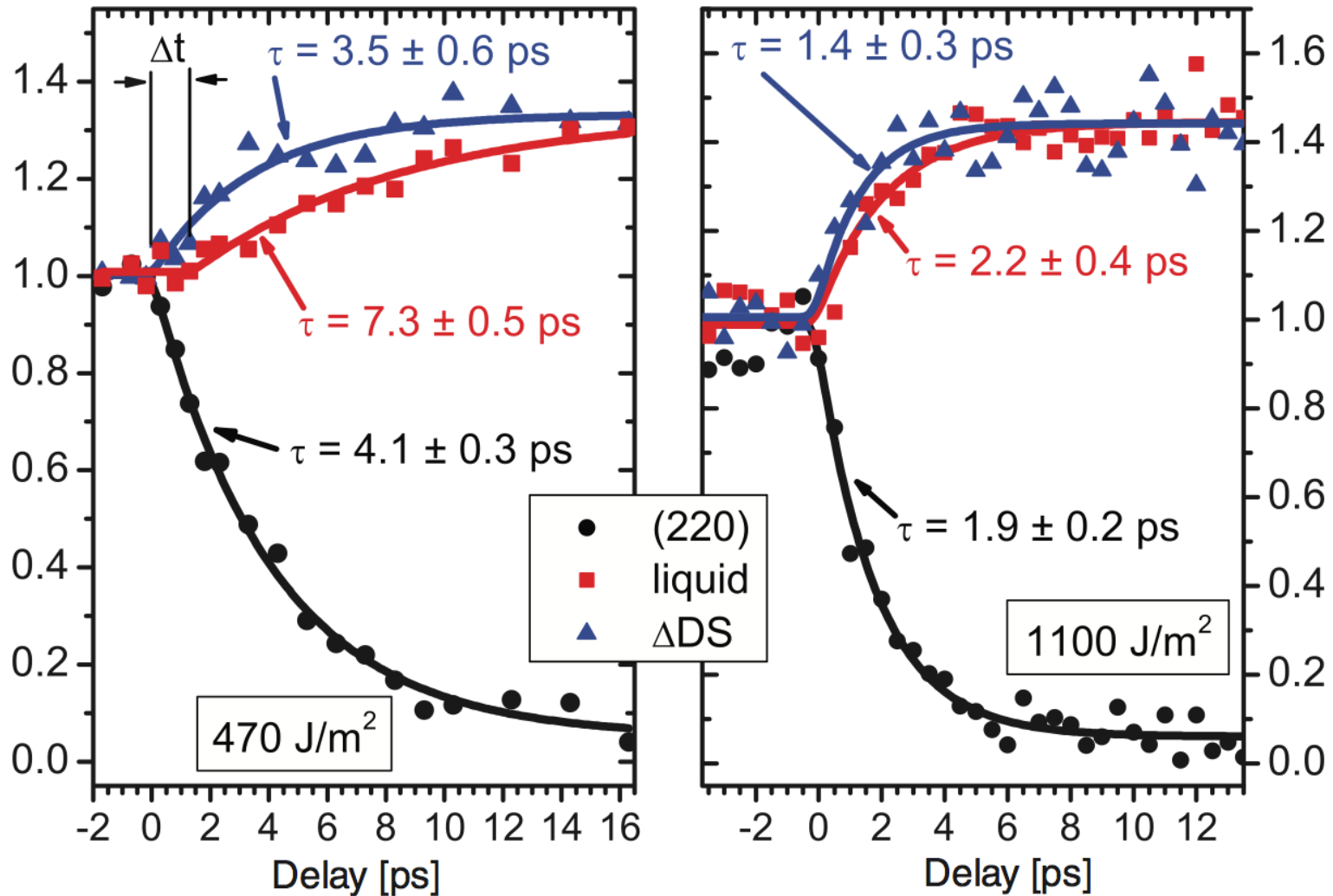
R. Ernstorfer, D. Miller et al, Science 323 1033 (2009)



