Melt-front description of melting in polycrystalline materials

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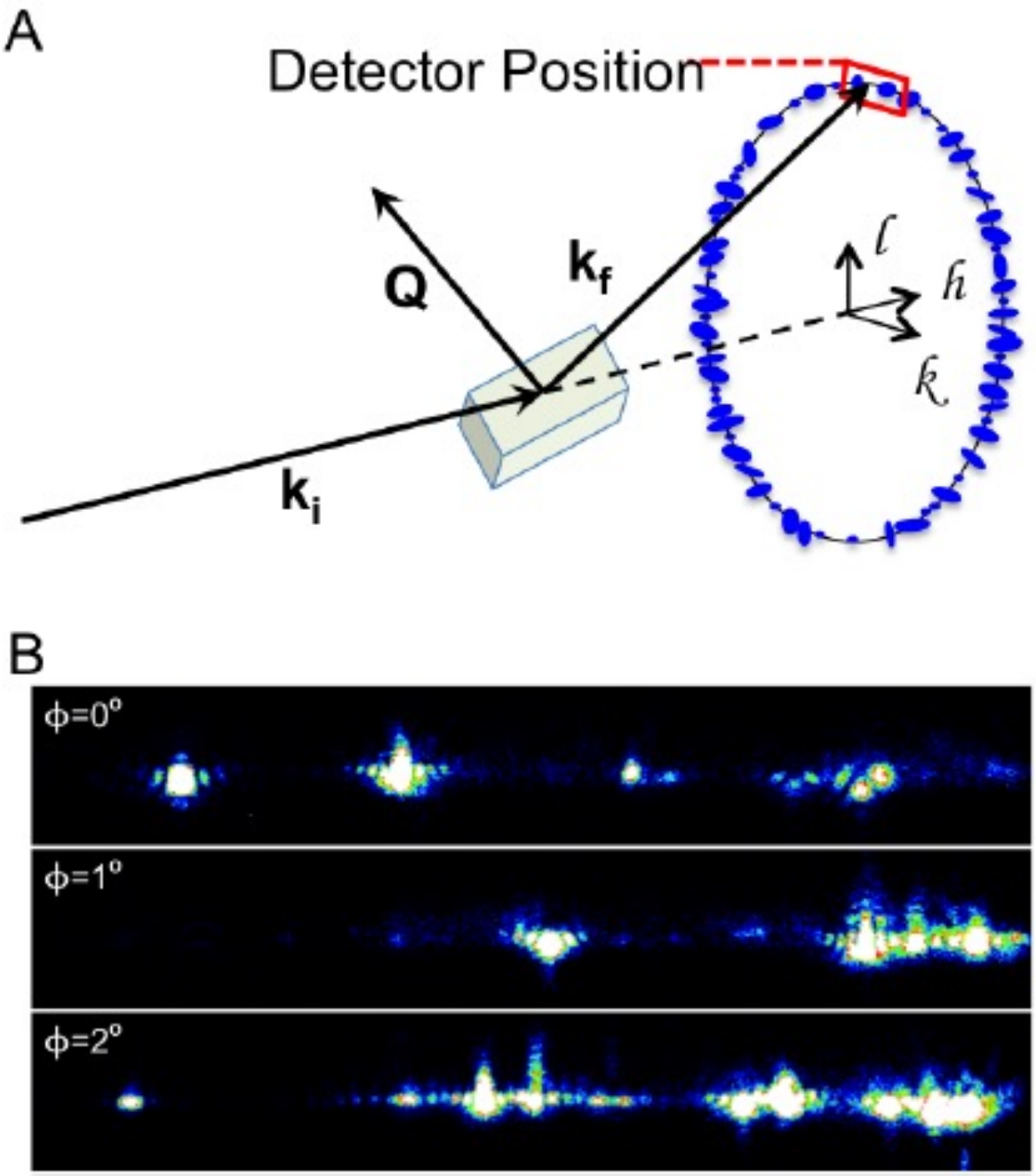
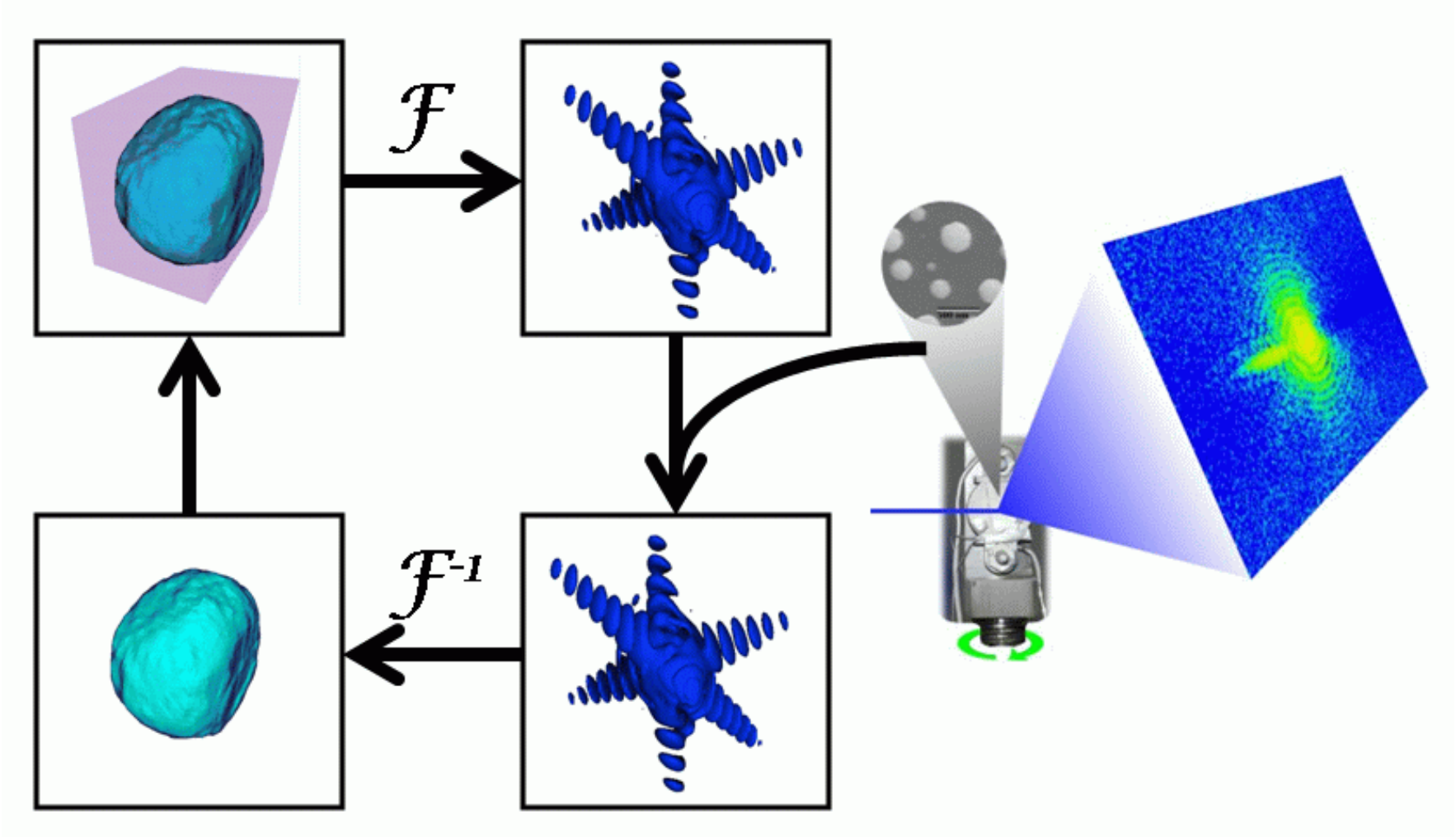
Sogang University
POSTEC

First User Meeting
PAL-XFEL
Pohang, January 2021


A
Detector Position
Q
k_f
k_i
l
h
k
B
ϕ=0°
ϕ=1°
ϕ=2°

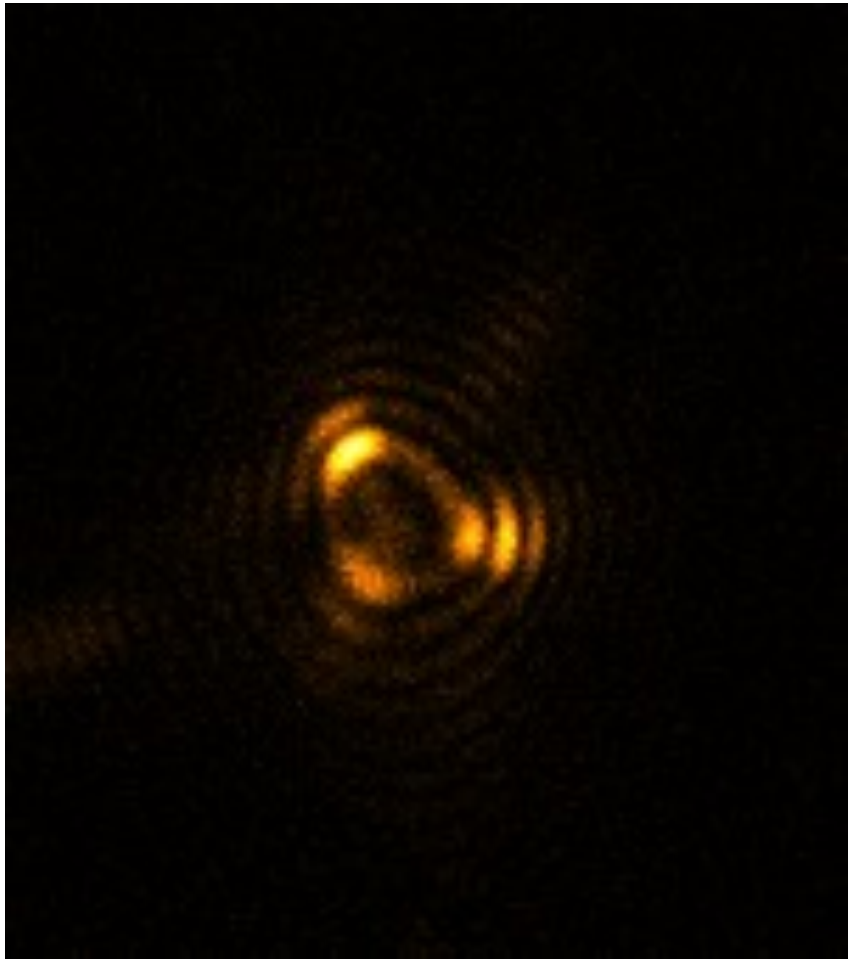
Generic "Error Reduction" method

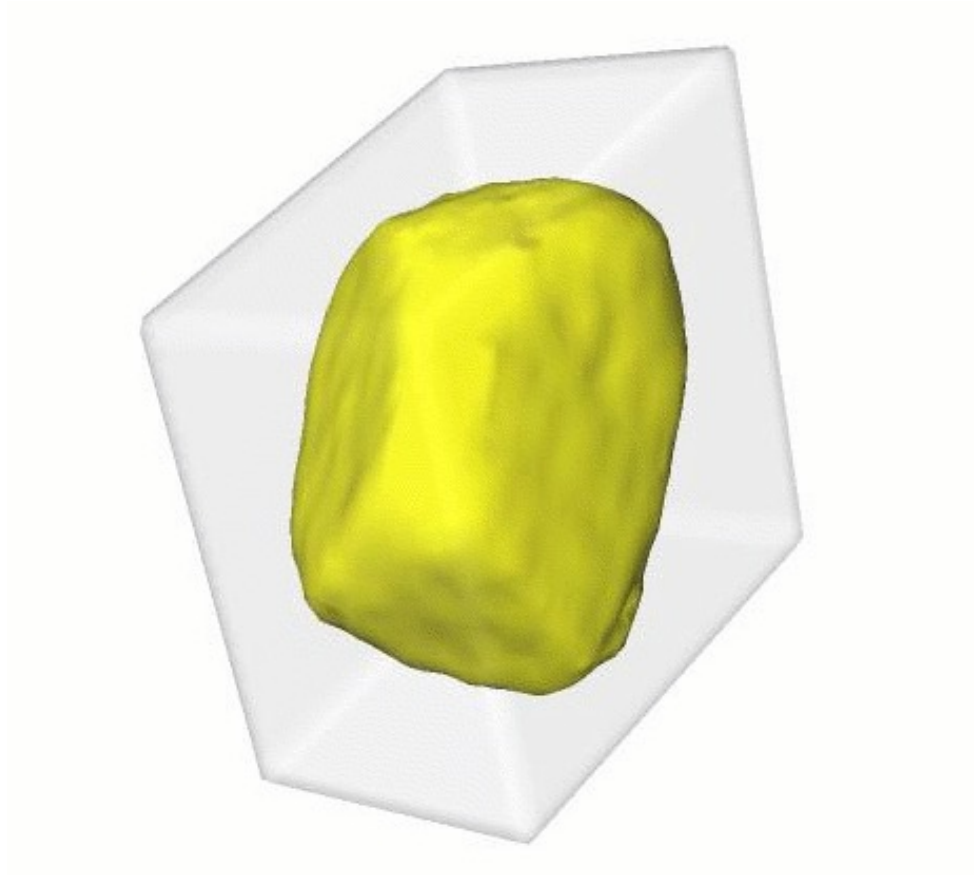


J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

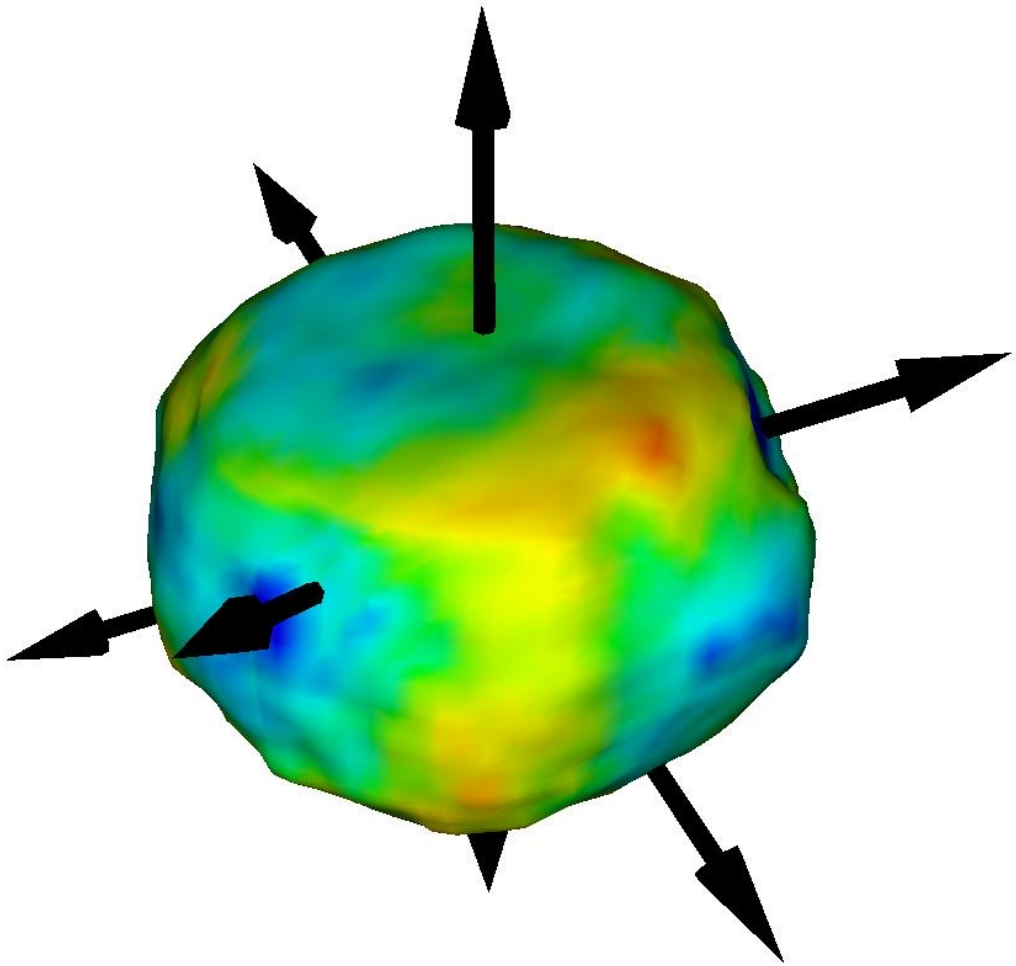
Gold nanocrystal reconstruction

showing support used for 20 HIO followed by 10 ER



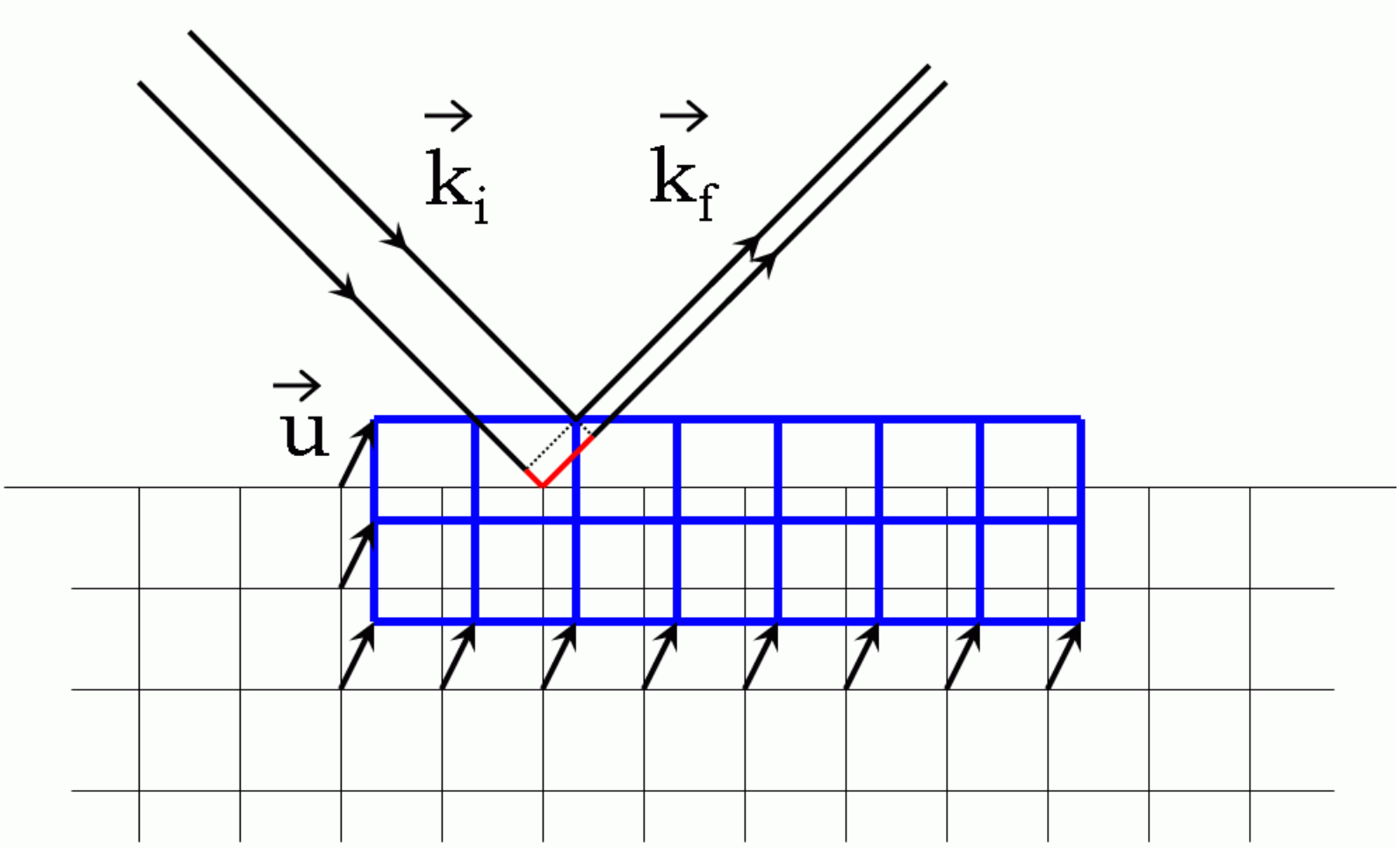


Phase isosurface of residual strain



Sensitivity to strain

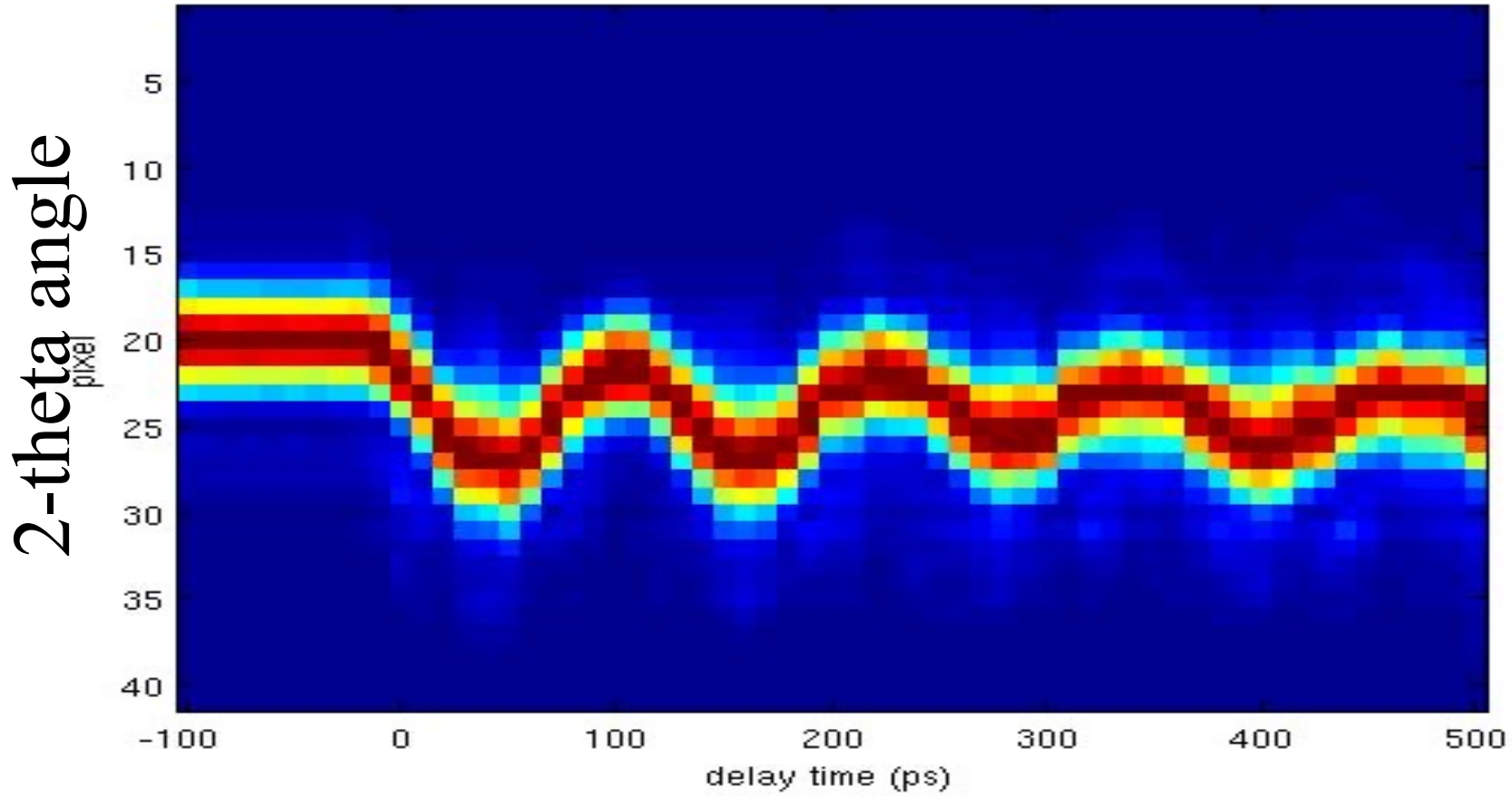
$$\Delta\varphi = \mathbf{k}_f \cdot \mathbf{u} - \mathbf{k}_i \cdot \mathbf{u} = \mathbf{Q} \cdot \mathbf{u}$$



