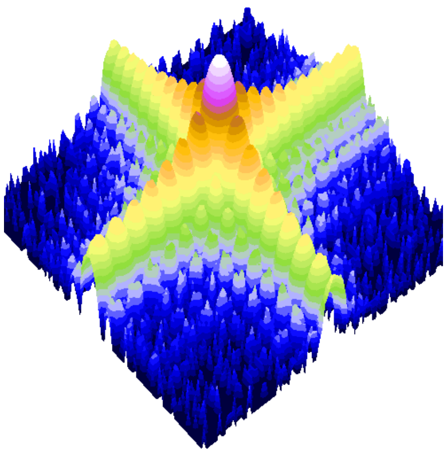
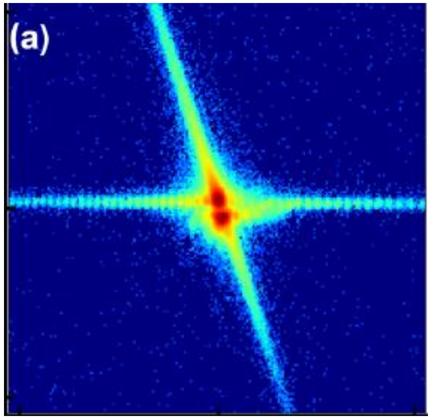
Charge And Spin Density Waves In The Light Of Coherent X-Rays





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ECRYS 2014

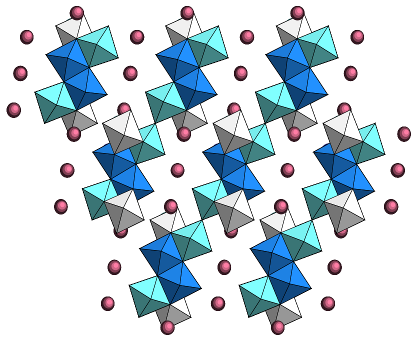
Motivation

Coherent x-ray diffraction :

Study **specific** periodic modulations (q selectivity) through the **phase defects** they contain

X-ray diffraction: the modulation can be of any kind: atomic lattice, CDW, etc…

$K_{0.3}MoO_3$



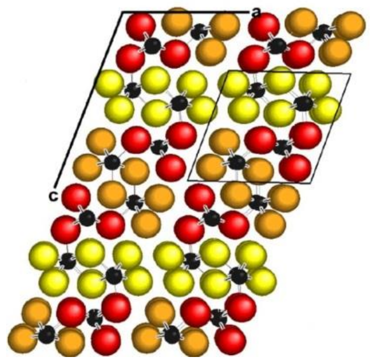
Static & sliding CDW

→ CDW dislocation

→ *Soliton lattice* in sliding state

Le Bolloc'h et al., PRL ***95****, 116401 (2005)*
Le Bolloc'h et al., PRL ***100****, 096403 (2008)*
V. Jacques et al., PRB ***85****, 035113 (2012)*

$NbSe_3$



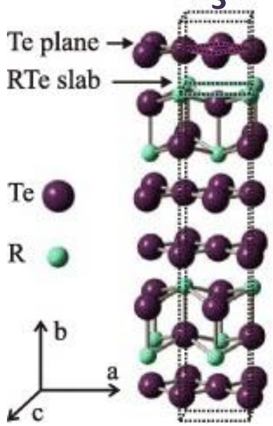
Sliding CDW

→ Stages of sliding

→ *Defects* prior to sliding

Pinsolle et al. PRL ***109****, 256402 (2013)*

$TbTe_3$



Sliding CDW

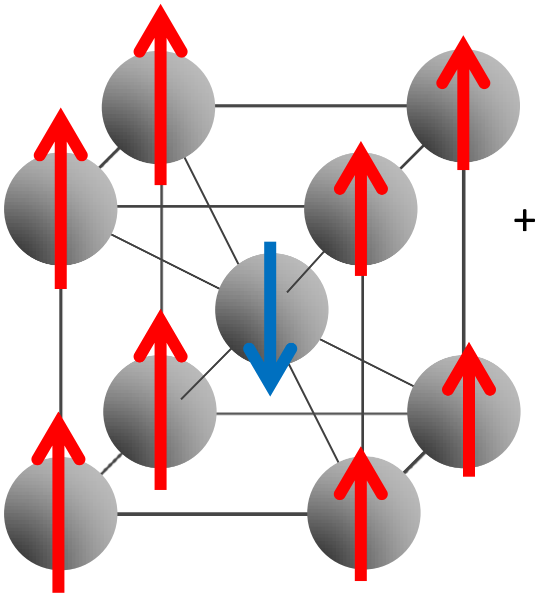
→ Stages of sliding

→ *CDW defects* all the time

(cf David's talk)

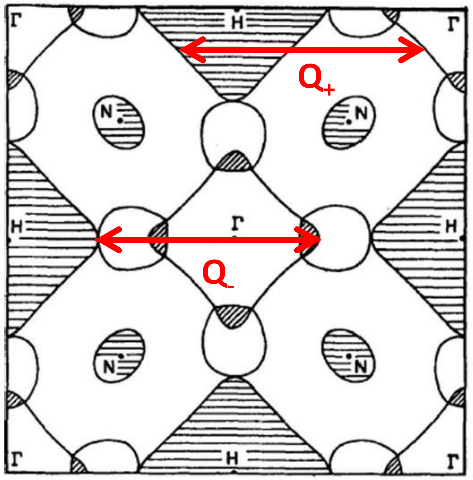
What about a magnetic modulation like a SDW with respect to defects?