K. Robinson, ATF-UED

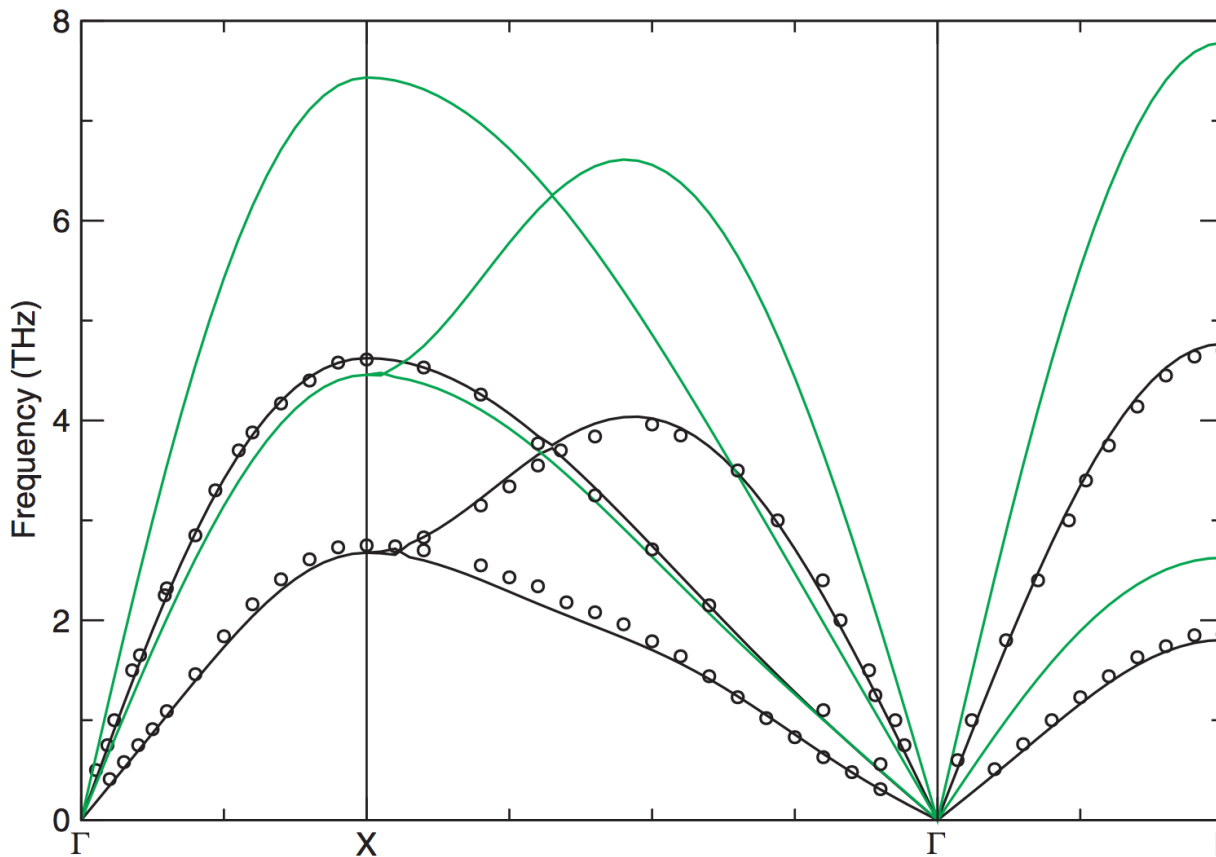
Transient Melting of Au (by UED)

R. Ernstorfer, D. Miller et al, Science 323 1033 (2009)



Calculated Phonon band structure of Au electron heating ($T=6\text{eV}=7\times 10^4\text{K}$)

Recoules et al PRL 96, 055503 (2006)