Pump-probe at LCLS (XPP)

Justin Wark, Loren Beitra, Alexander Korsunsky, Ross Harder, David Fritz ,
Sebastien Boutet, Jesse Clark, Garth Williams, Brian Abbey, Andy Higginbotham,
Diling Zhu, Henrick Lemke, Mattieu Chollet, Marc Messerschmidt

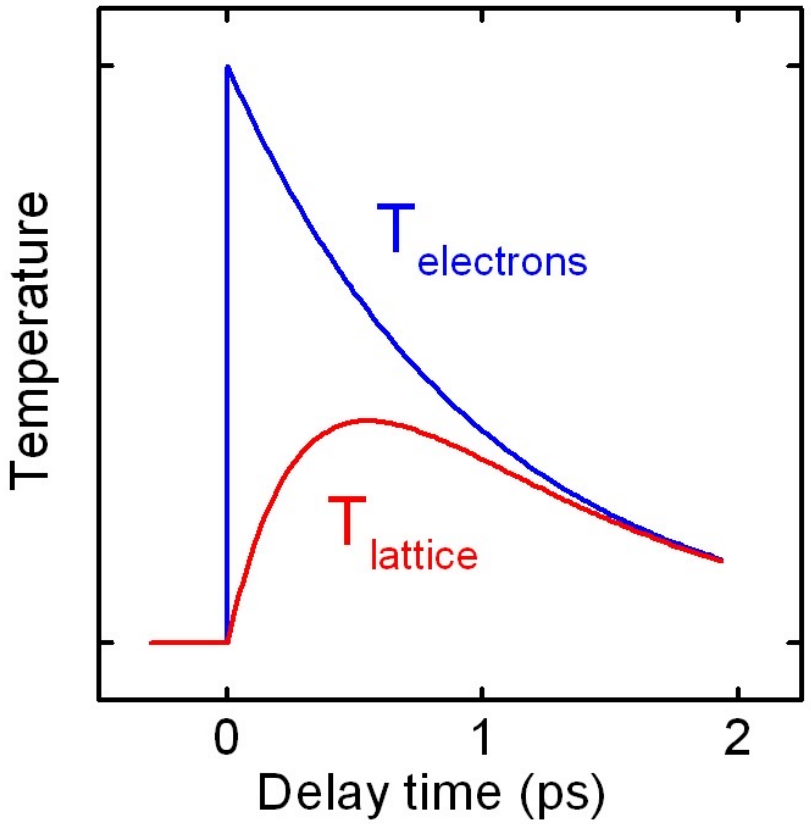
250nm Single Gold Crystal



"Two-temperature" model

I. K. Robinson et al, Journal of Optics **18** 054007 (2016)

J. K. Chen et al, Int J. Heat Transfer **49** 307 (2006)



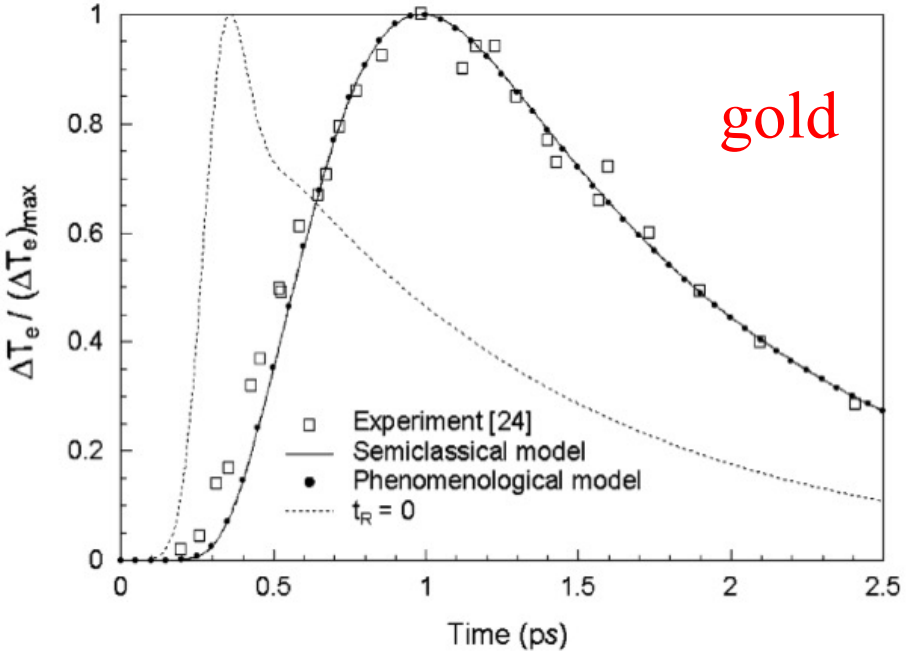
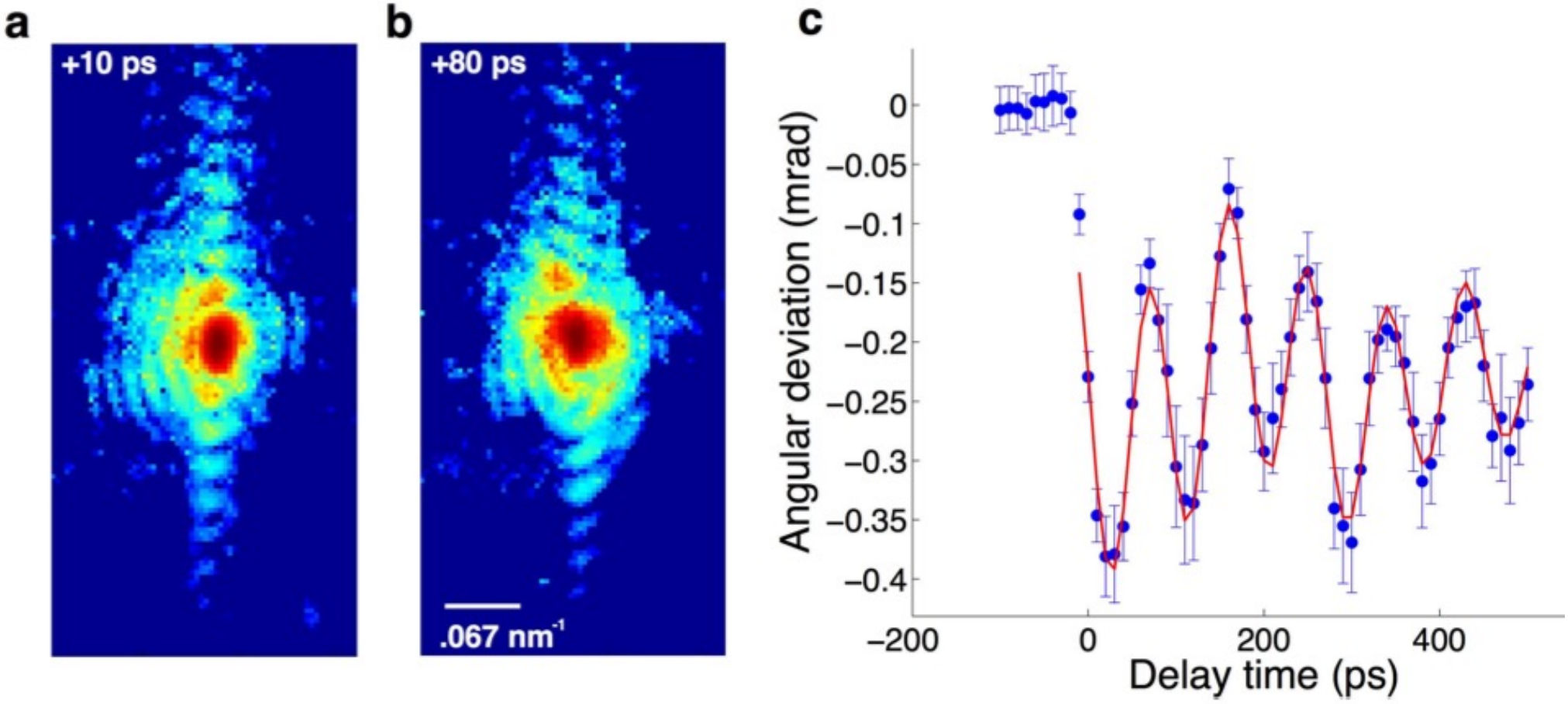


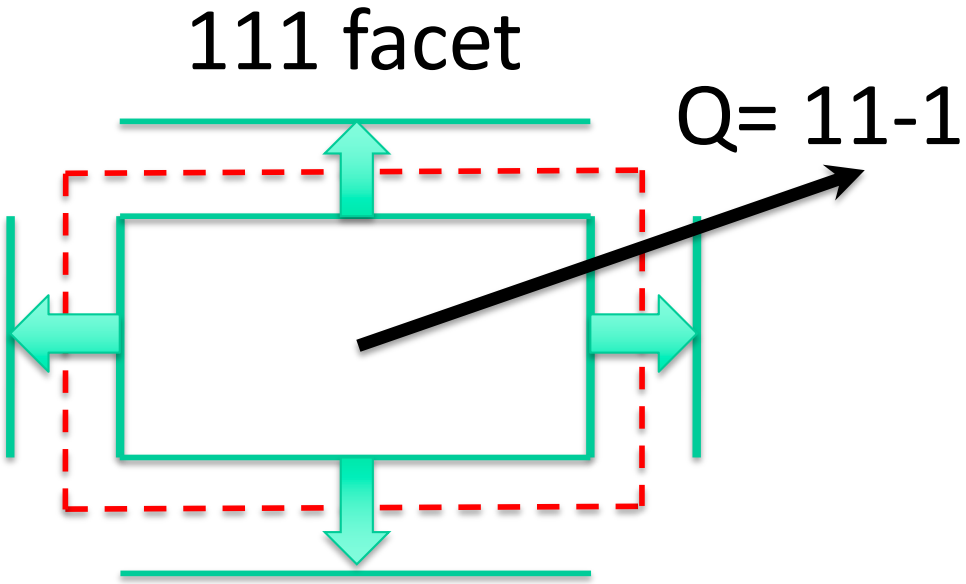
Fig. 2. Comparison of the change in electron temperature at the front surface of an 80-nm gold film irradiated by a 2.8 mJ/cm^2, 800 nm, 150-fs laser pulse.

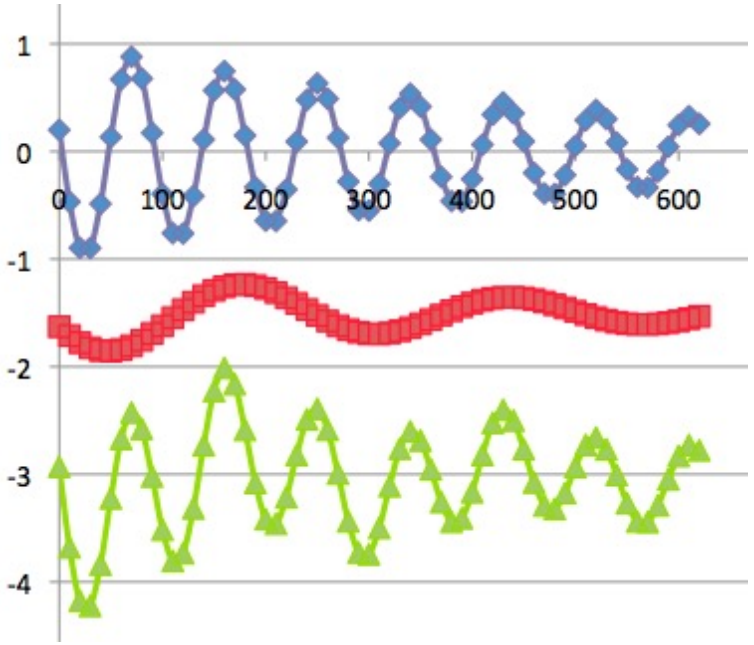
Time resolved Bragg peak position



Two Normal Modes of Vibration

$$S(\tau) = \sum_{n=1}^{N} A_n \exp\left[-(\tau/\tau_{d,n})^2\right] \cos\left(\omega_n \tau + \varphi_{0,n}\right)$$



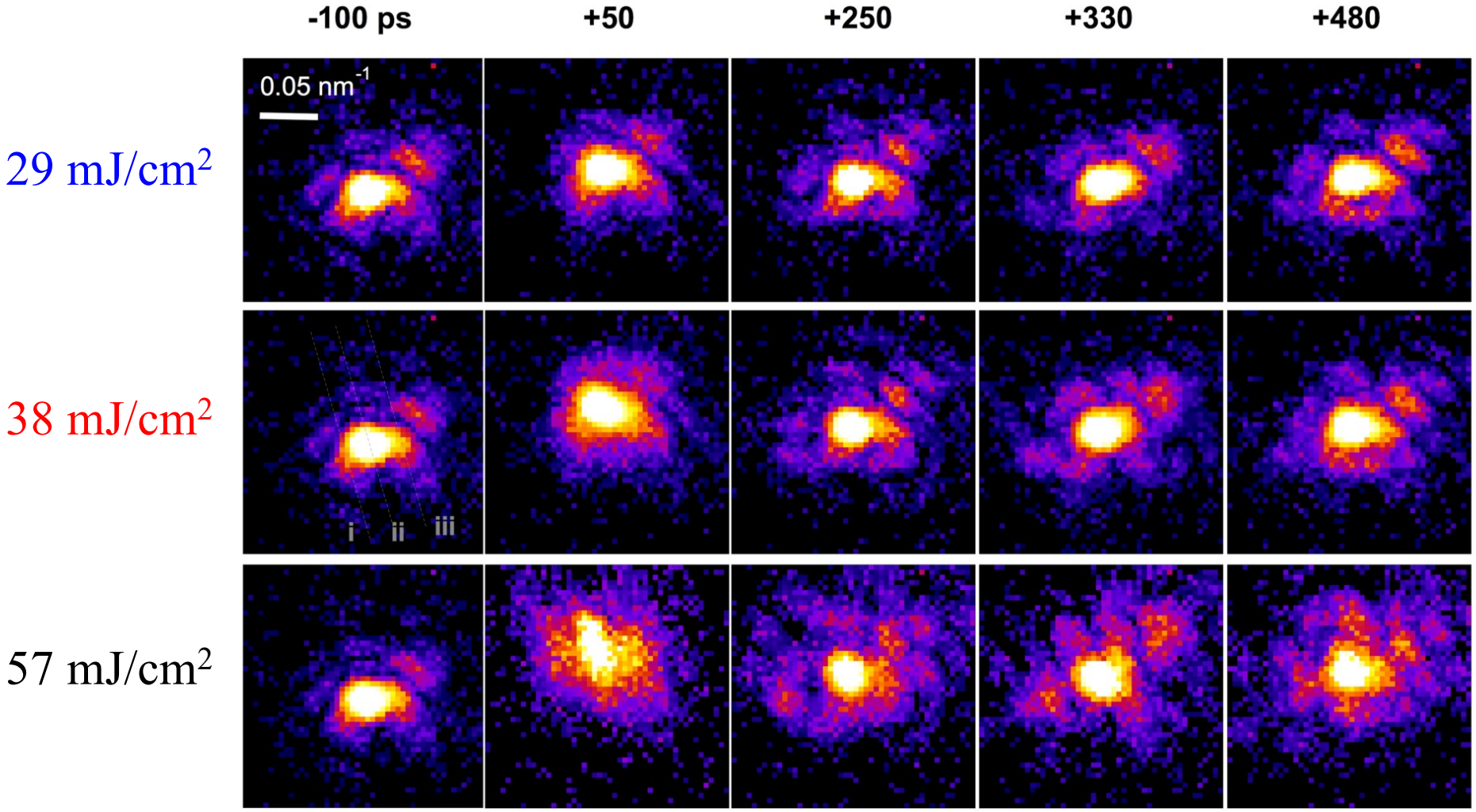


T_1 = 90ps h_1 = 145nm c_S = 3240 m/s

T_2 = 259ps h_2 = 420nm

Dependence on Laser Fluence

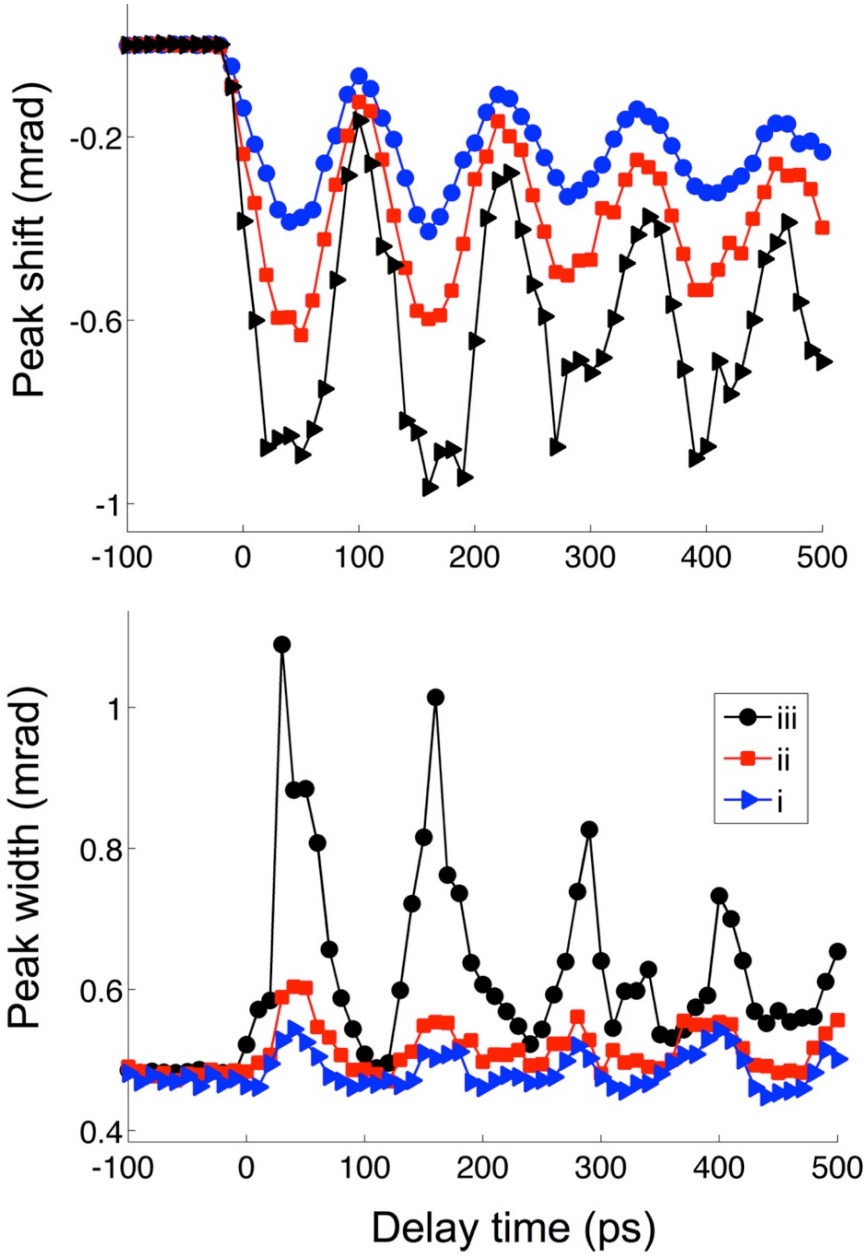
Jesse Clark et al, PNAS **112** 7444 (2015)