Chromium : a SDW/CDW 3D compound



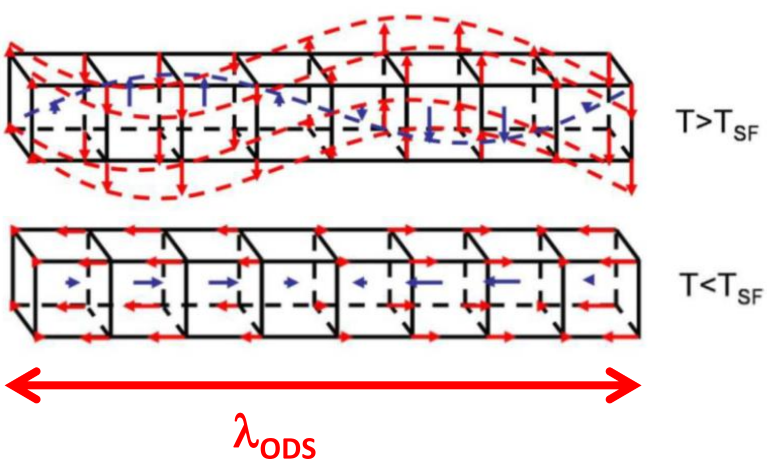
For $T<T_N$:
AF
+ incommensurate SDW along <001>:
➔ Periodic modulation of |**m**|

*Corliss et al, PRL **3**, 211 (1959)*
*Overhauser, PRL **4**, 226 (1960)*

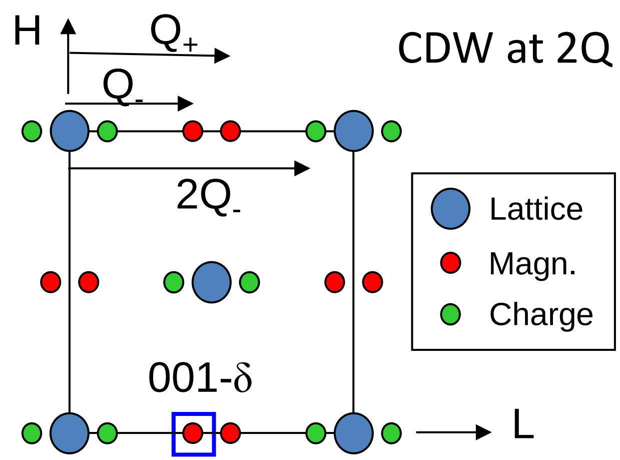


Cr Fermi surface

Two transitions :
T_N = 311K
T_{SF} = 123K



In diffraction, for single-Q samples:



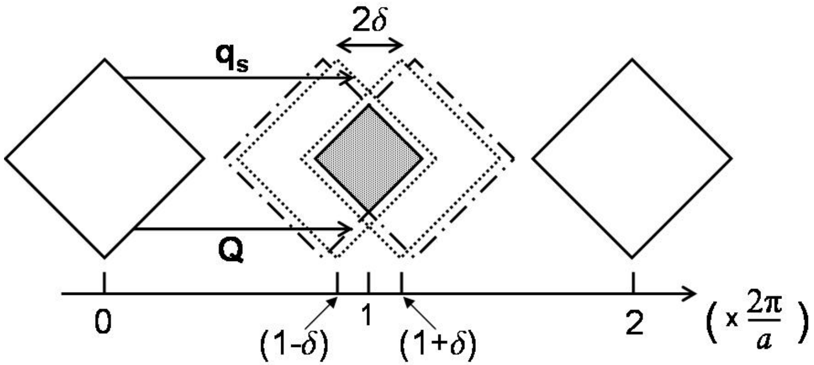
*Tsunoda et al., Solid State Comm. **14**, 287 (1974)*

How does the CDW appear?

SDW: modulation with wavevector Q + harmonics nQ.
- n even: charge component
- n odd: spin component

3 bands model

The CDW @ 2nQ are SDW harmonics that lead to a periodic lattice distorsion



Young and Sokoloff, J. Phys. F: Metal Phys., **4**, 1304 (1974)

Magnetostriction

The SDW creates a strain wave with wave vector 2Q due to magnetoelastic coupling to the lattice

Cowan, J. Phys. F: Metal Phys., **8**, 423 (1978)

Aim: use novel techniques to get a new vision of CDW/SDW coupling in Cr: ***coherent x-ray diffraction*** and ***time-resolved x-ray diffraction***

Aim of the experiment

Can we learn something looking at both SDW and CDW through their defects using coherent x-ray diffraction?