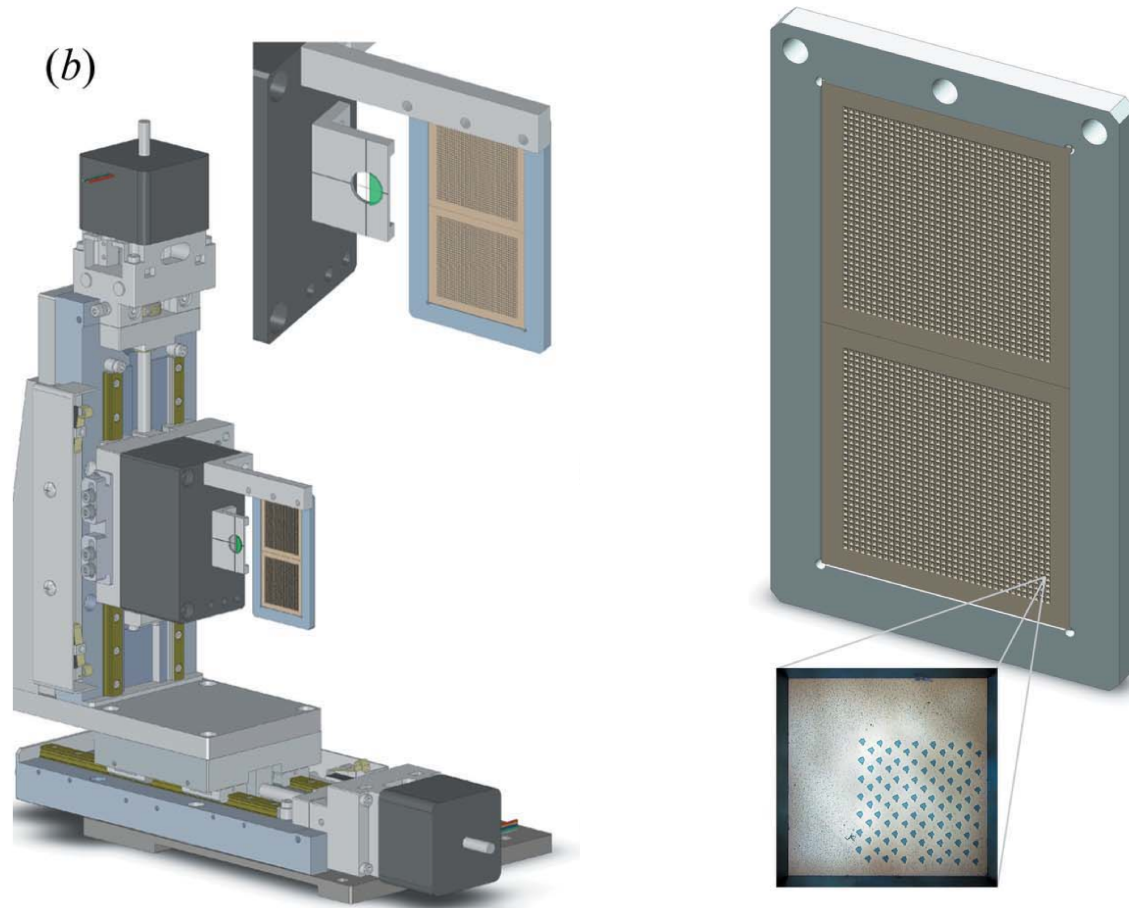


Hot theory
DFPT few fs

RT theory +
Neutron
scattering
experiment

MAXIC chamber for SACLA

Changyong Song et al, J. Appl. Cryst. **47** 188 (2014)



Total scattering

Lars Ehm (SBU)

Experimentally observable total structure factor:

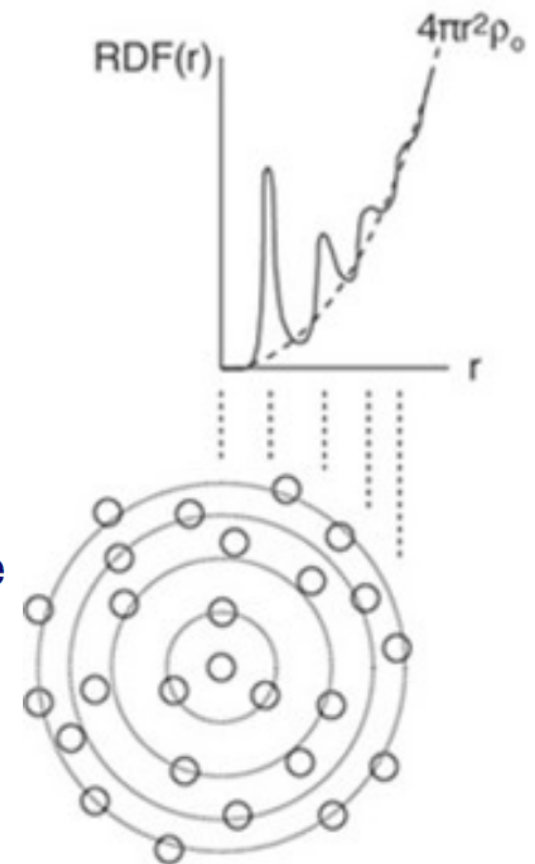
$$S(Q, \omega) = \frac{1}{2\pi\hbar} \int G(r, t) \exp\{i(Q \cdot r - \omega t)\} dr dt$$