Dependence on Laser Fluence

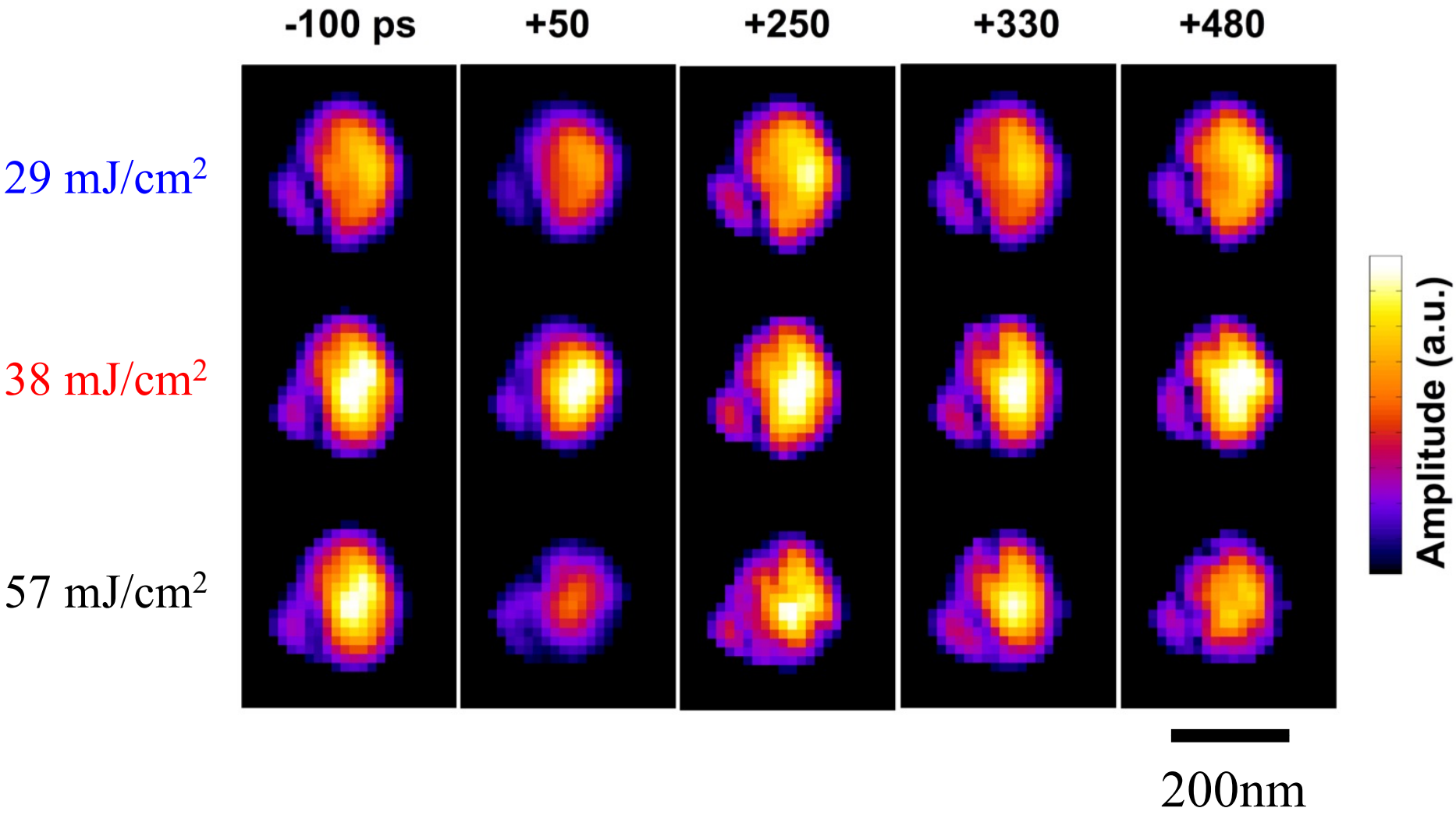
Jesse Clark et al, PNAS **112** 7444 (2015)

29 mJ/cm^2
38 mJ/cm^2
57 mJ/cm^2



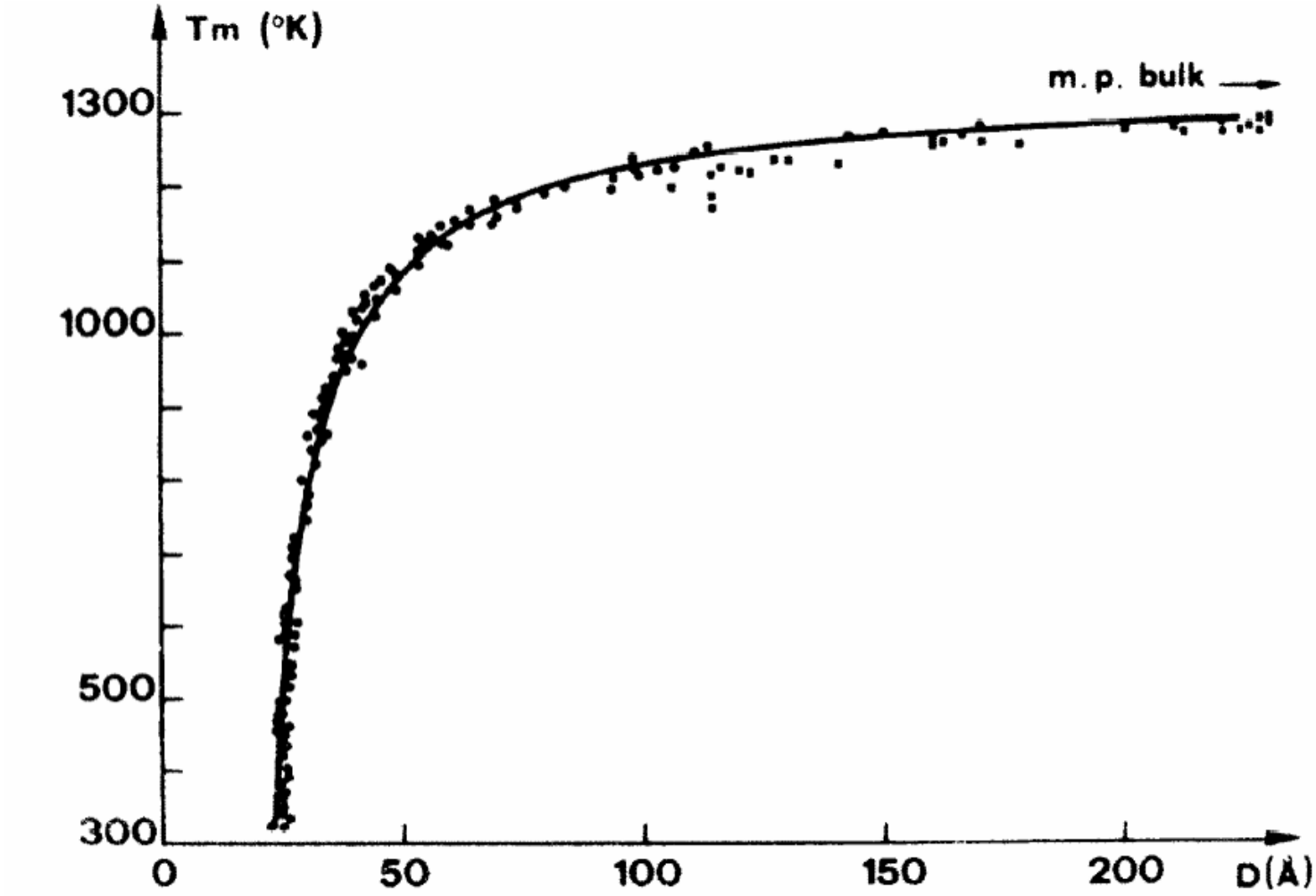
Dependence on Laser Fluence

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

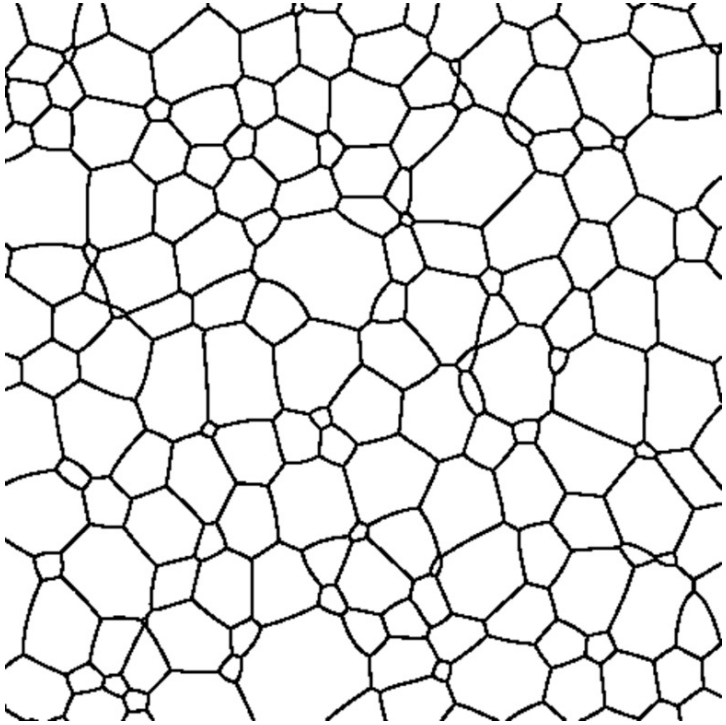


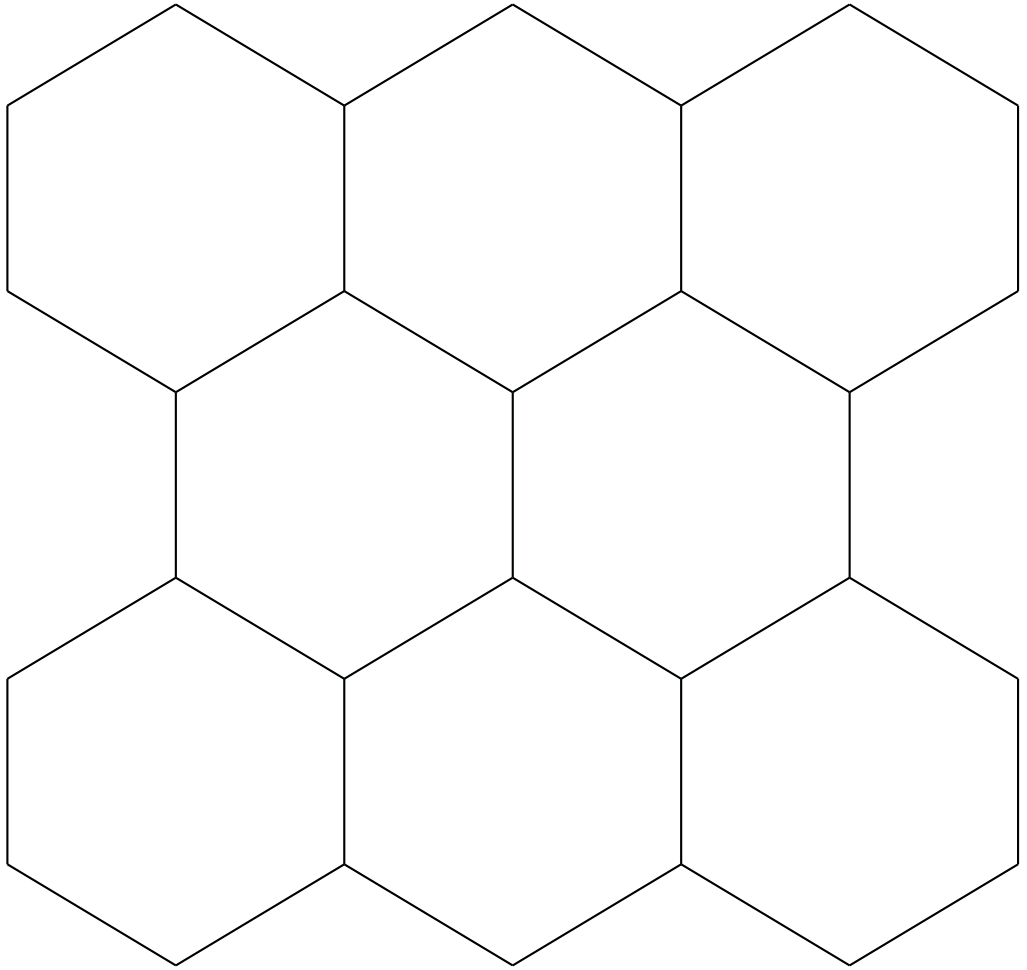
Size-dependent Melting of Au Particles

P. Buffat and J-P. Borel, Phys. Rev. A 2287-97 (1975)



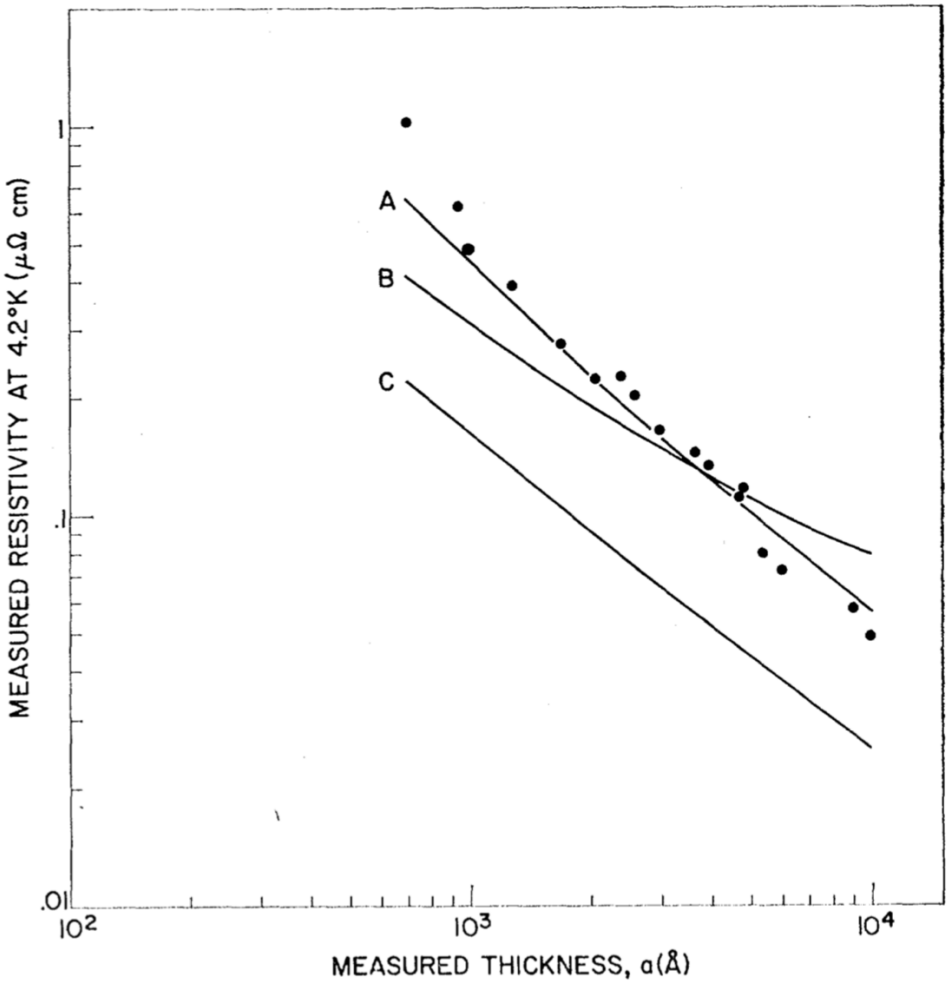
Grain Boundary Melting ?



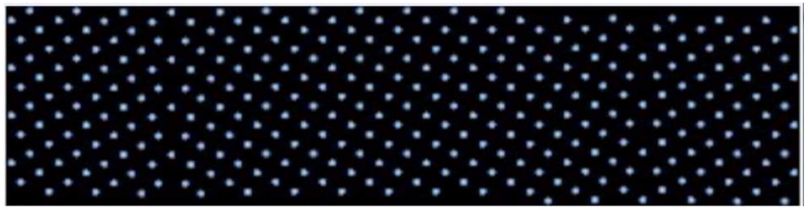


Resistivity of Al Thin Films

A. F. Mayadas and M. Shatzkes, PRB **1** 1382 (1970)



- "Universal curve" of MFP vs electron energy
- Thermal MFP removed at low temperature
- Grain size proportional to thickness (model)

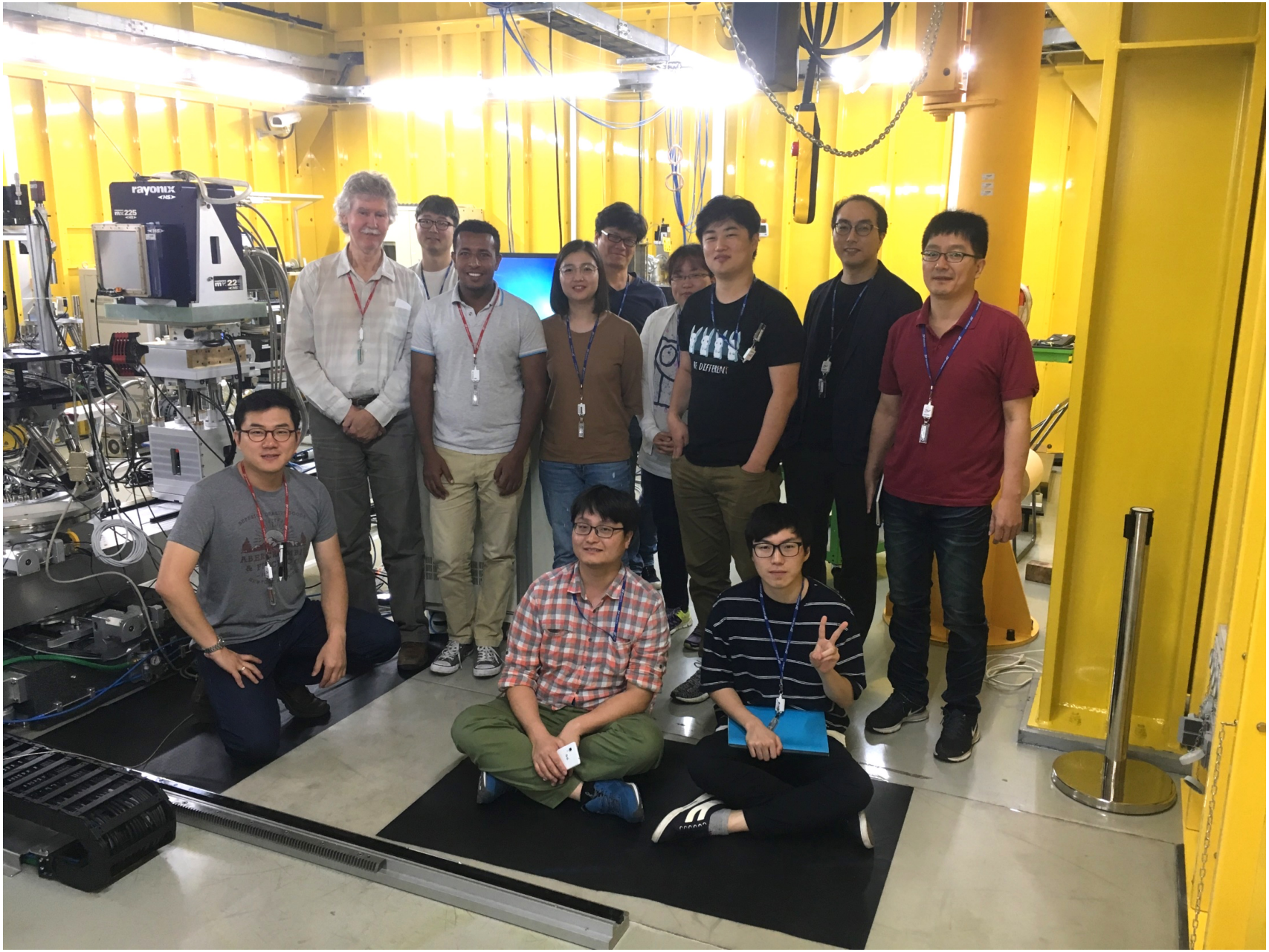


Questions about Melting

- Can we see the liquid phase?
- Are there transient liquid structures (water)?
- How fast does melting take place?
- Where does the melting start?
- How does the 2TM couple to the lattice?
- Role of sample geometry?

PAL XFEL Control Room

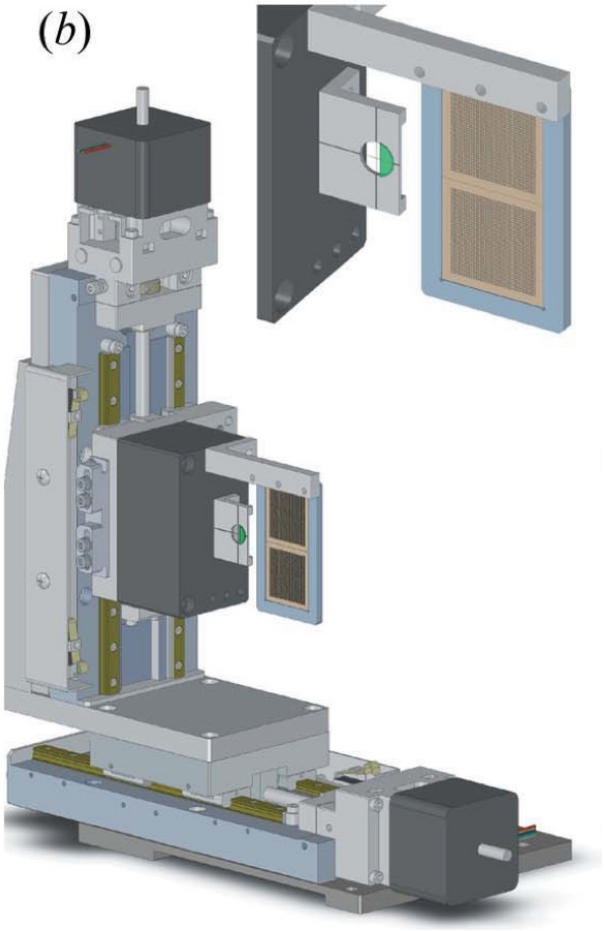
Sunam Kim, Jae Hyuk Lee, Yongsam Kim, Jaeku Park, Sang-Youn Park, Intae Eom, Hyojung Hyun, Tae-Yeong Koo, Jaehun Park, Daewoong Nam and Sang Soo Kim