Total scattering → Bragg and diffuse scattering

Fourier transform → Pair Distribution Function

What do we get from PDF?

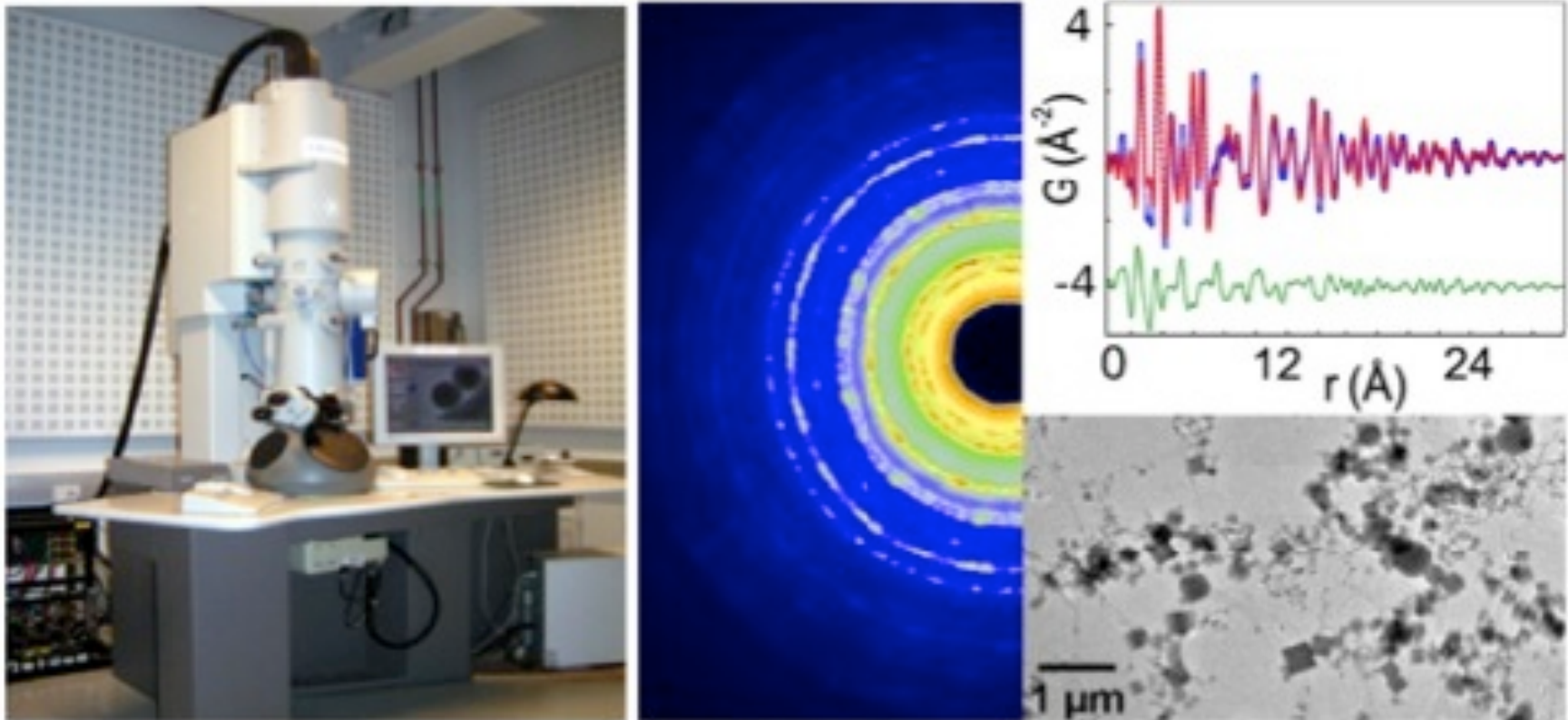
- Probabilities of finding atom pairs separated by distance r
 - Short, intermediate, and long-range structure
- Nanocrystalline materials
- Fit structural models
- Crystal size



Electron Pair Distribution Function

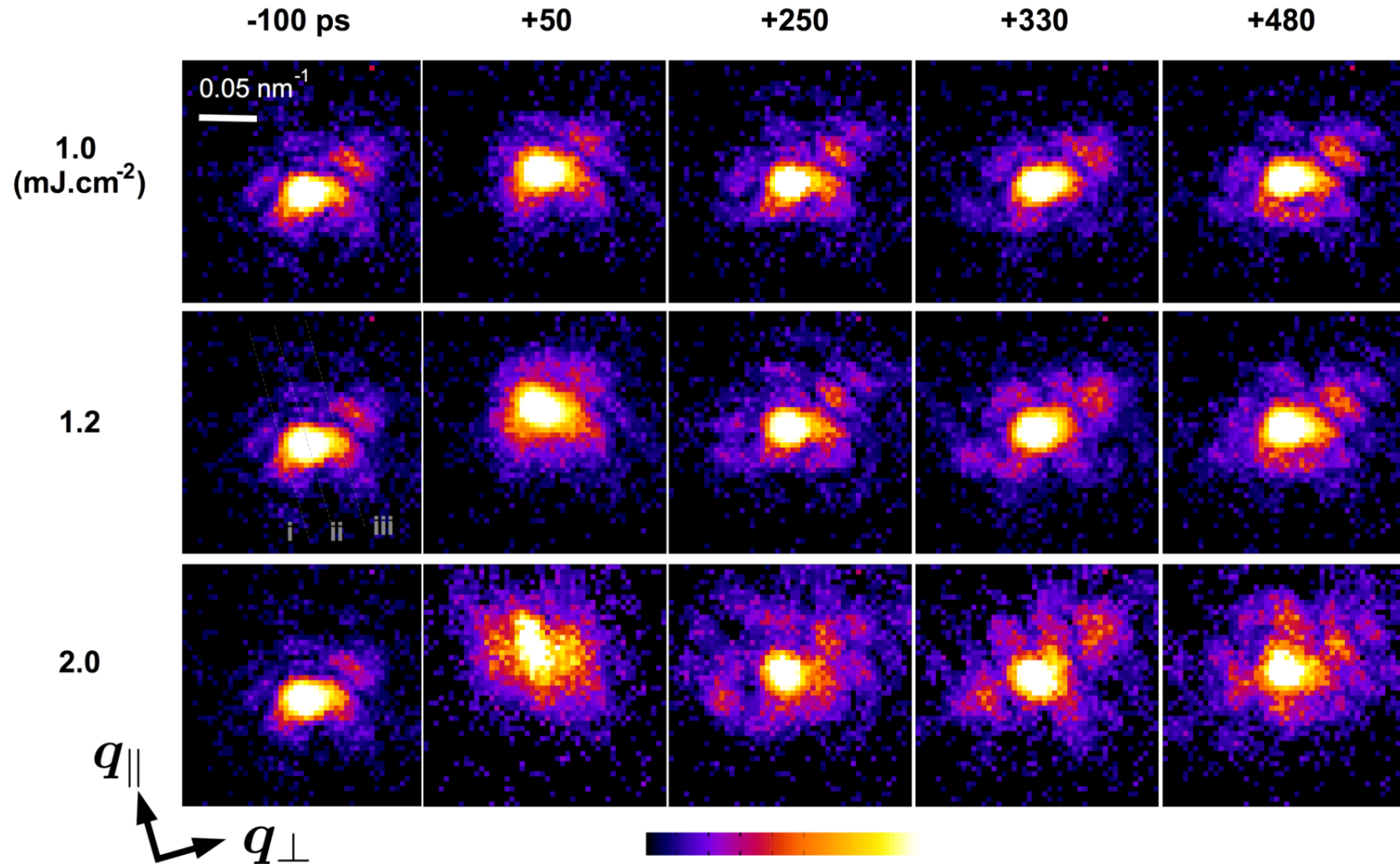
M. Abeykoon et al, Z. Kristallogr. **227** 248 (2012)