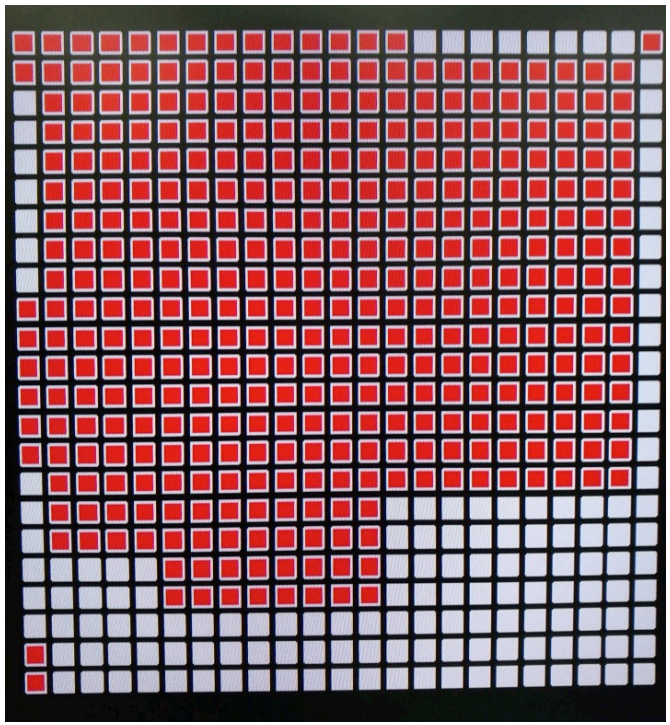

rayonix

Scan Stage for MAXIC chamber

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

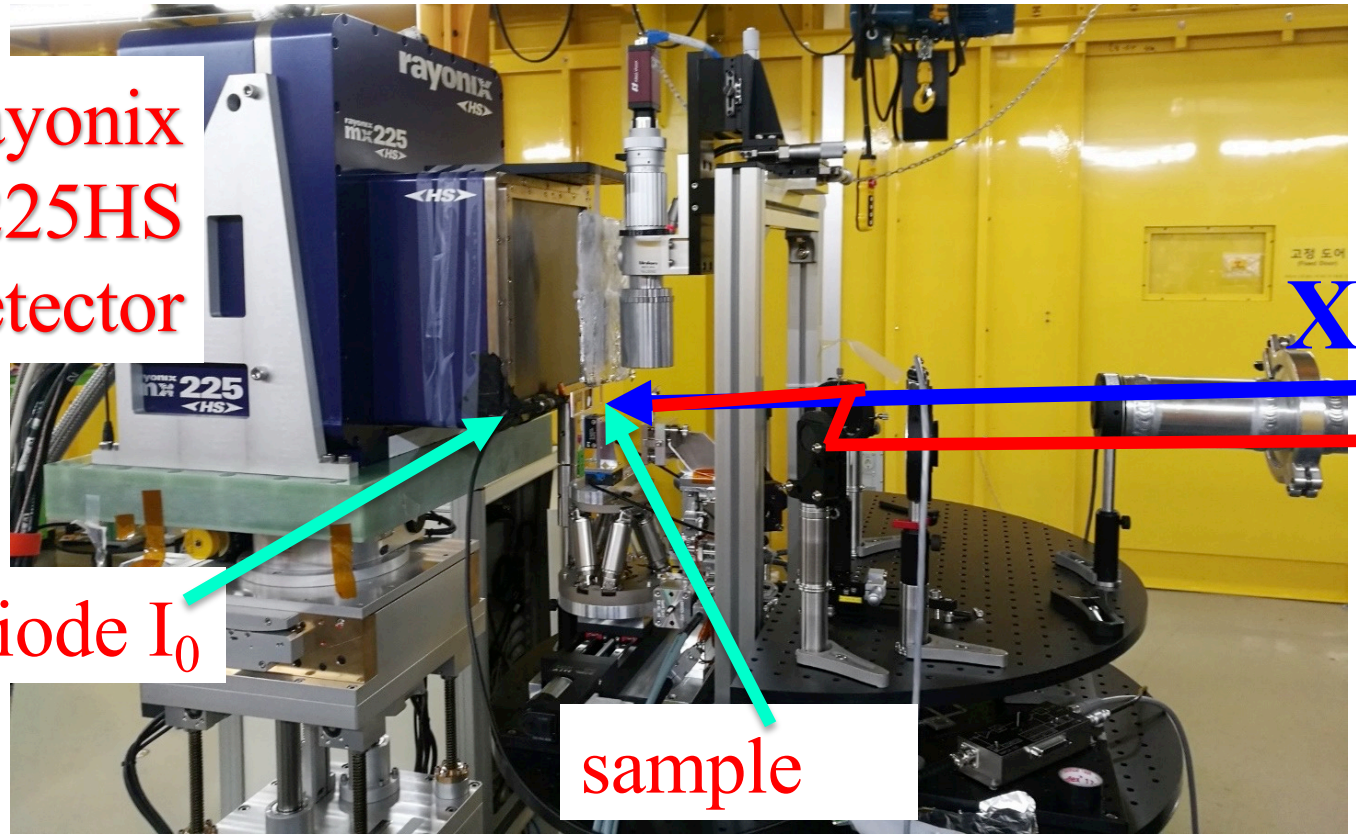
Daewoong Nam, scanning software



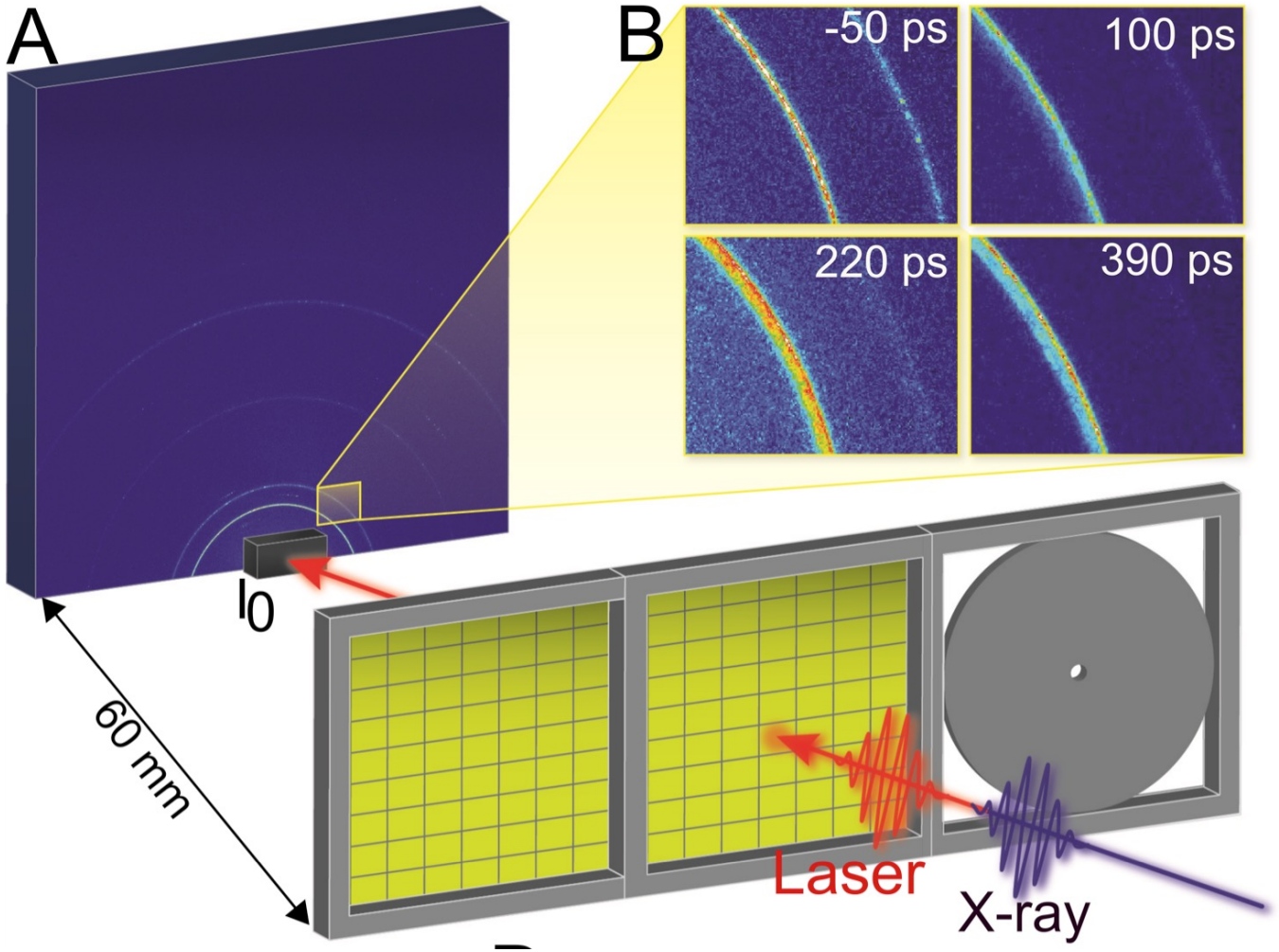


23x23 windows

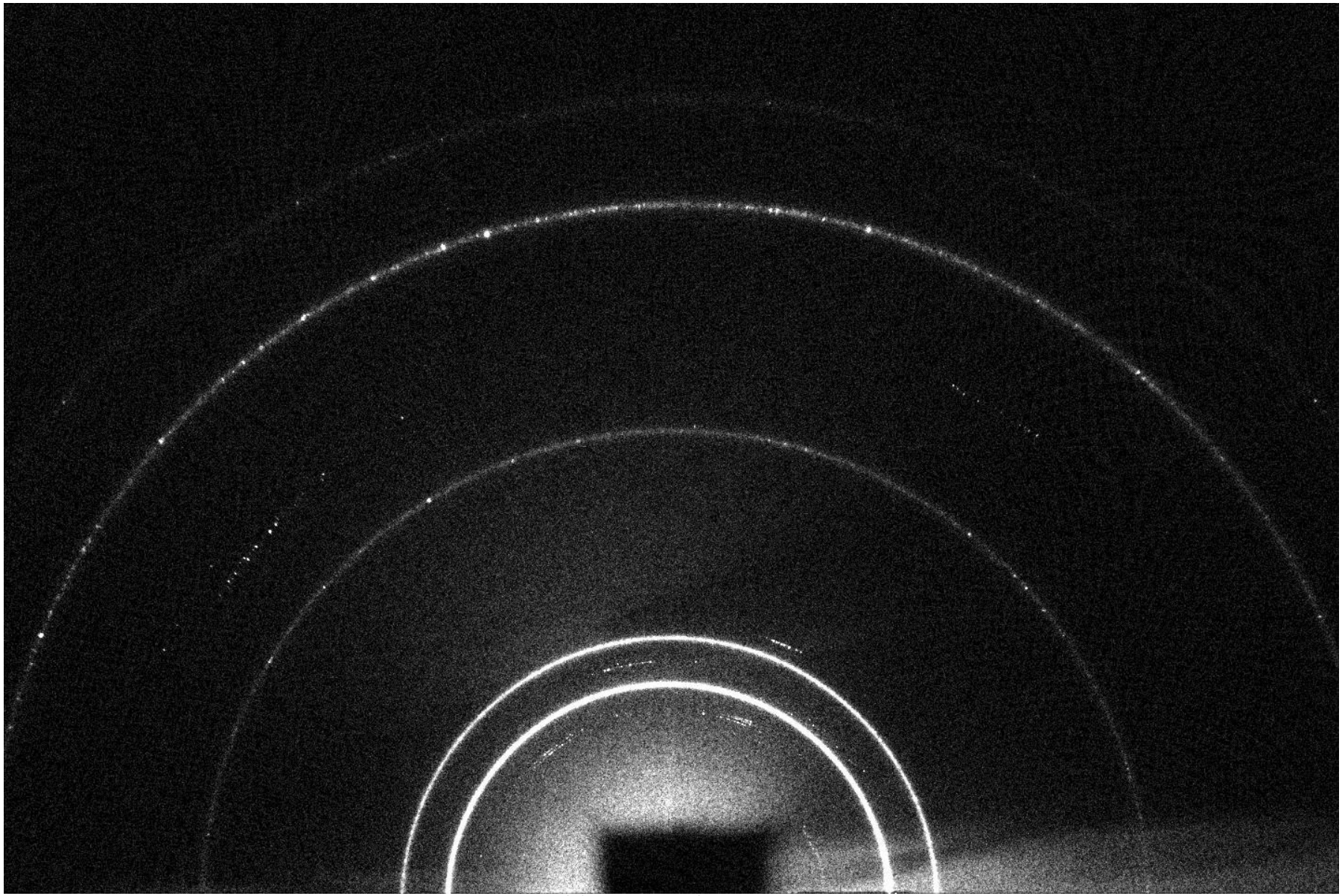
Experimental set-up at PAL-XFEL September 2017