NaCl TEM, ED and ePDF



Pump Probe Au Nanocrystal Diffraction

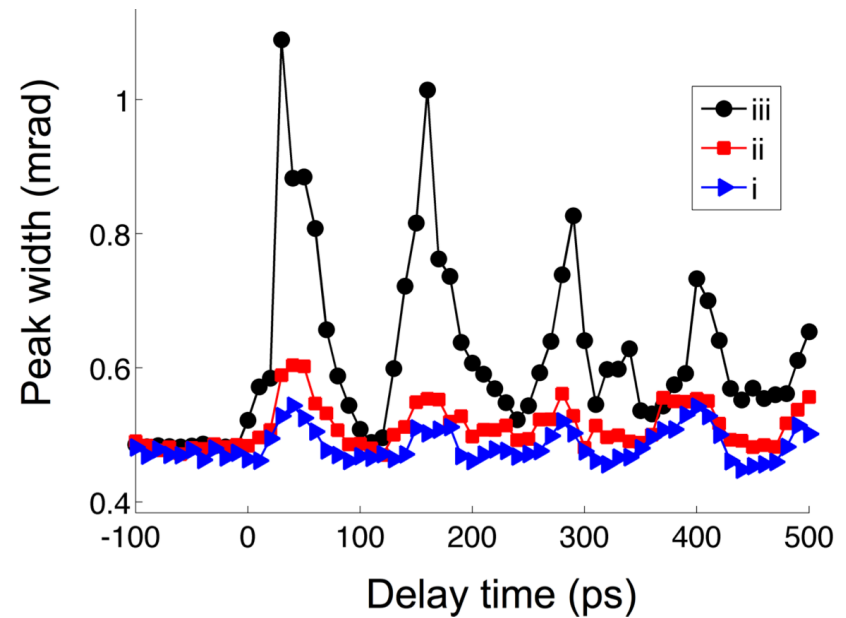
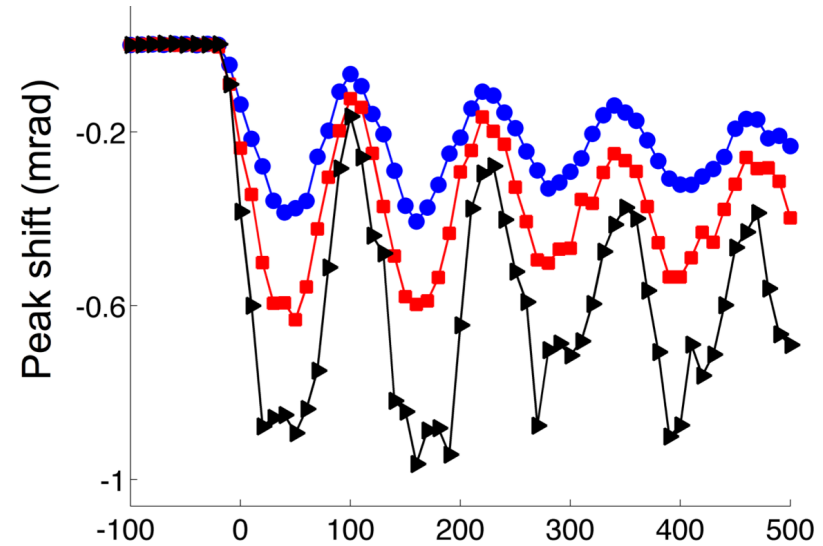
Jesse Clark et al, PNAS **112** 7444 (2015)



Dependence on Laser Fluence

Jesse Clark et al, PNAS **112**
7444 (2015)

1.0 mJ cm⁻²
1.4 mJ cm⁻²
2.0 mJ cm⁻²



Dependence on Laser Fluence

Jesse Clark et al, PNAS **112** 7444 (2015)