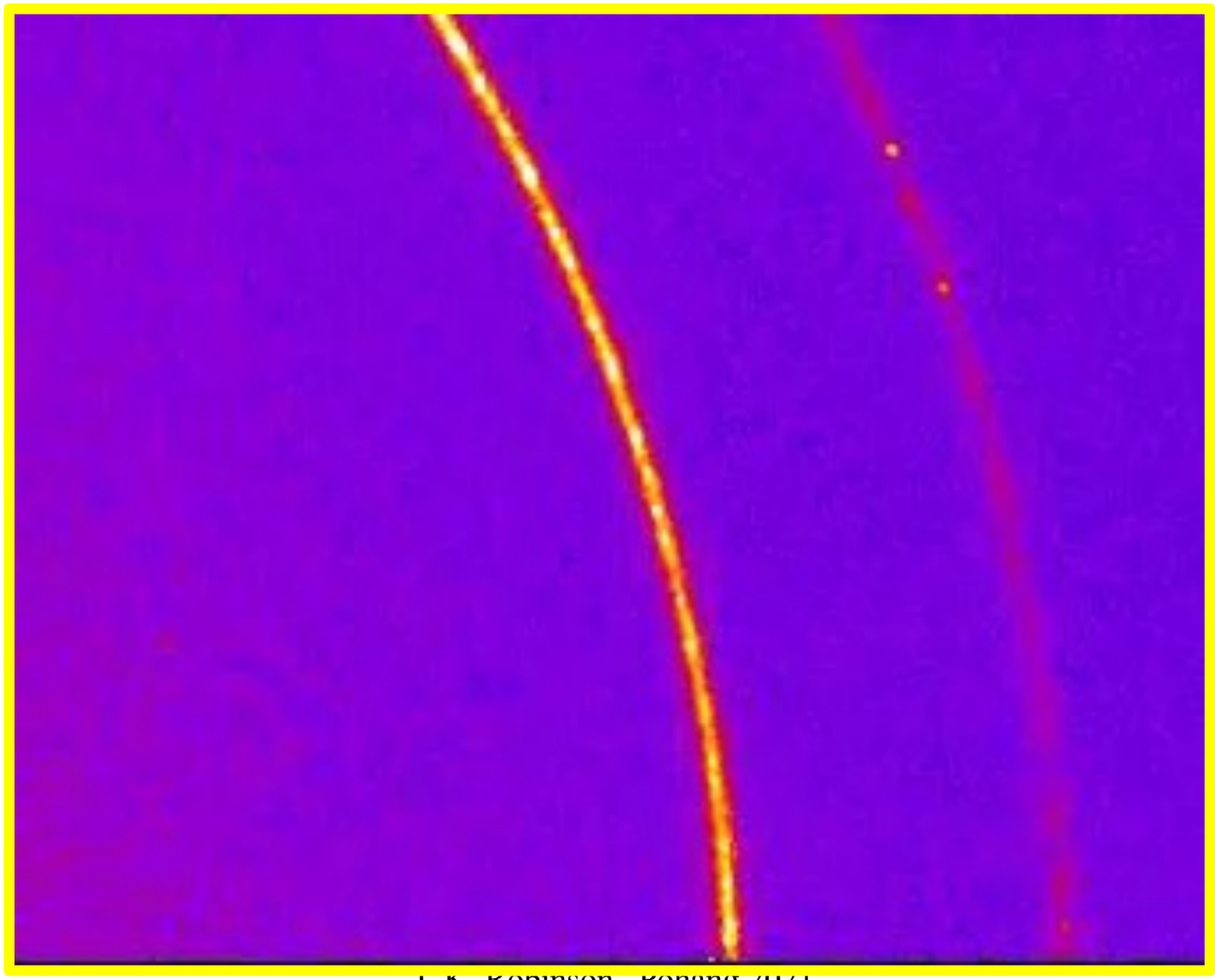
Powder Diffraction Geometry



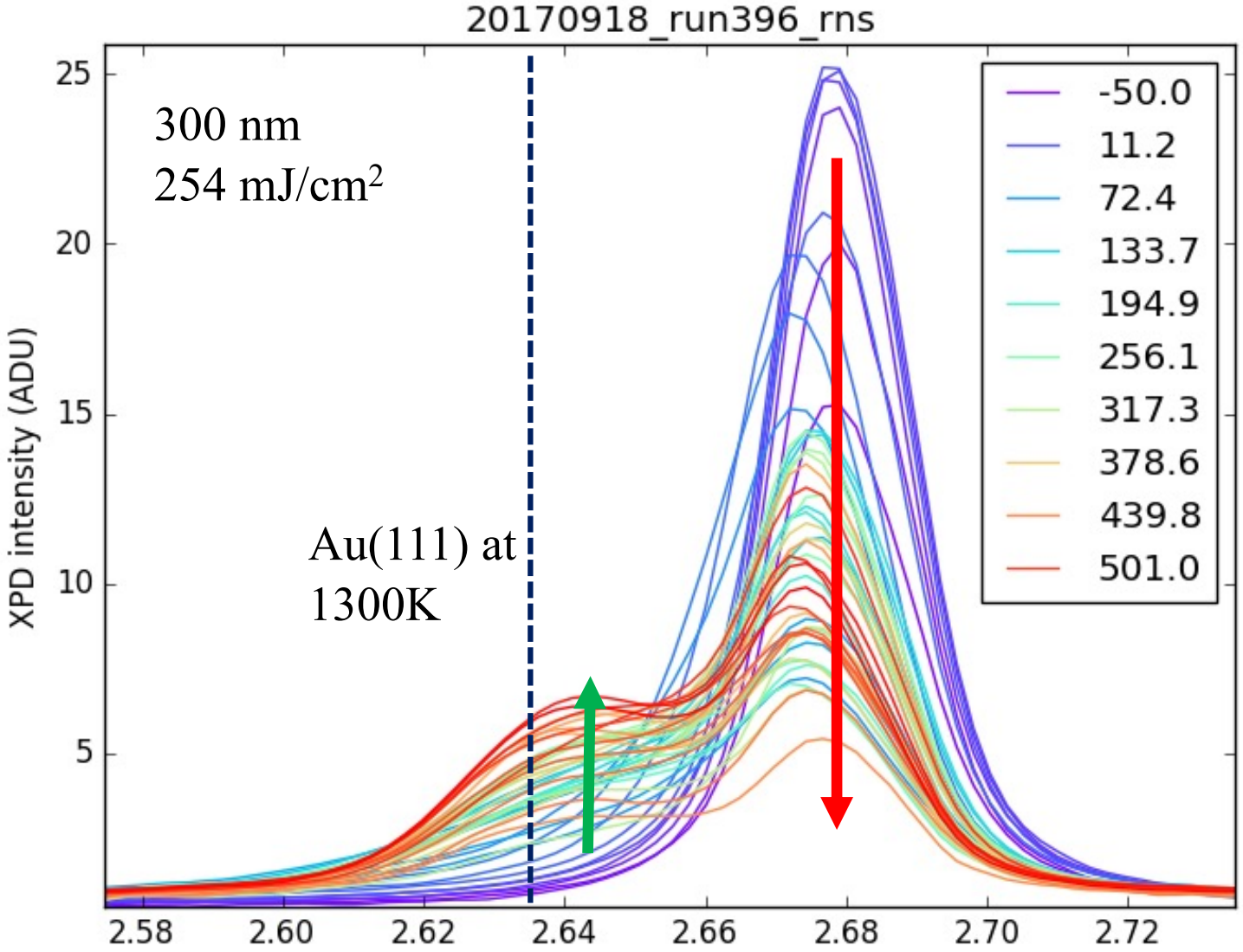
Raw data #397 300nm film



Raw data #396 300nm film, 254 mJ/cm^2



PyFAI integration around ring



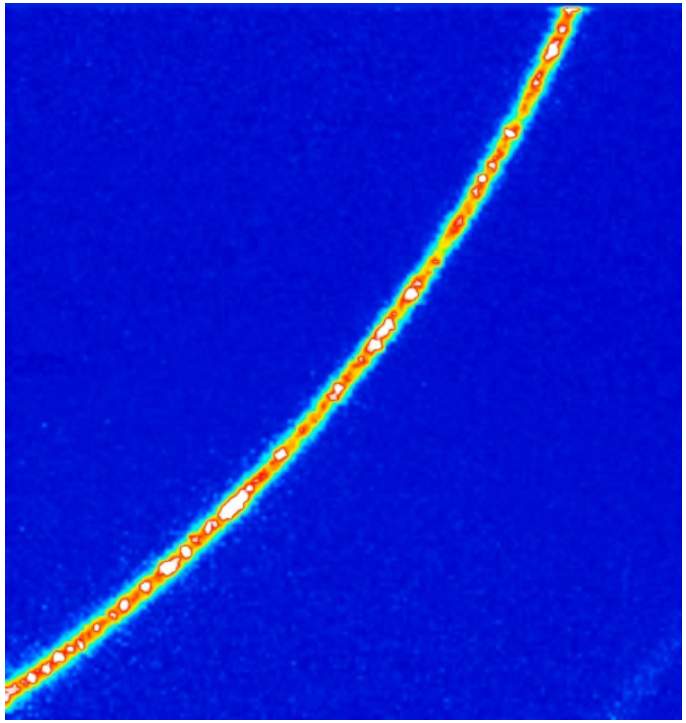
Average grain size ≥ 30nm

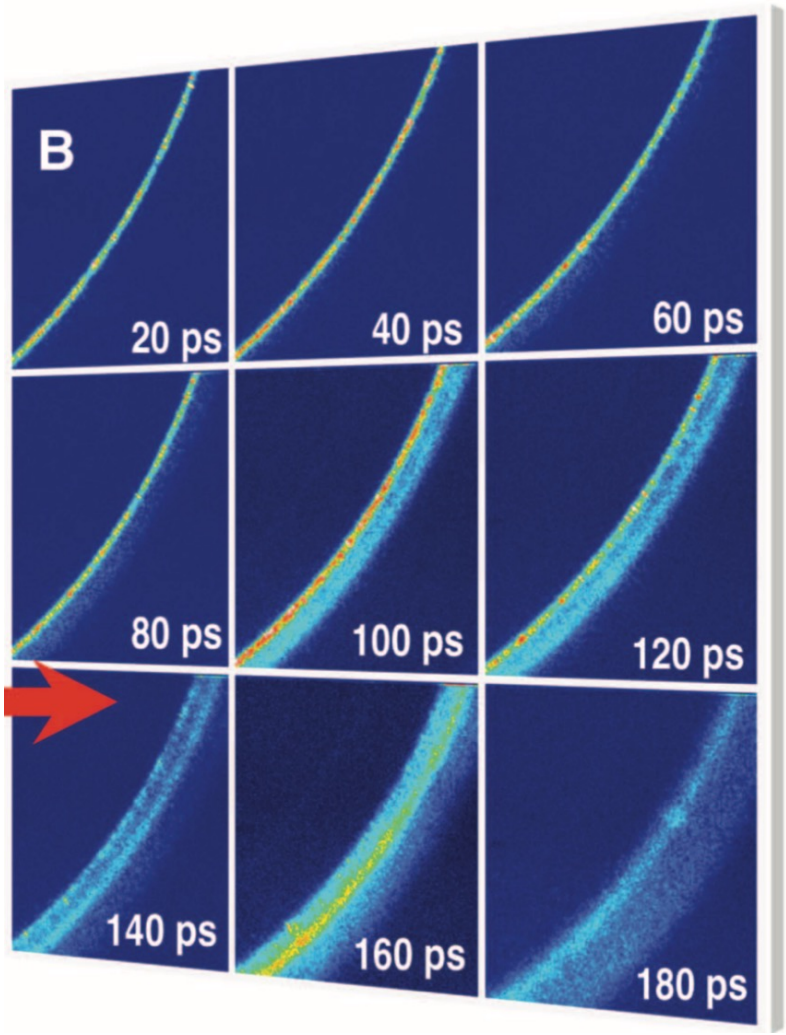
New peak ~3x broader

Thin Film of Cu at CXI, LCLS

D. Milathianaki et al, Science **342** 220 (2013)

38 J/cm^2 170ps

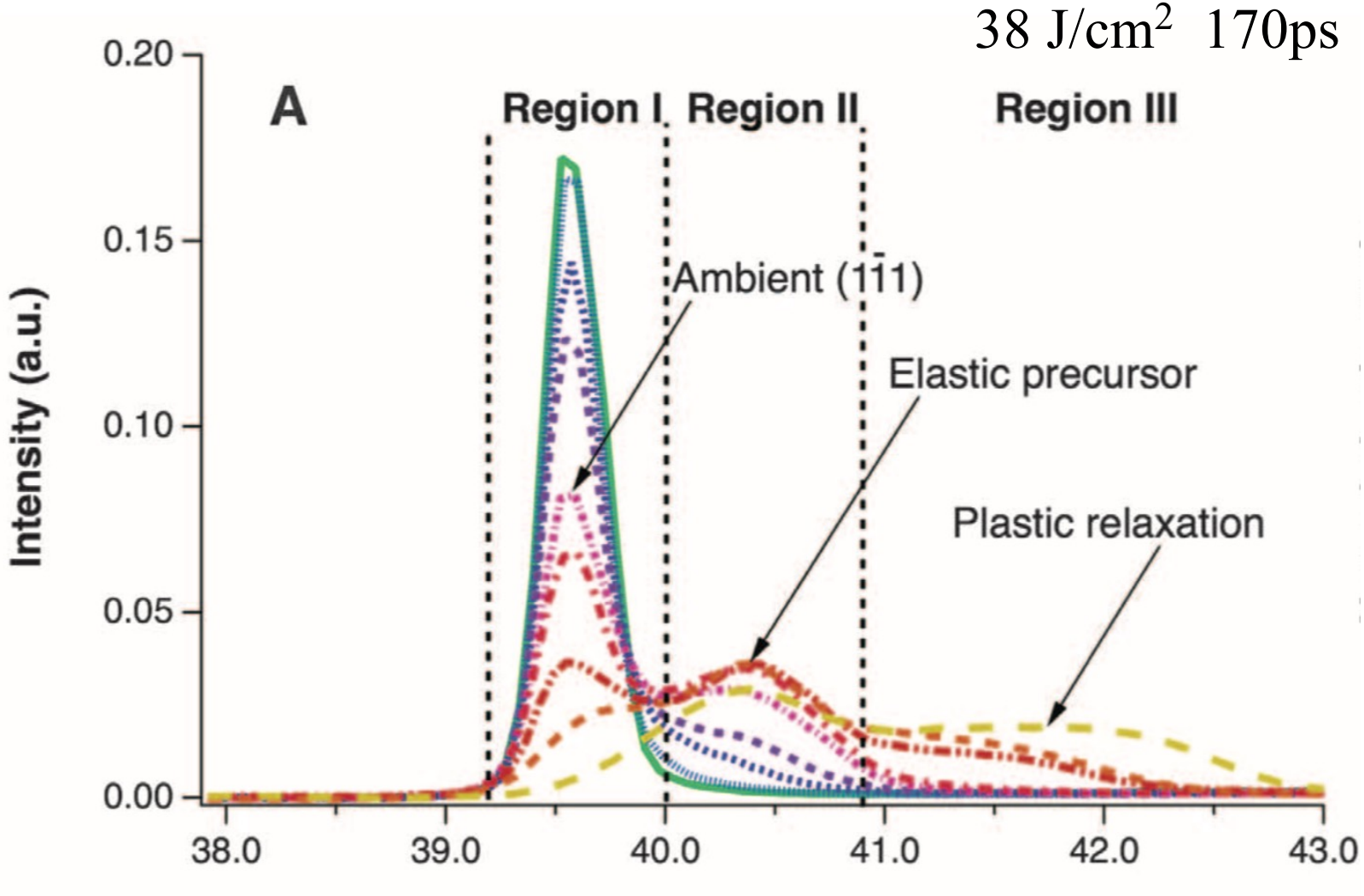




Thin Film of Cu at CXI, LCLS

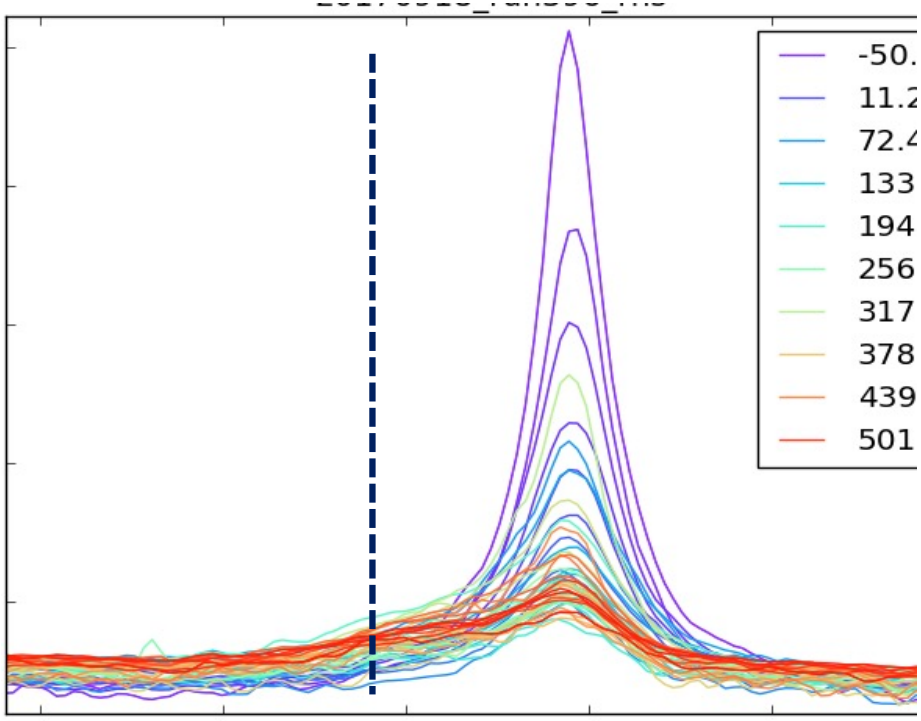
D. Milathianaki et al, Science **342** 220 (2013)

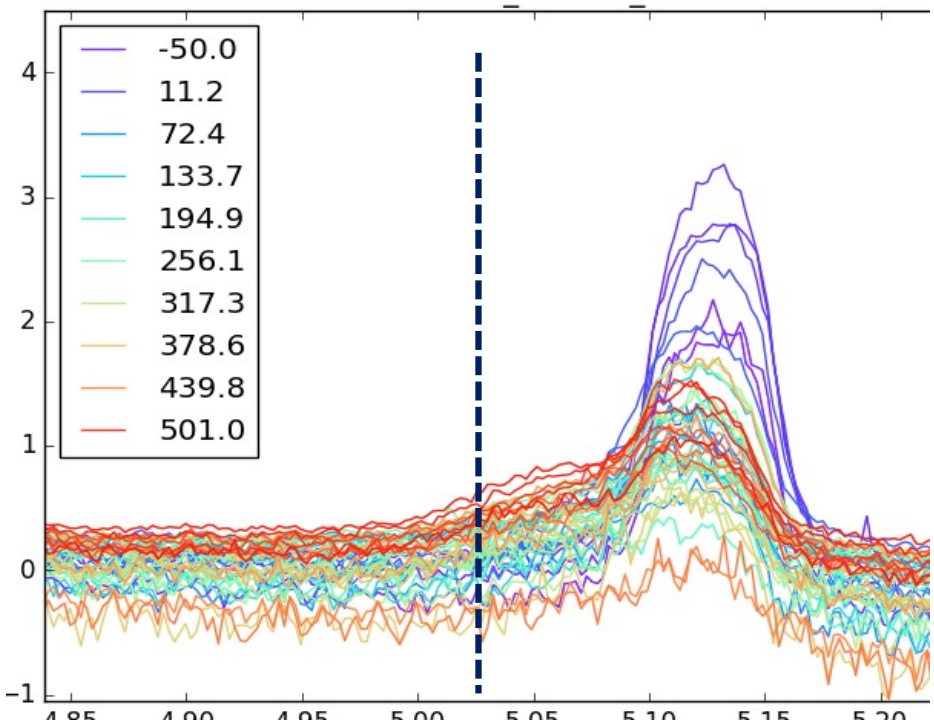
38 J/cm^2 170ps



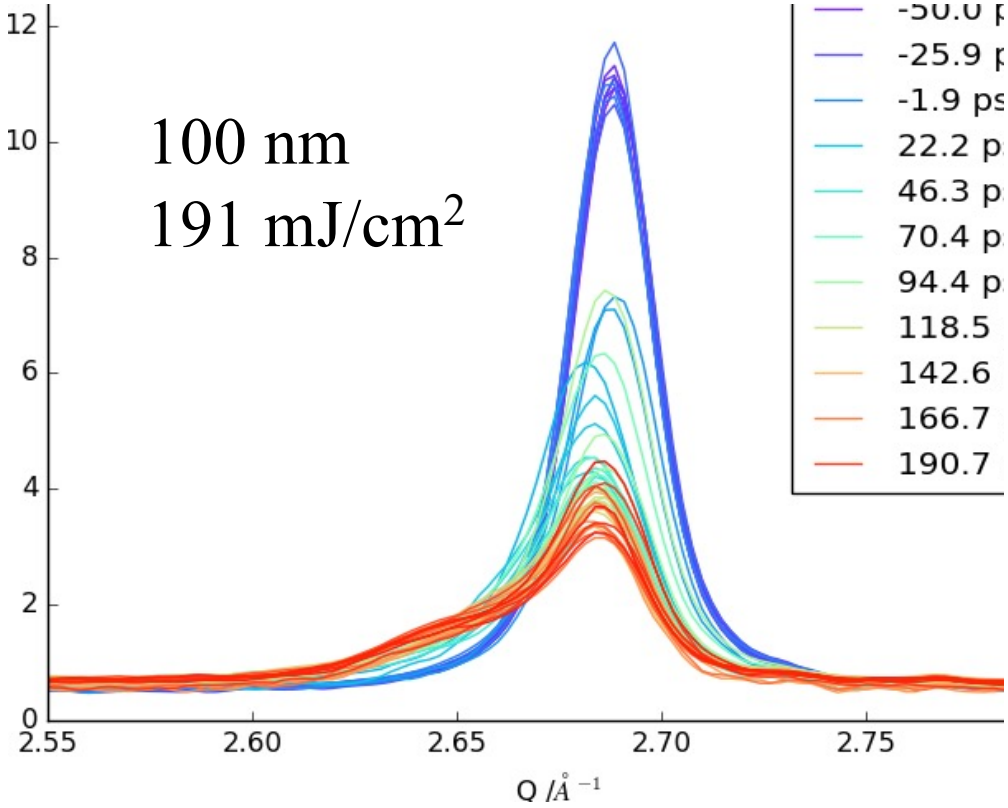
200 and 311 peaks

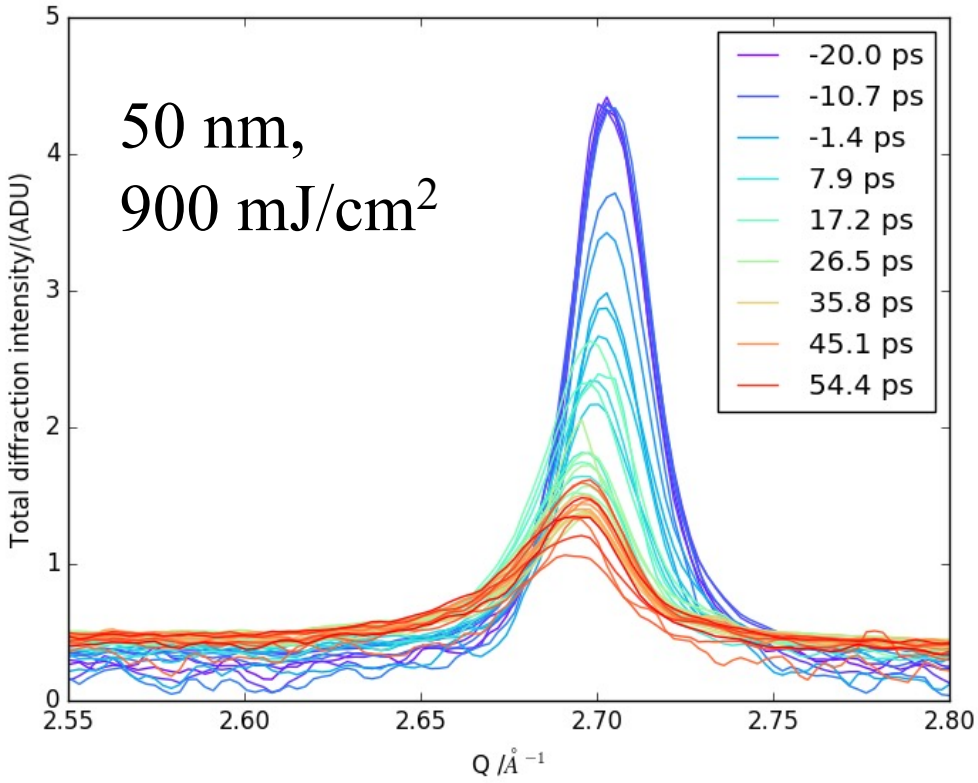
#396 300nm film, 254 mJ/cm^2



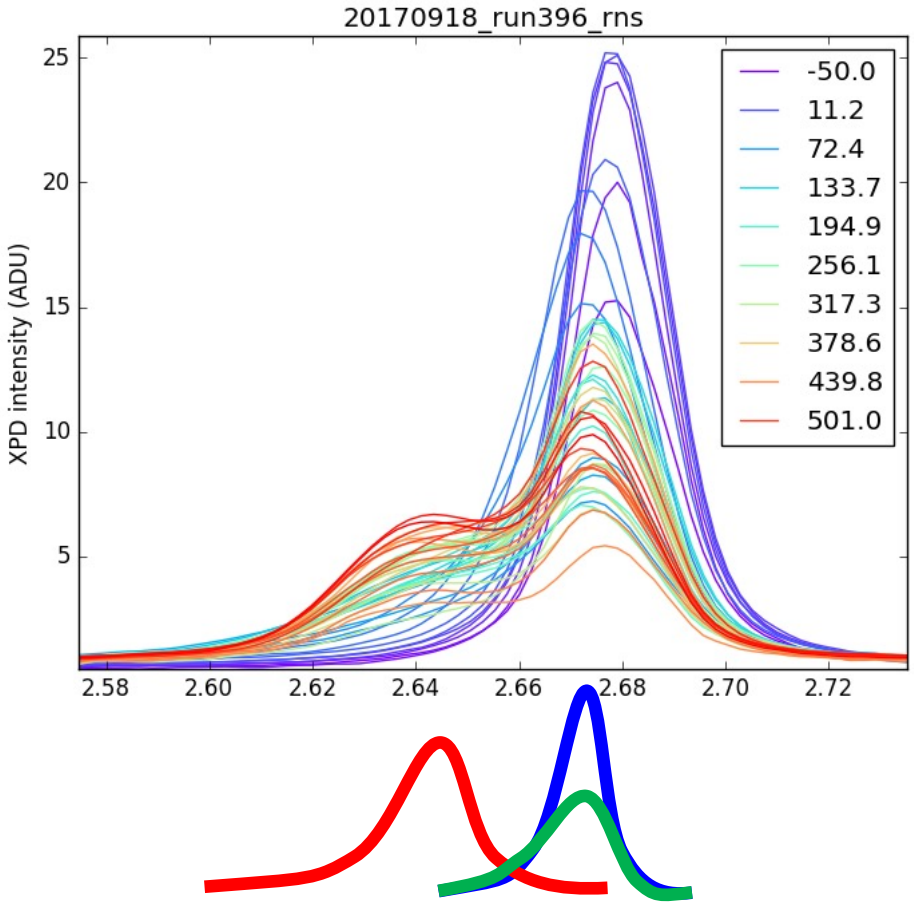


Thinner films, #416 and #382



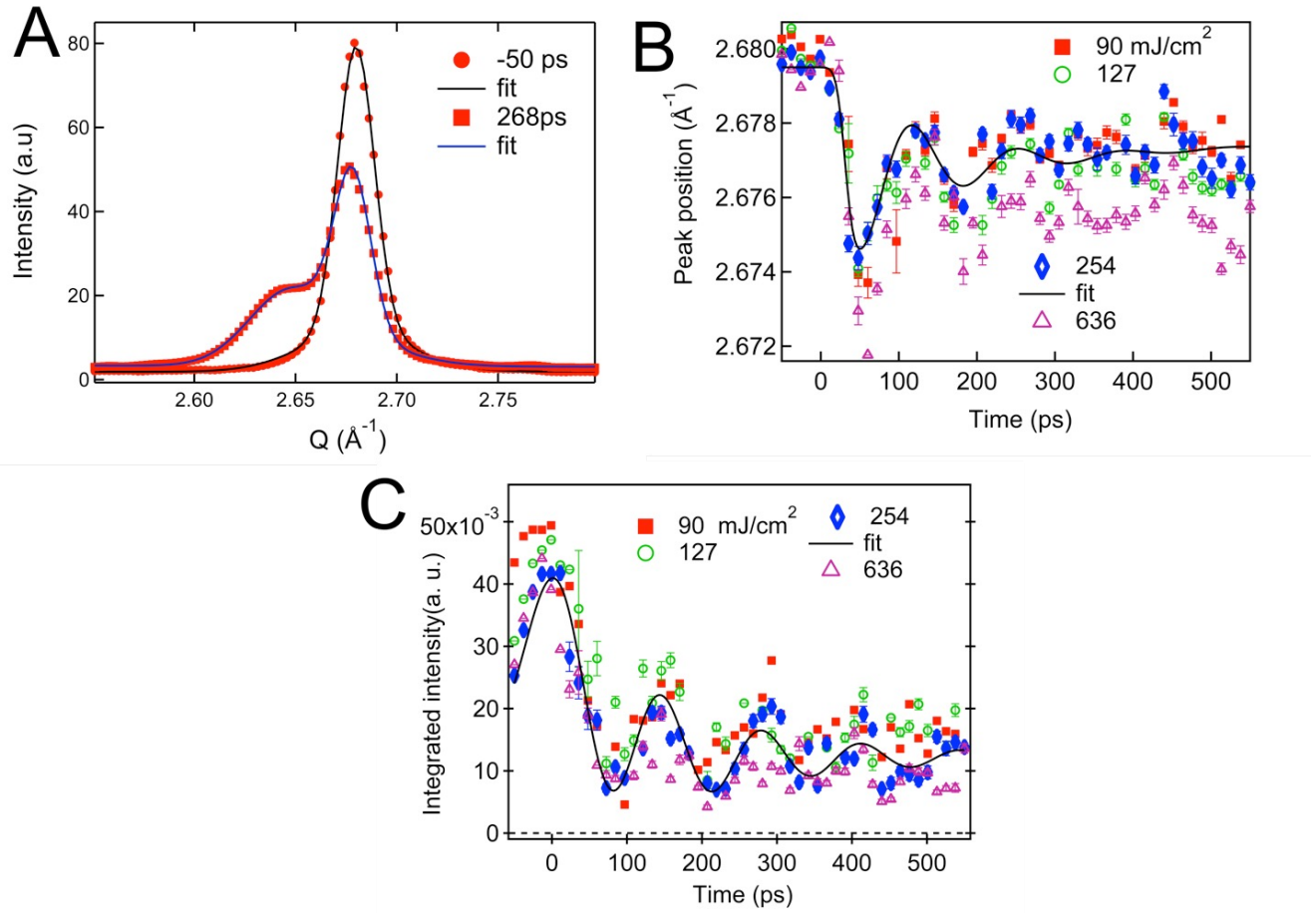


Gaussian ftting procedure



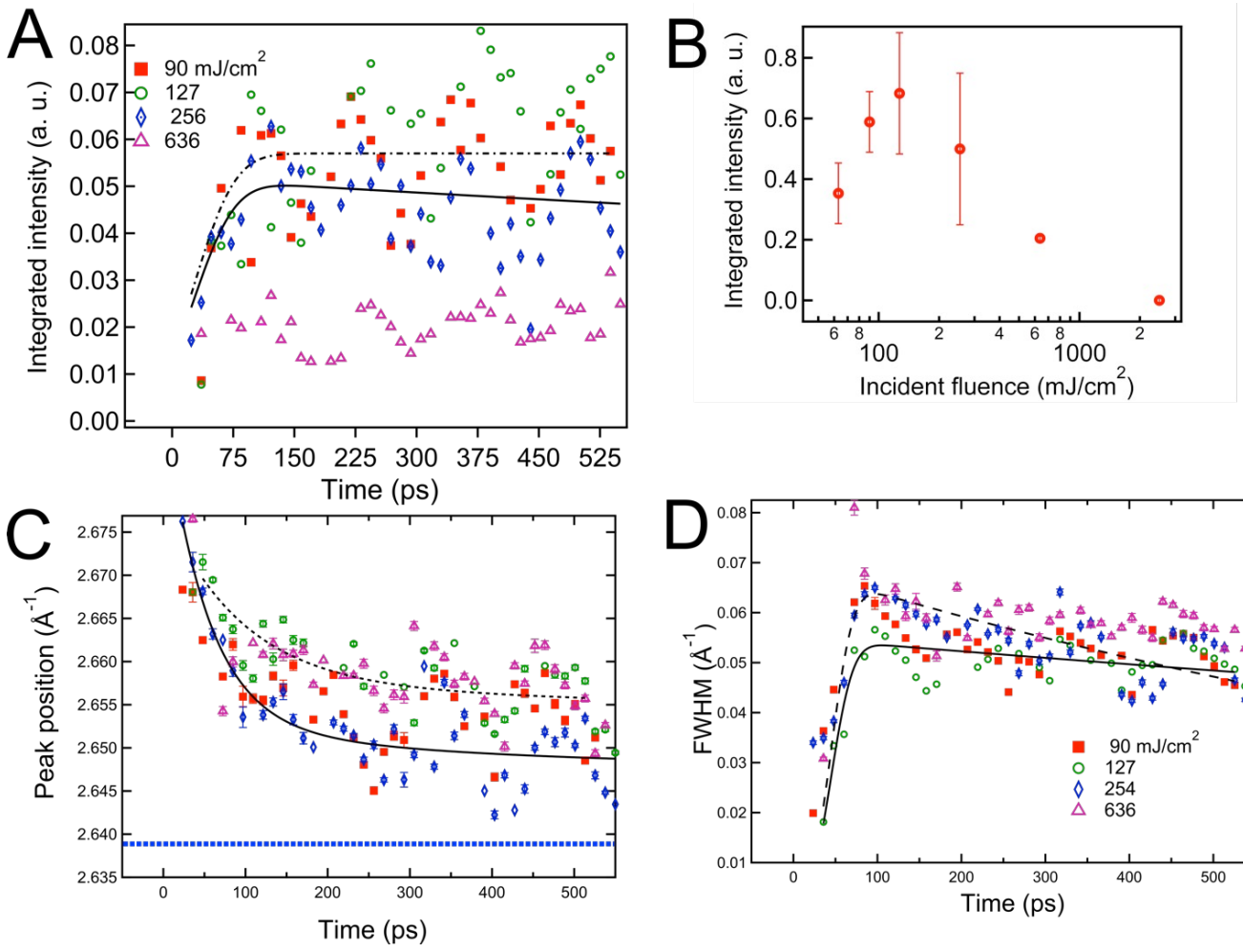
- Crystal Peaks (2x)
  - fixed widths
  - fixed height ratio
  - variable position
- "New" Peak
  - variable width
  - variable height
  - variable position

Response of the Crystal 111 peak



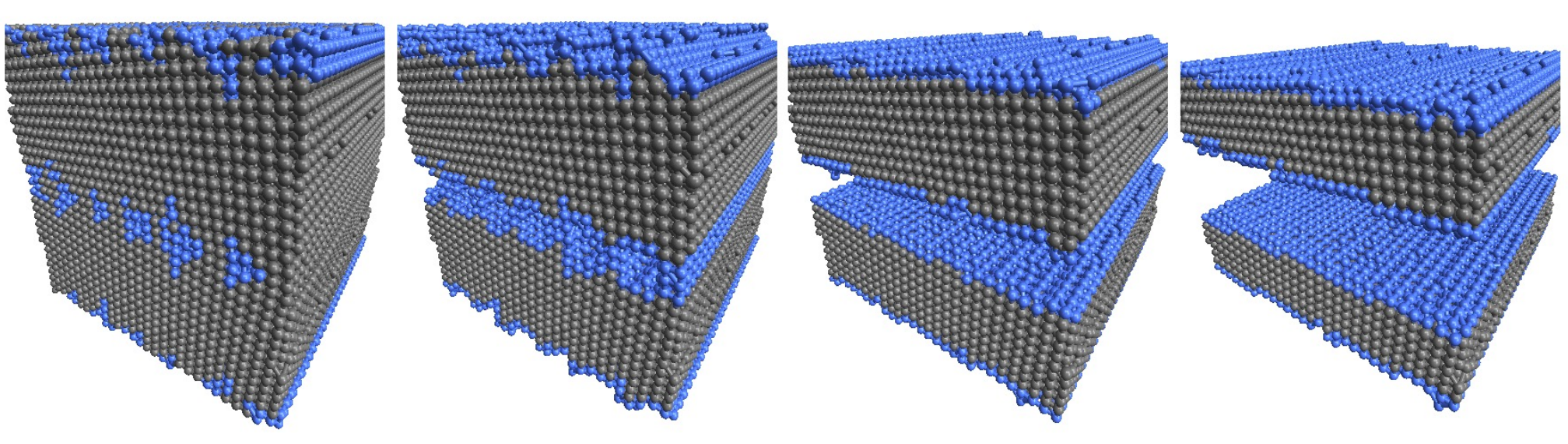
Response of New Peak

Material trapped at the melting point



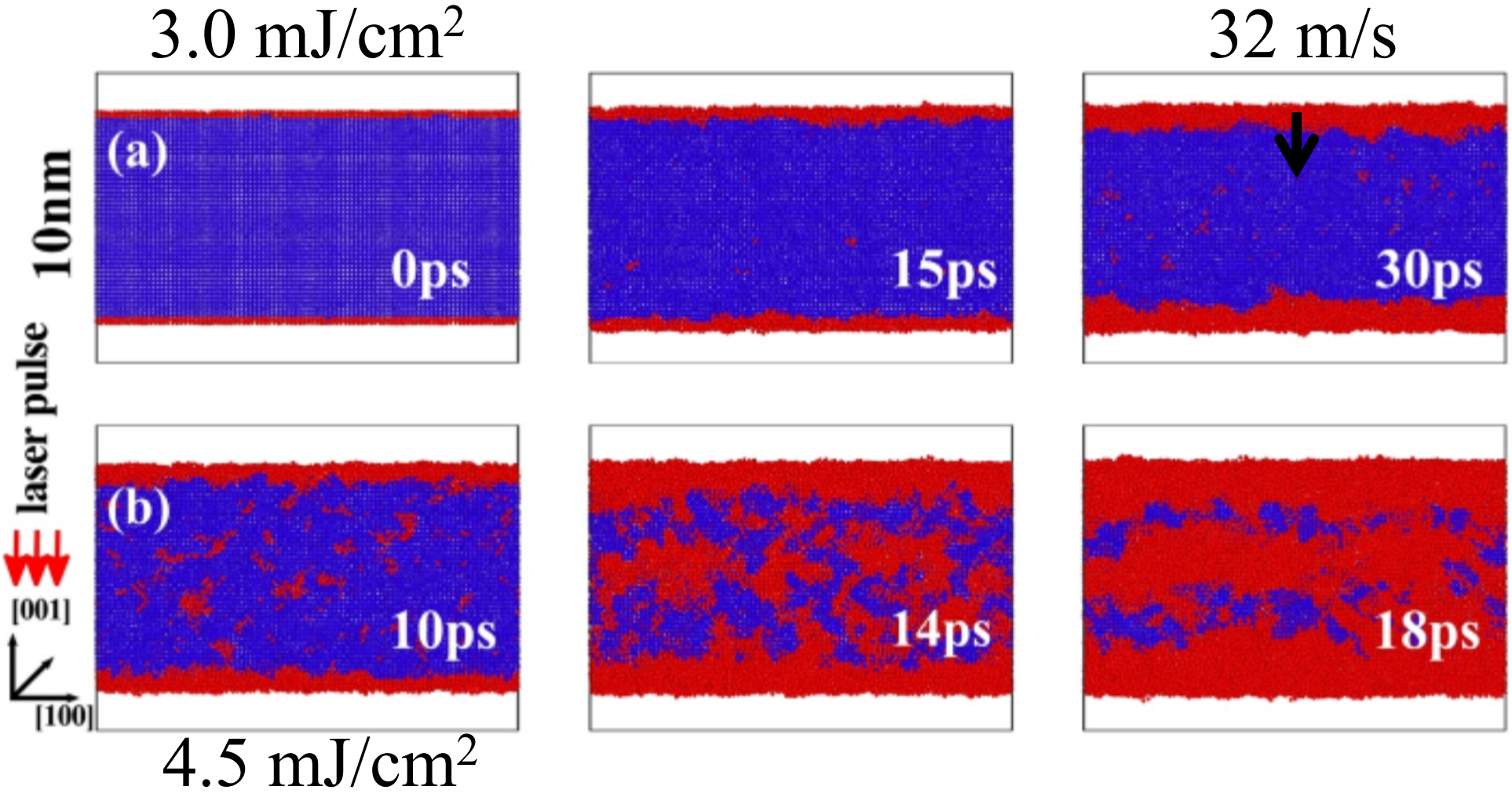
Force-Field Simulation of GB melting

J. Berry, K. Elder and M. Grant, PRB 77 224114 (2008)

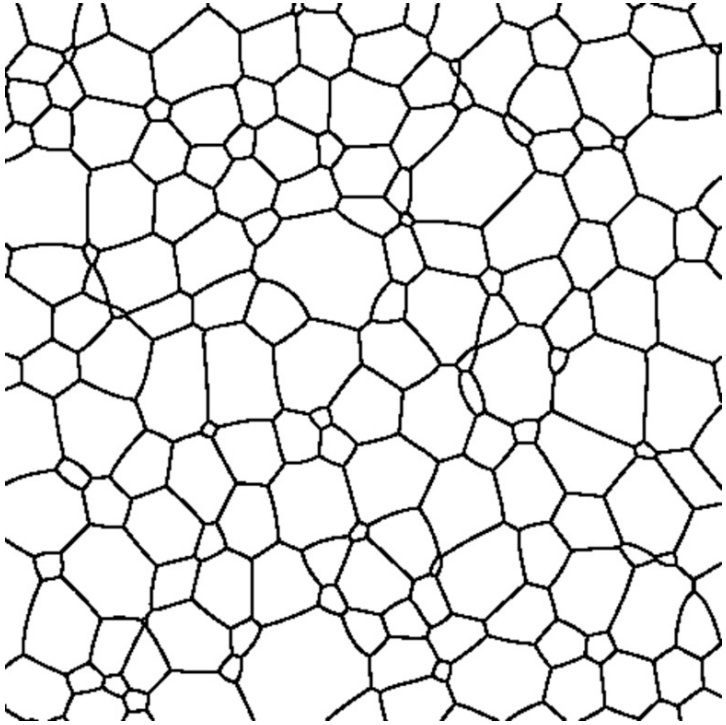


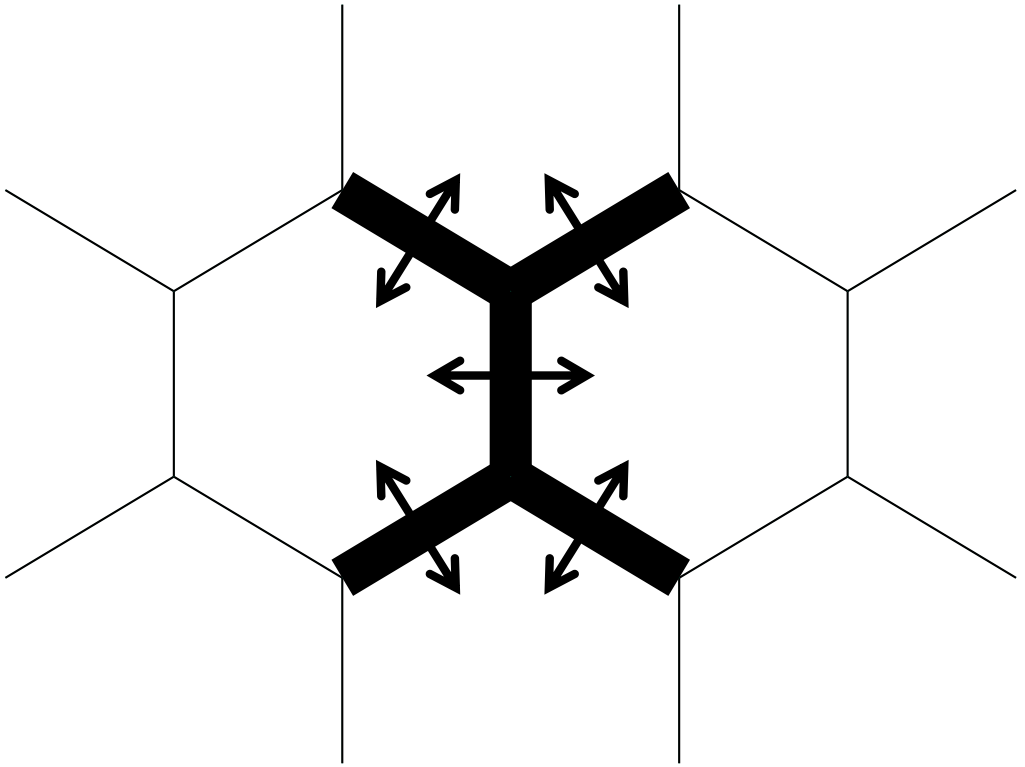
2TM-MD (EAM) simulation Au slab

Giret et al, APL **103** 253107 (2013)

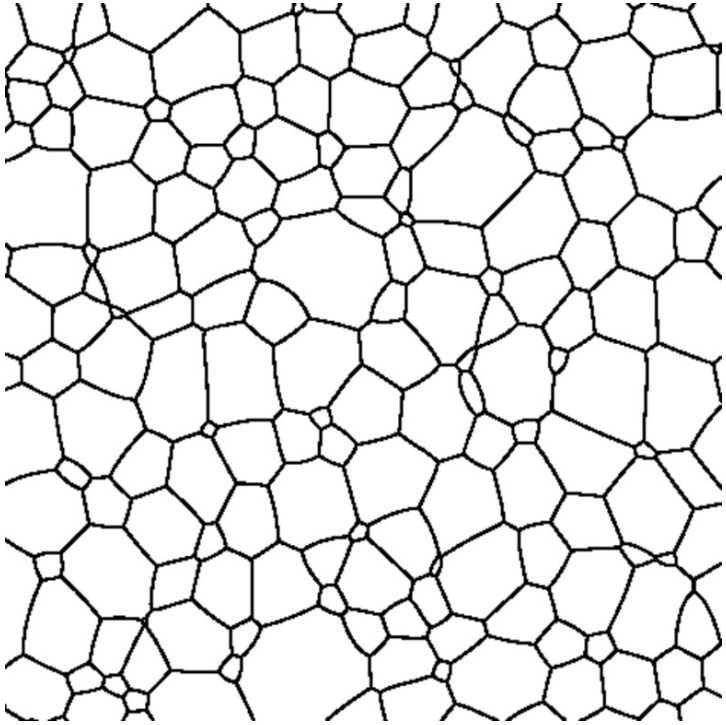


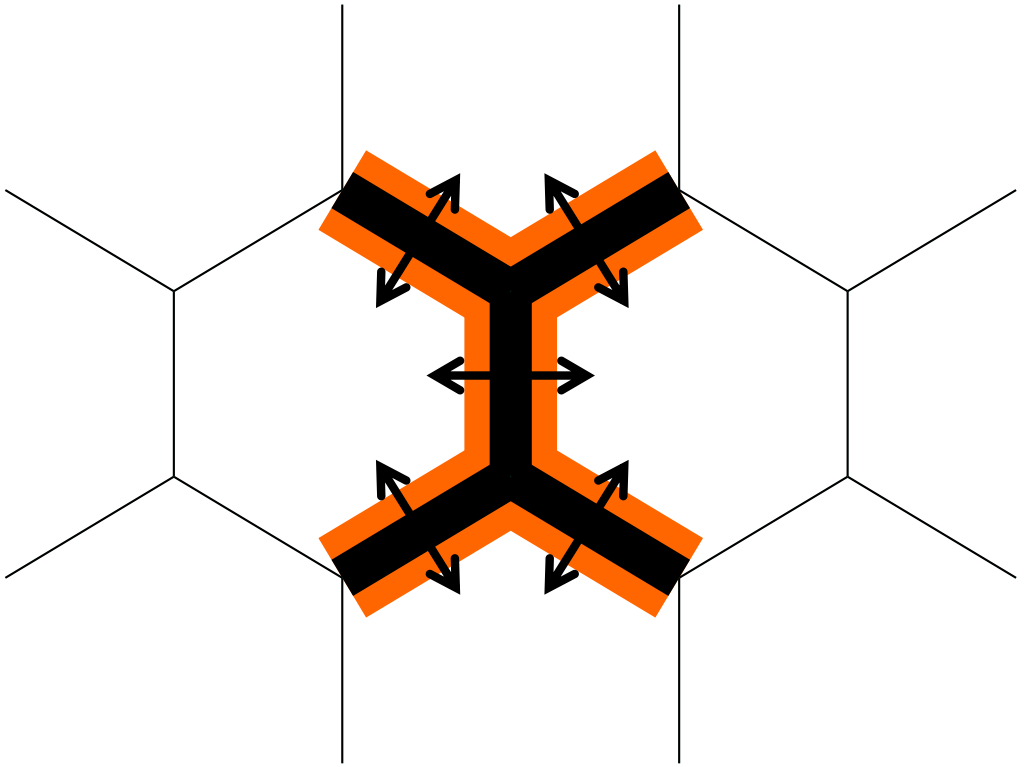
Grain Boundary Melting





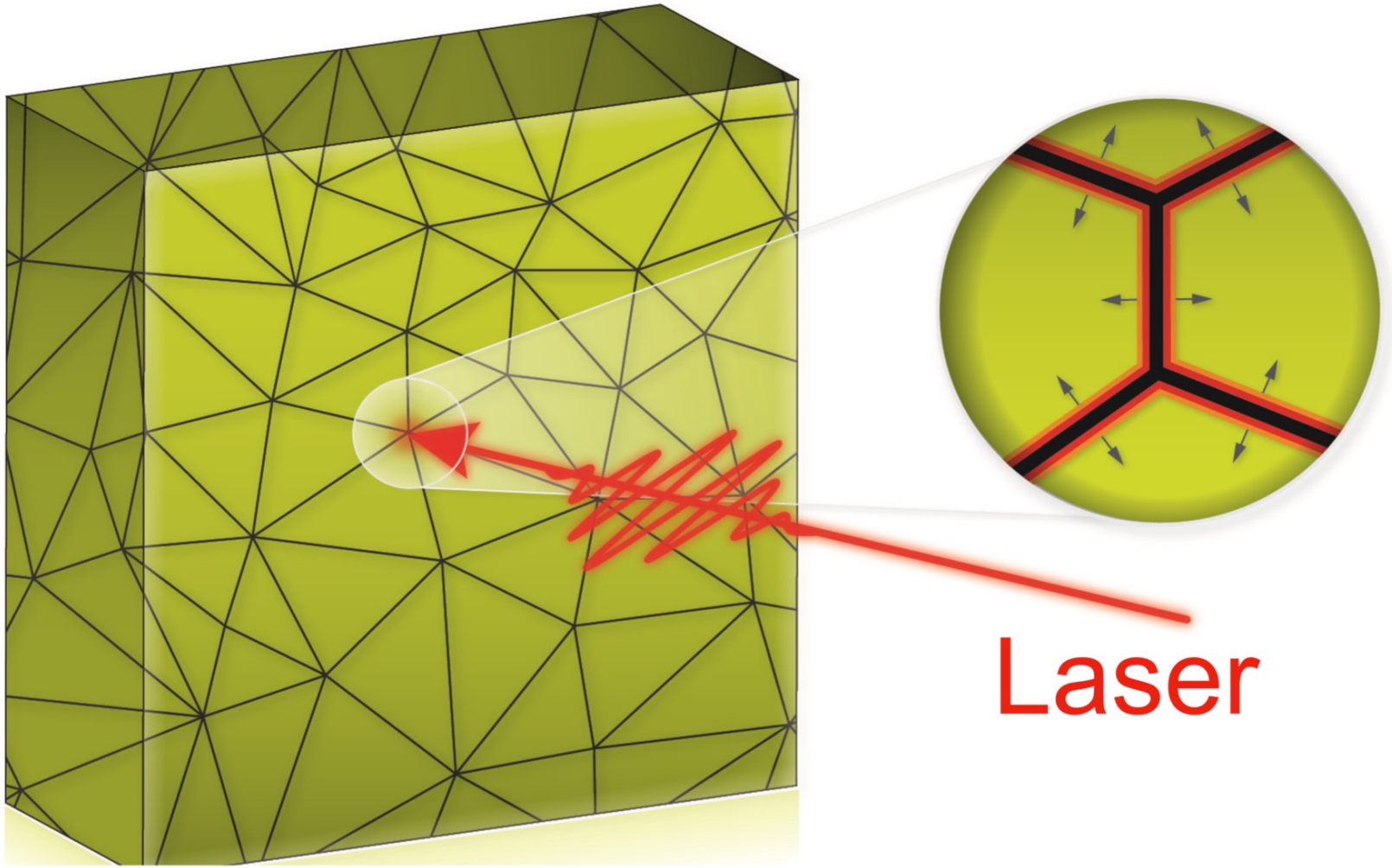
Grain Boundary Melting





Grain Boundary Induced Melting

T. A. Assefa et al Science Advances 6 eaax2445 (2020)



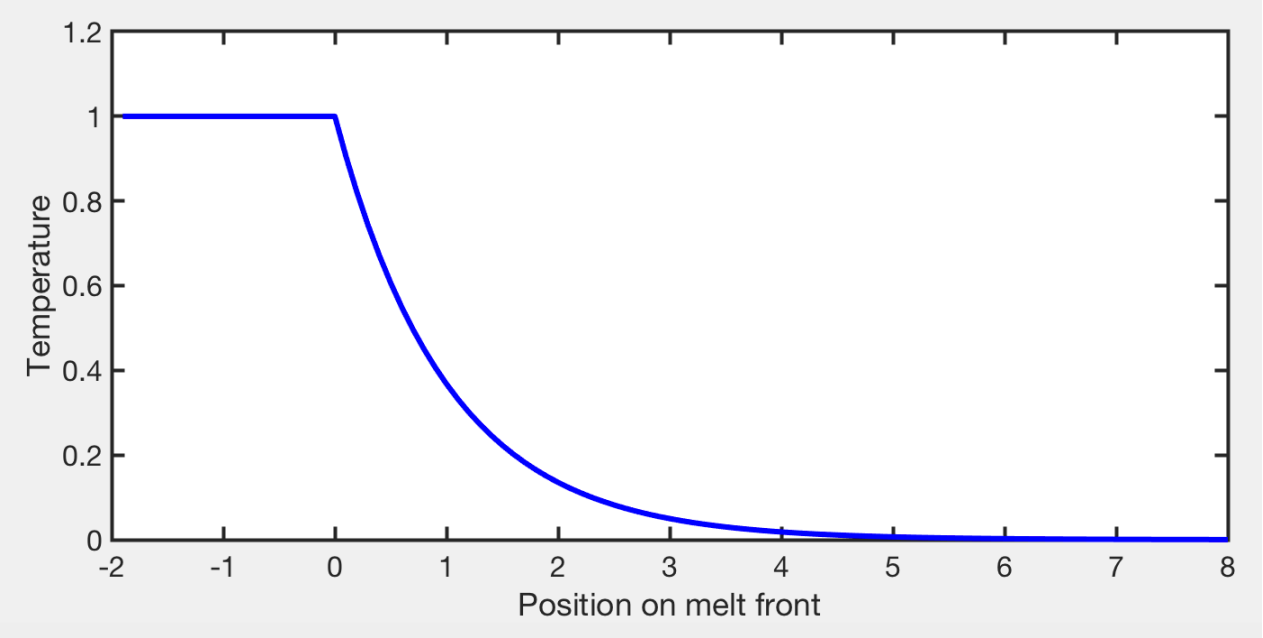
Temperature next to Melt Front

$$T(x) = \int_0^\infty \frac{e^{(x-vt)^2/4\alpha t}}{\sqrt{4\alpha t}} dt$$

Heat equation

$$\alpha = \frac{k}{c_p \rho}$$

Diffusivity



v=1

α=1

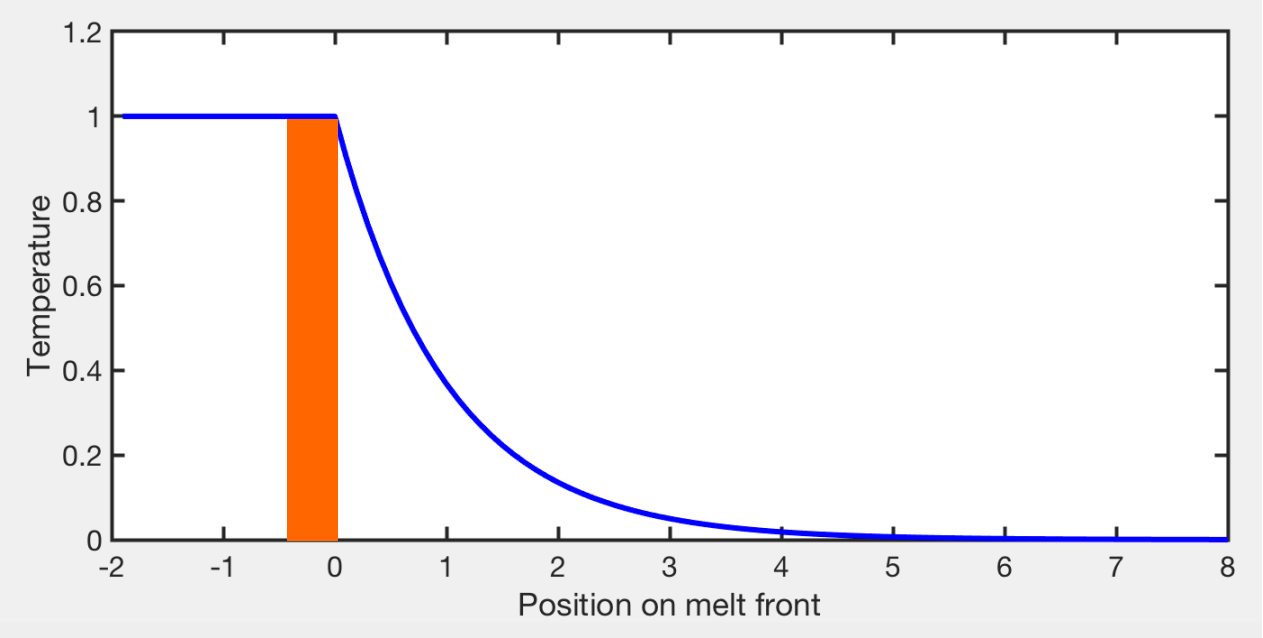
Temperature next to Melt Front

$$T(x) = \int_0^\infty \frac{e^{(x-vt)^2/4\alpha t}}{\sqrt{4\alpha t}} dt$$

Heat equation

$$\alpha = \frac{k}{c_p \rho}$$

Diffusivity

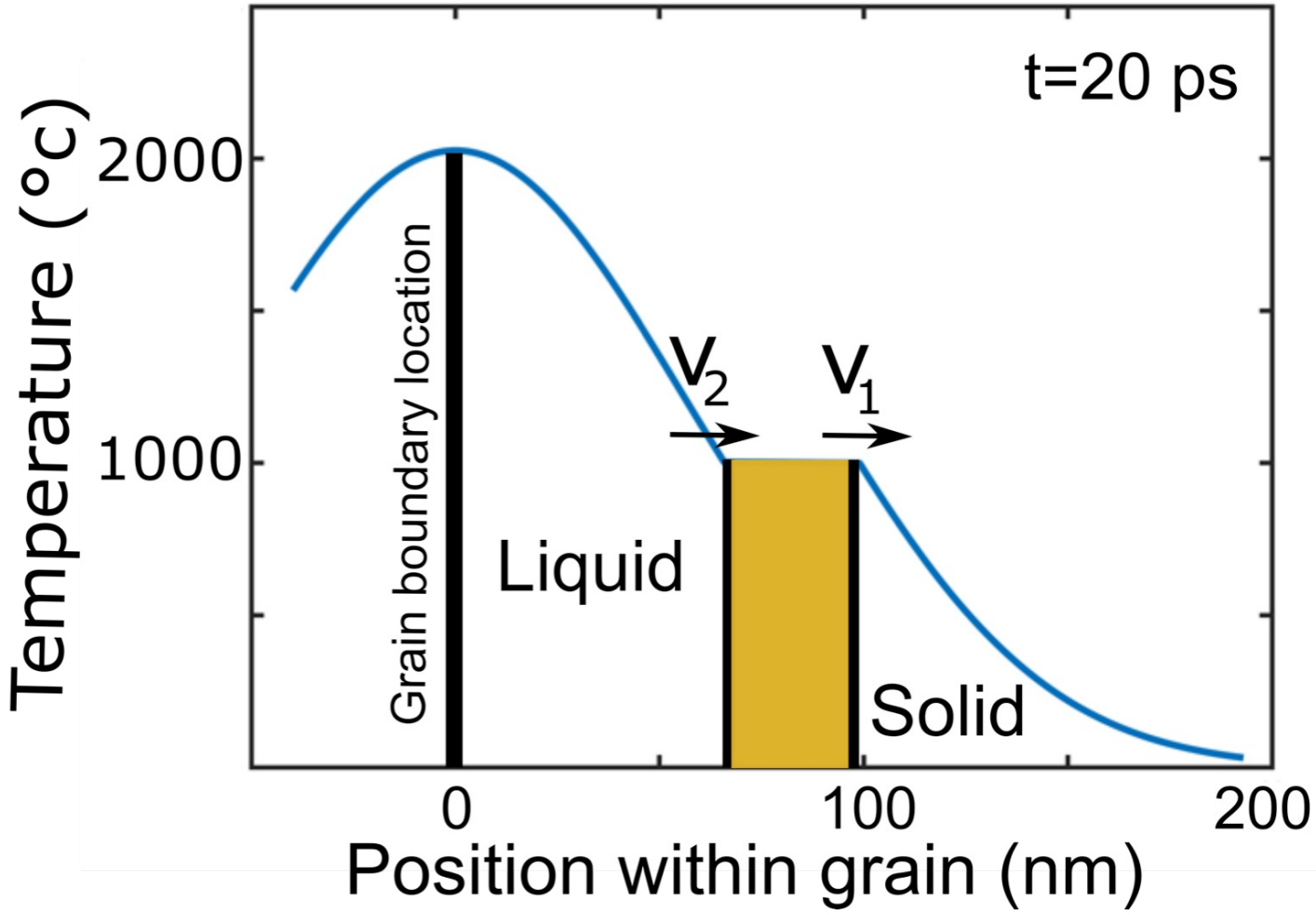


v=1

α=1

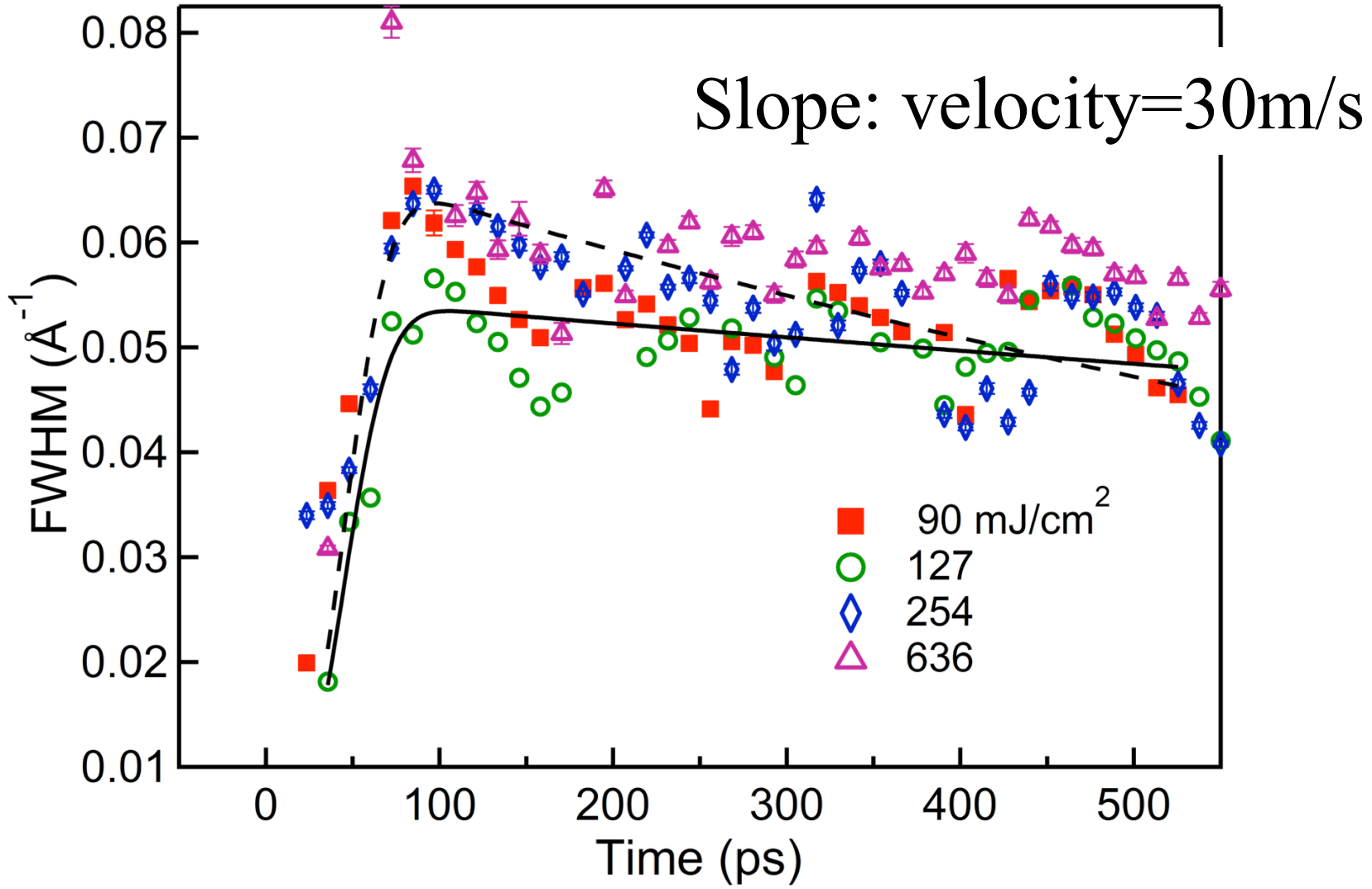
Grain Boundary Induced Melting

T. A. Assefa et al Science Advances 6 eaax2445 (2020)

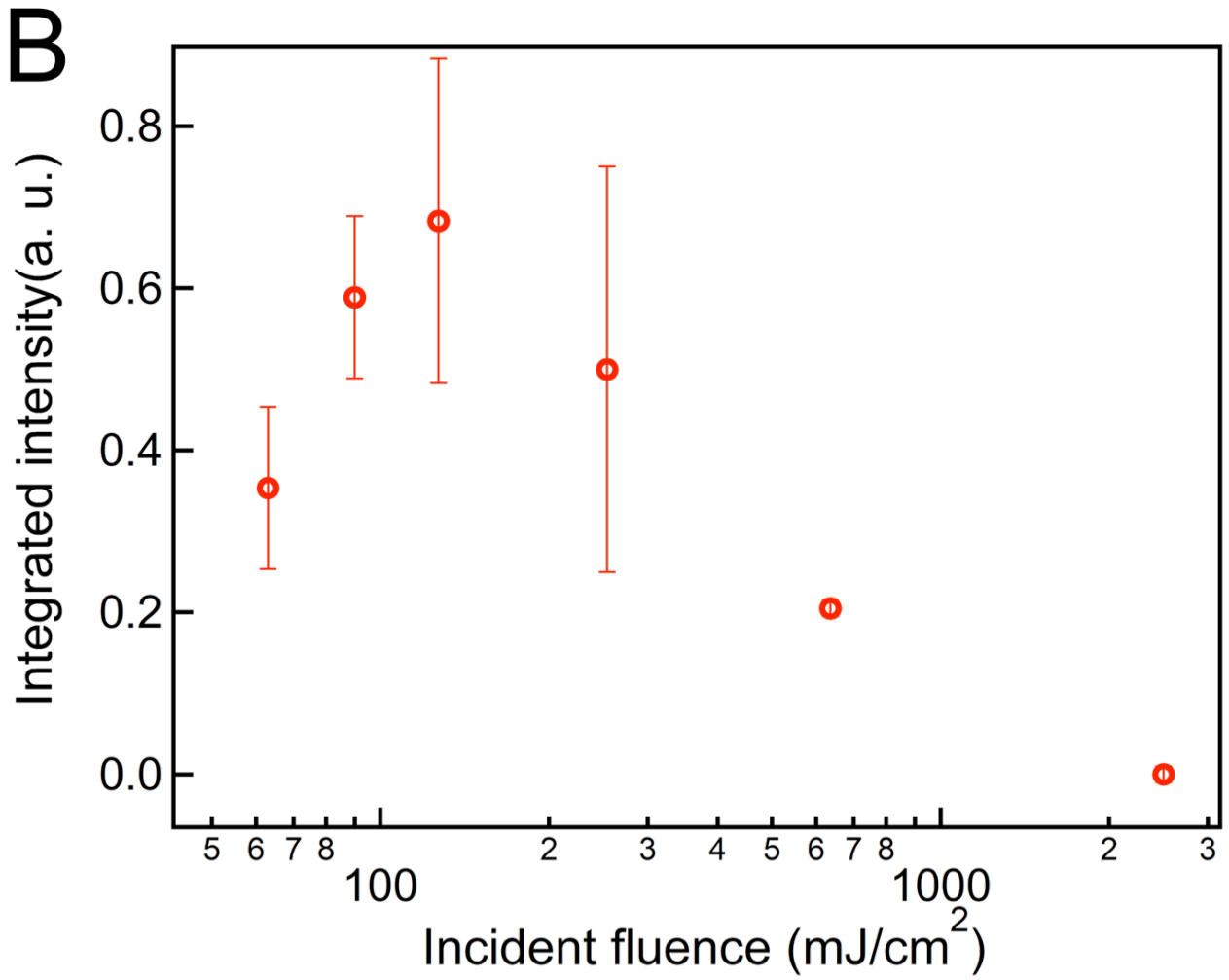


Width of new "Melt-Front" Peak

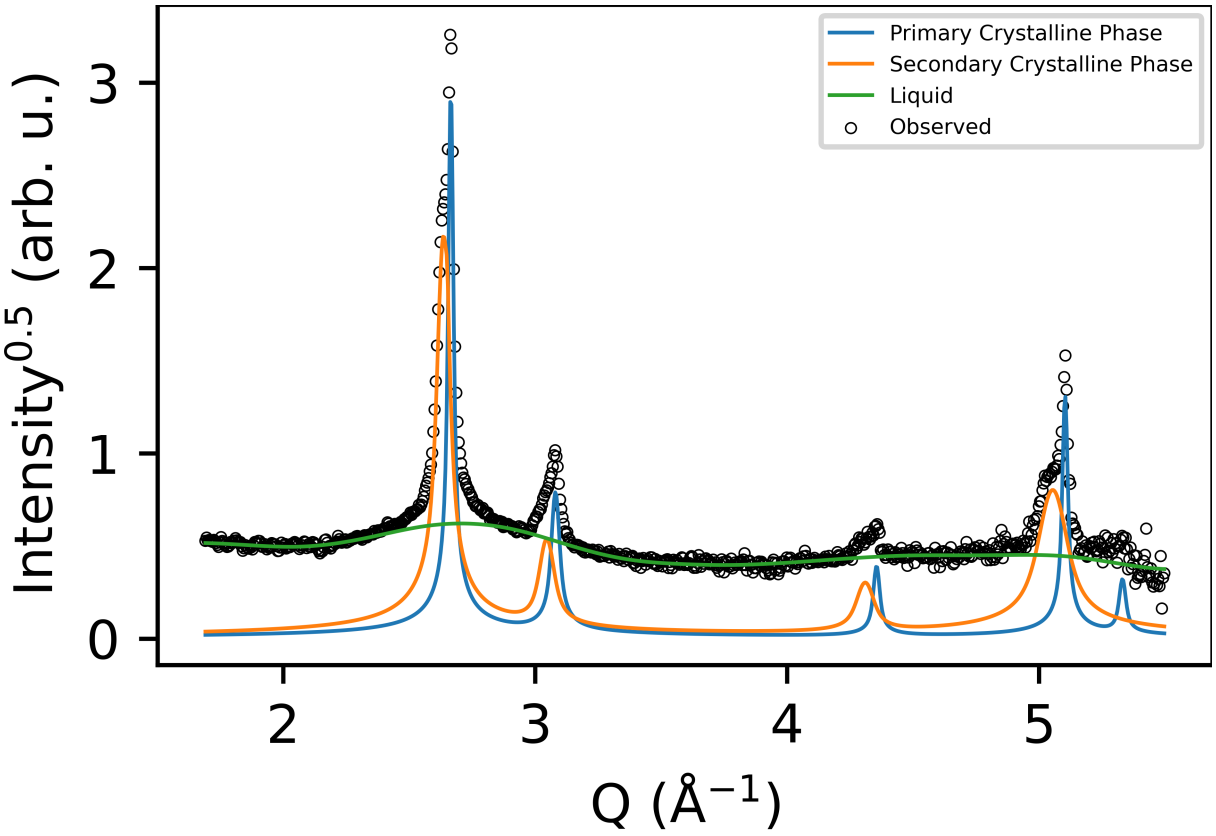
T. A. Assefa et al Science Advances 6 eaax2445 (2020)



Fluence dependence of New Peak



Extracting the diffuse signal

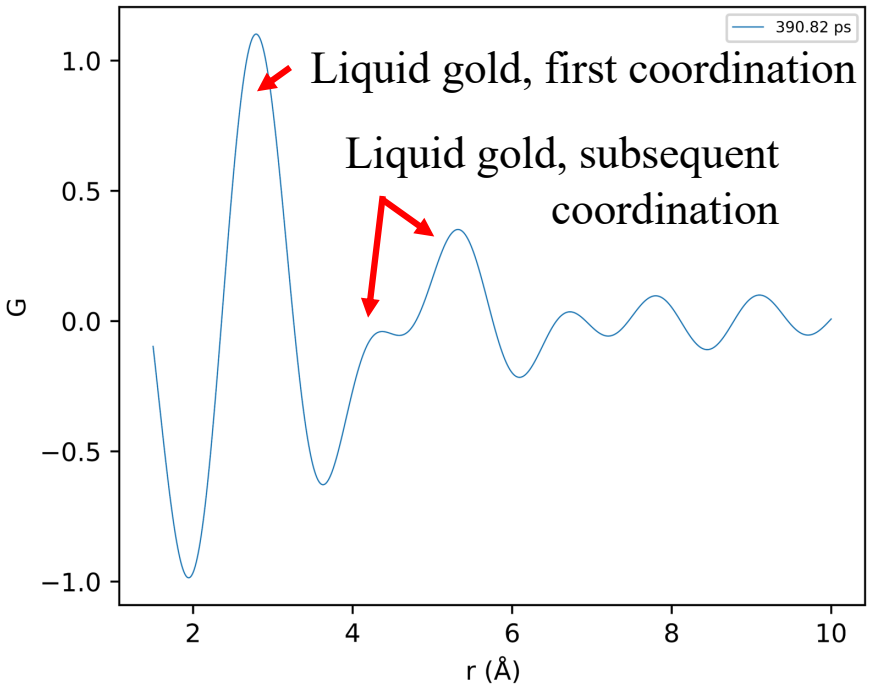


- Raw data plotted, 231 ps, square root intensity scale
- Unconstrained peak fitting approach
- Remove Bragg components

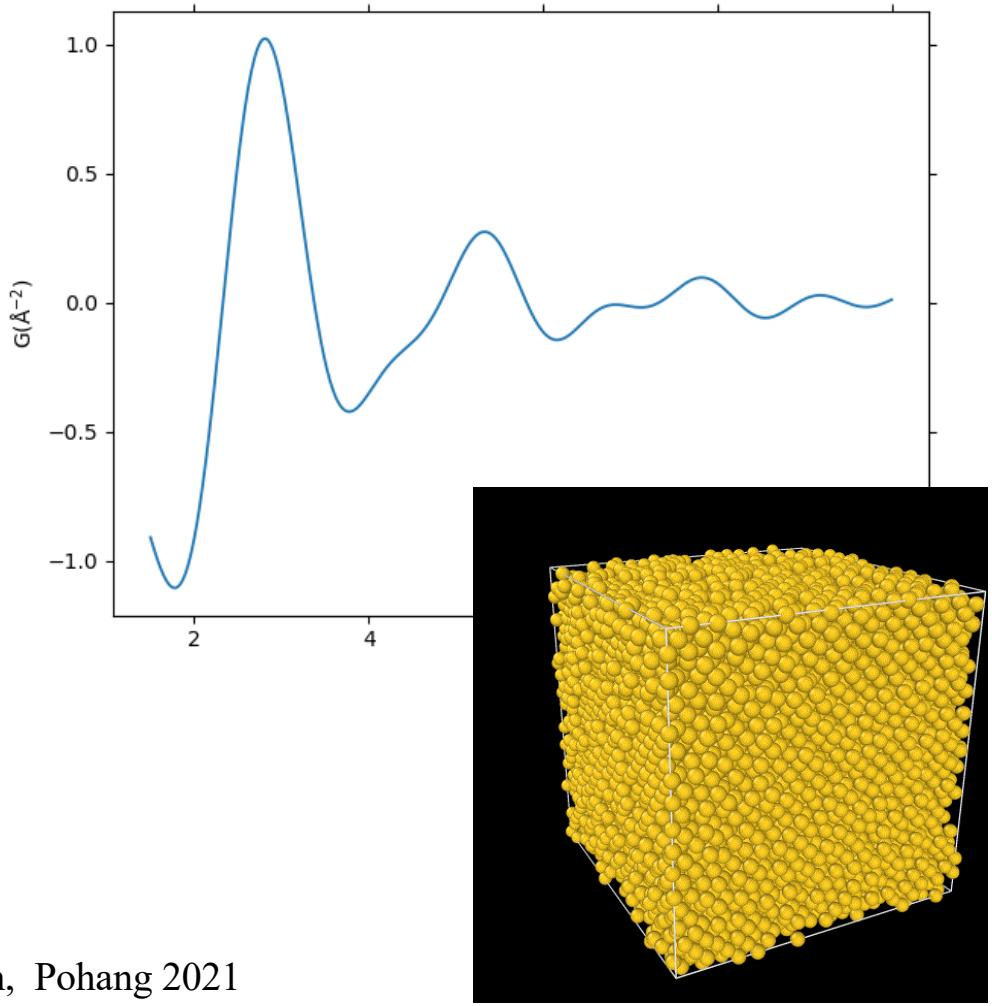
Is this liquid gold PDF ?

R. Koch unpublished

Observed

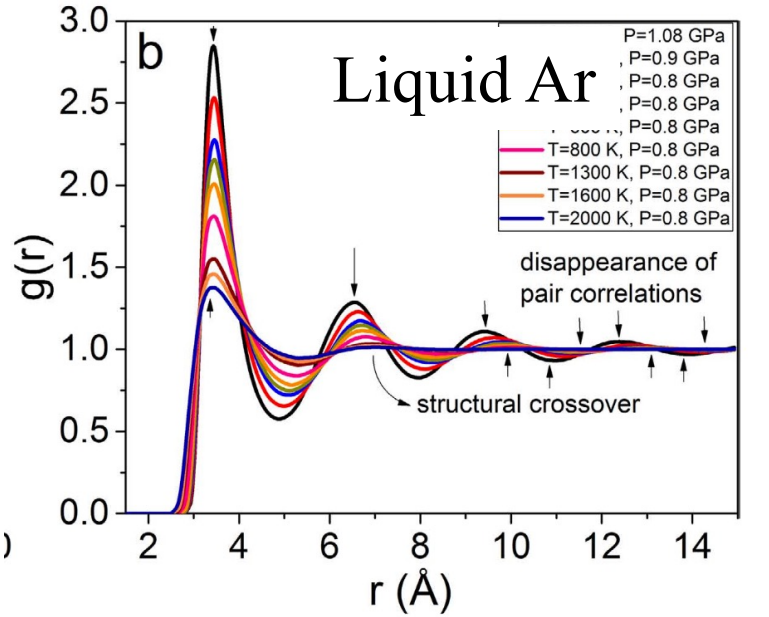


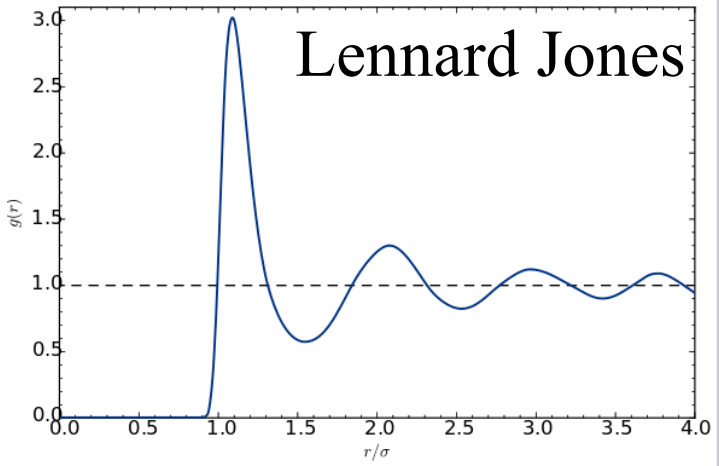
Simulated



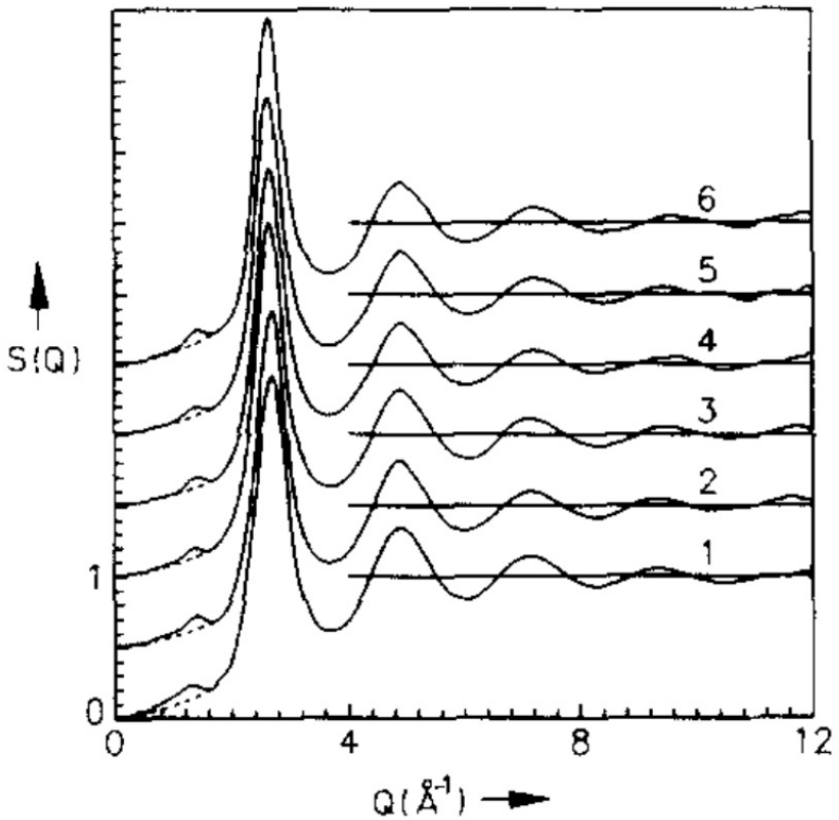
I. K. Robinson, Pohang 2021

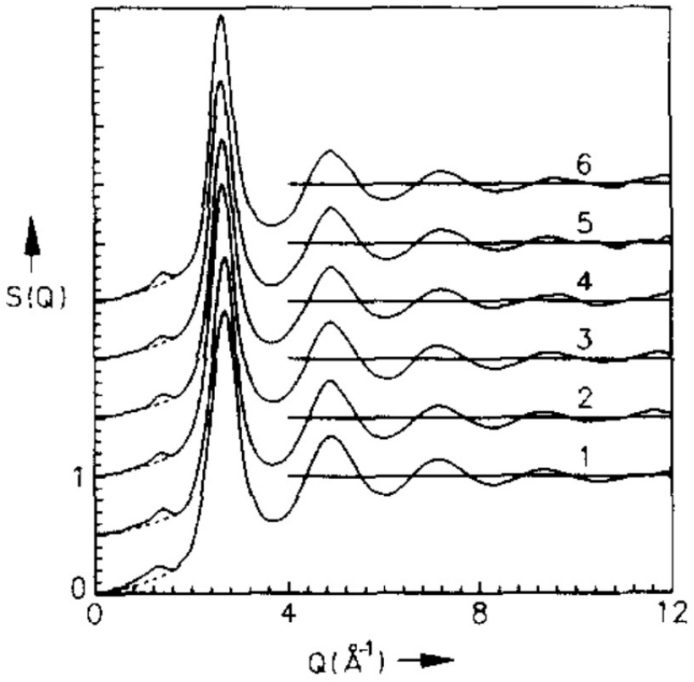
Other Liquid RDFs



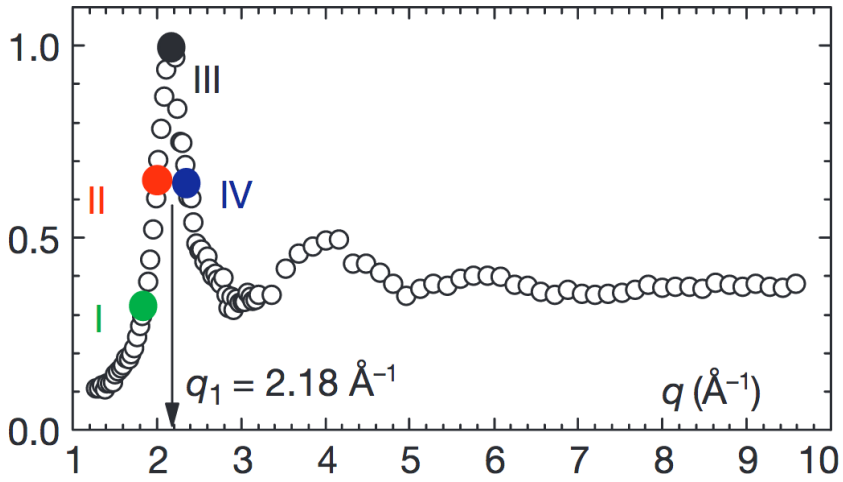


Au-Ge alloy

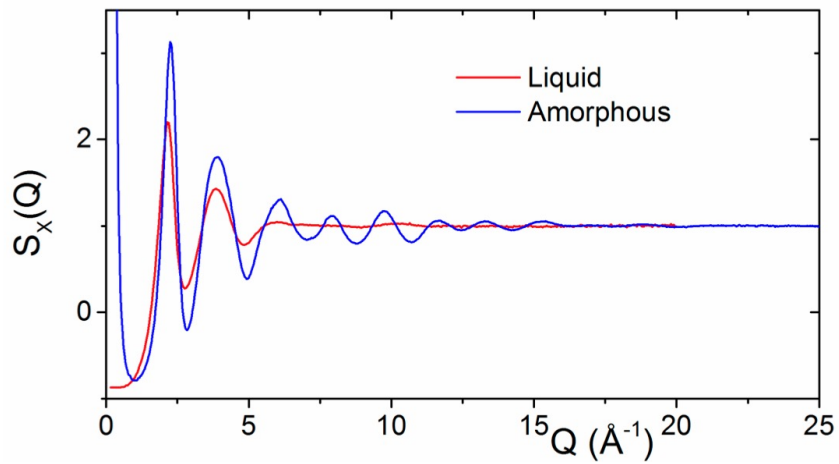




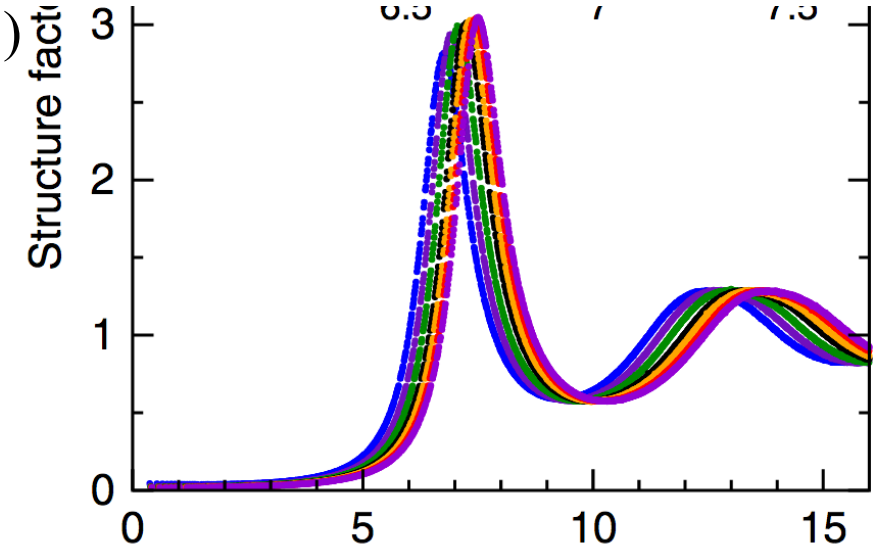
Liquid AuGe, Hoyer & Jodicke JNCS (1995)



Liquid Pb, Reichert et al (2000)



Liquid HfO_2, Gallington et al (2017)



LJ liquid, Pedersen et al (2016)

Melt-front description of melting in polycrystalline materials

- Laser induced disorder
- Three phases: liquid, solid, melt
- 2-phase inhomogeneous melting
- Energy transfer at Grain Boundaries
- Interface melting like nanoparticles
- Measured structure of Melt Front

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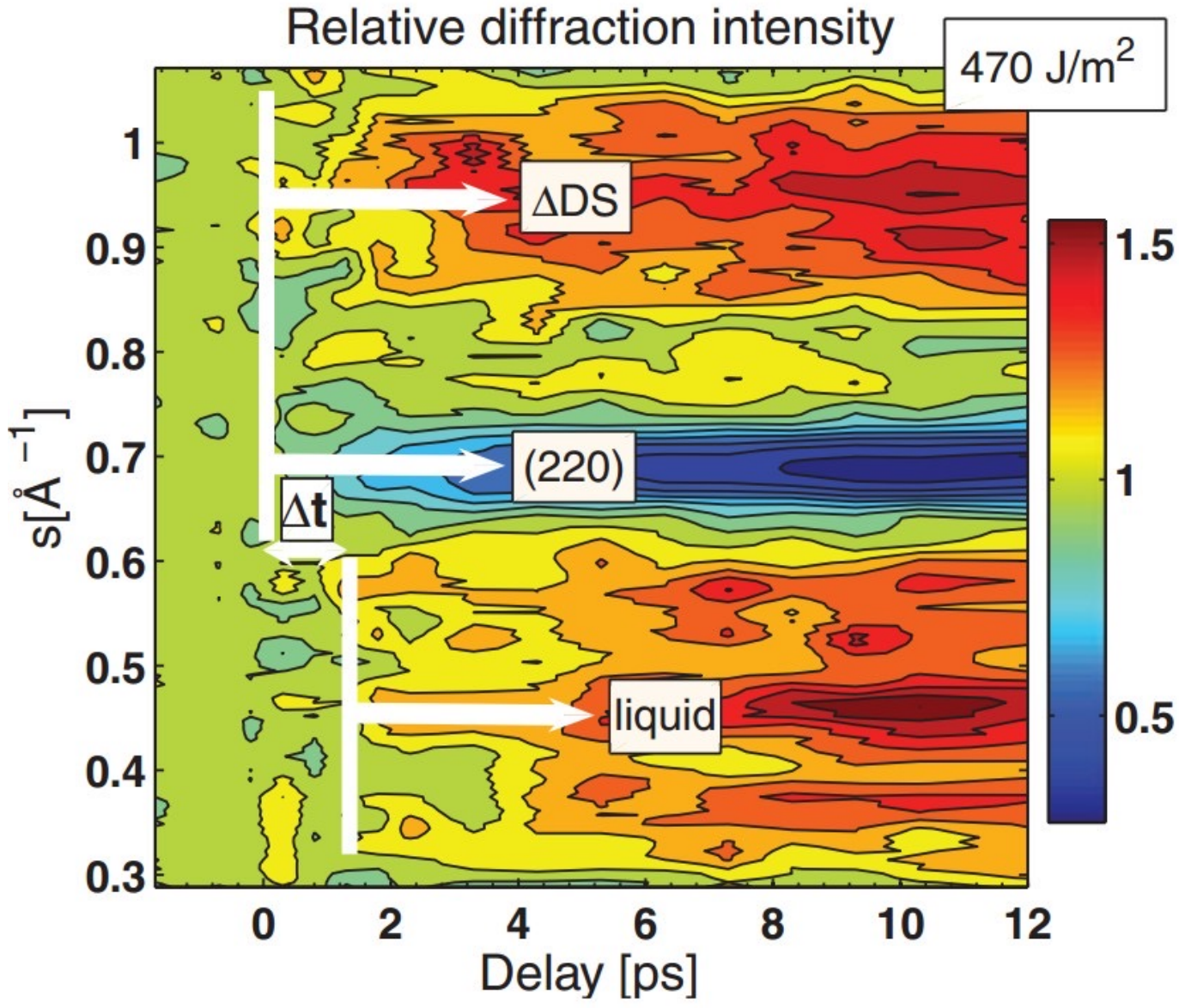
Mattieu Chollet
Marc Messerschmidt

Transient Melting of Au (by UED)

R. Ernstorfer, D. Miller et al, Science **323** 1033

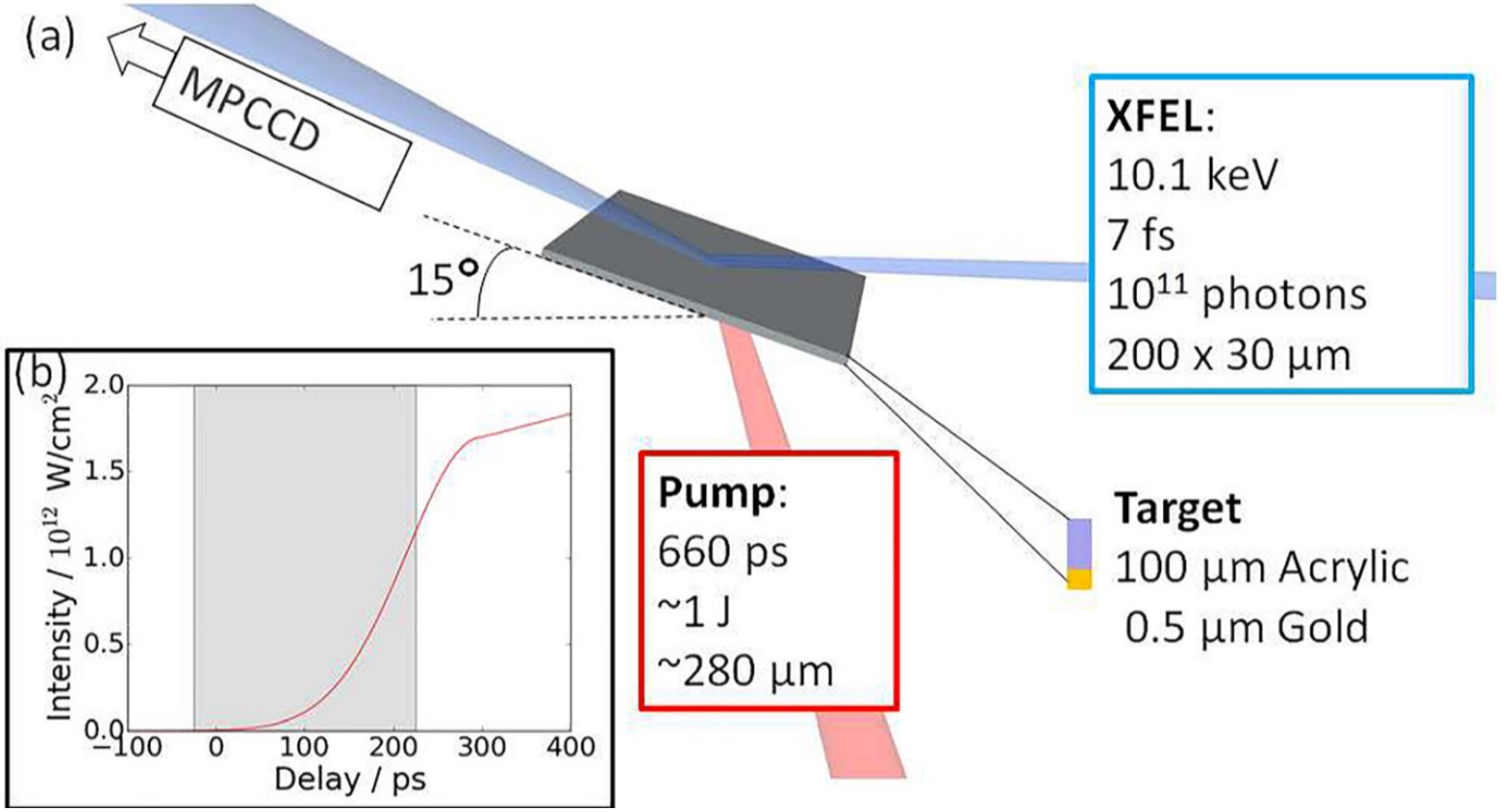


47 mJ/cm^2 absorbed

500nm Thin Film of Au at SACLA

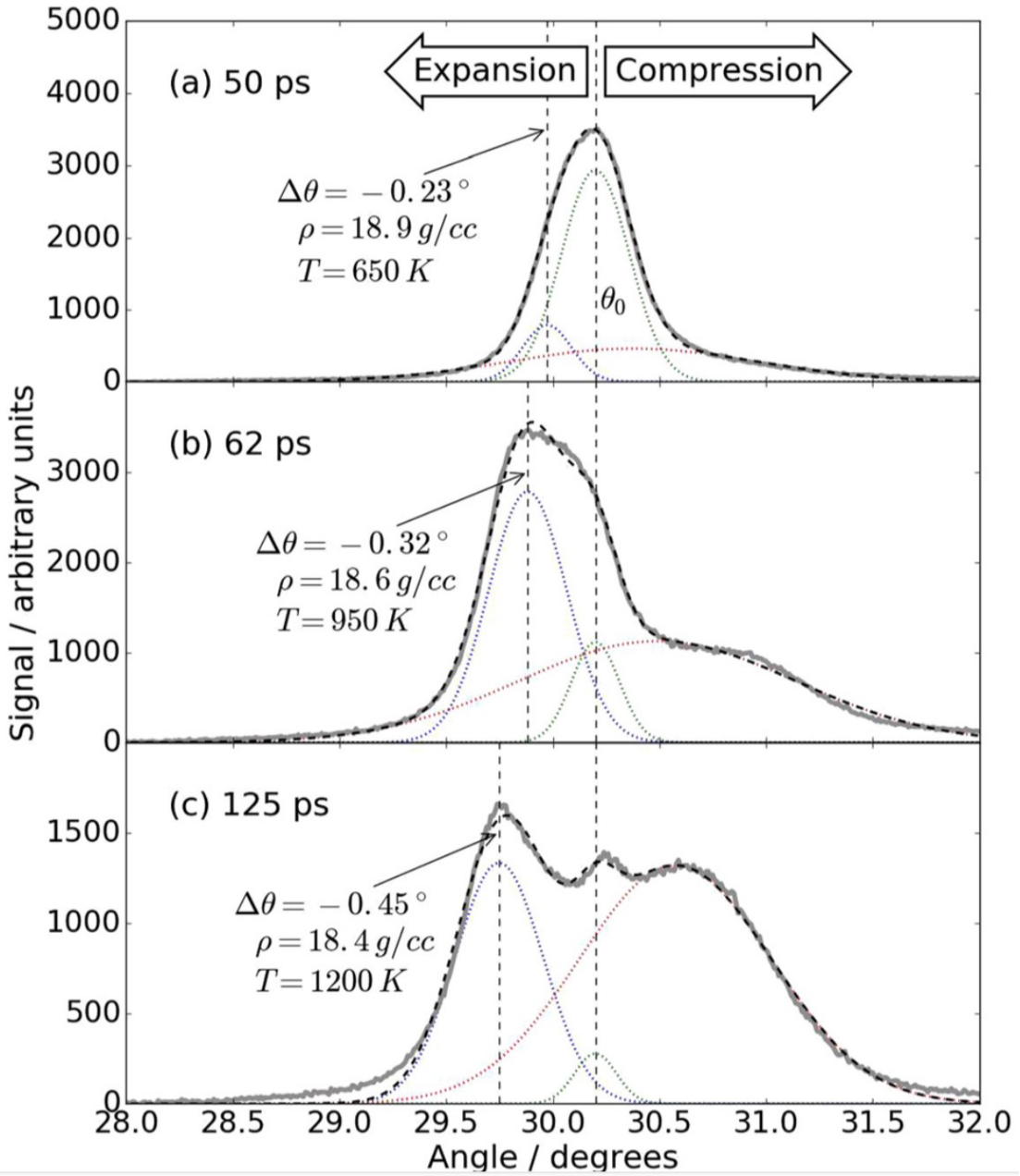
N. J. Hartley et al, APL **110** 071905 (2017)

5100 J/cm^2 660ps



500nm Thin Film of Au at SACLA

N. J. Hartley et al, APL **110** 071905 (2017)



5100 J/cm^2