FOR THIS EXPERIMENT WE MUST:

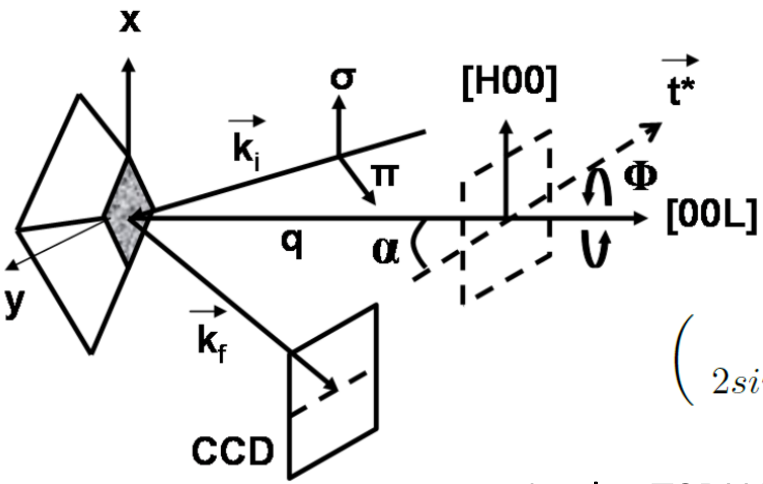
1. Use conditions for which x-rays are sensitive to magnetic modulation:
   ➔ **magnetic diffraction**

2. Be sensitive to defects: x-rays must have a well-defined phase:
   ➔ **coherent x-rays**

3. Probe the same volumes for SDW and CDW:
   ➔ **simultaneous diffraction conditions**

Magnetic diffraction

Using a ***polarized x-ray beam***, it is possible to probe a magnetic order with x-rays



Magnetic scattering matrix:

$$M(\theta) = \begin{pmatrix} M_{\sigma\sigma'} & M_{\pi\sigma'} \\ M_{\sigma\pi'} & M_{\pi\pi'} \end{pmatrix} =$$

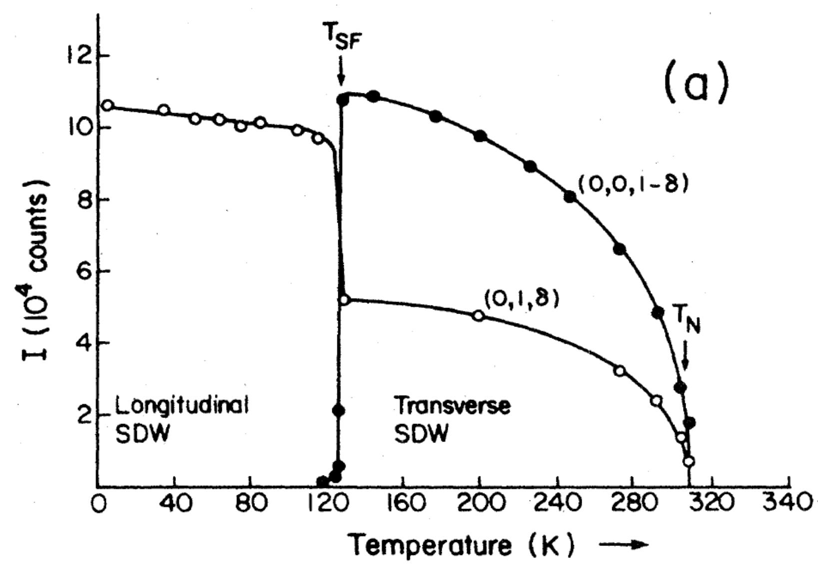
$$\begin{pmatrix} (sin2\theta)S_y & -2sin^2\theta[cos\theta(L_x+S_x)-sin\theta S_z] \\ 2sin^2\theta[cos\theta(L_x+S_x)+sin\theta S_z] & sin2\theta[2sin^2\theta L_y+S_y] \end{pmatrix}$$

In the TSDW phase: $A(\theta) = -i\frac{\hbar\omega}{mc^2}r_0\left(S_y\sin 2\theta - 2S_x\sin^2\theta\cos\theta\right)$

Magnetic cross section is very low

➔ Need to work in the conditions that maximize magnetic signal:

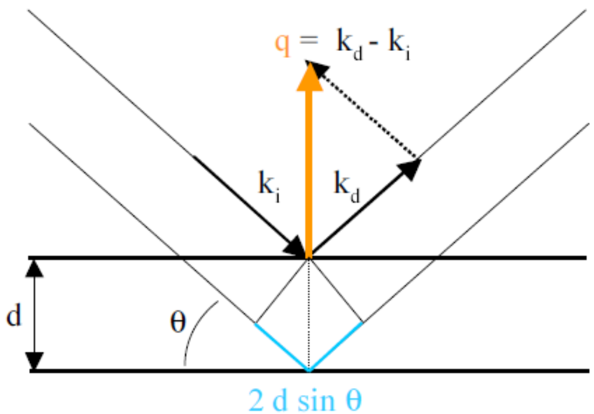
- Favorable ***temperature***
- ***Bright source***: synchrotron
- ***Polarized beam***: natural in synchrotrons
- ***Tune x-ray energy***: ok in synchrotrons



Why coherent x-ray diffraction?

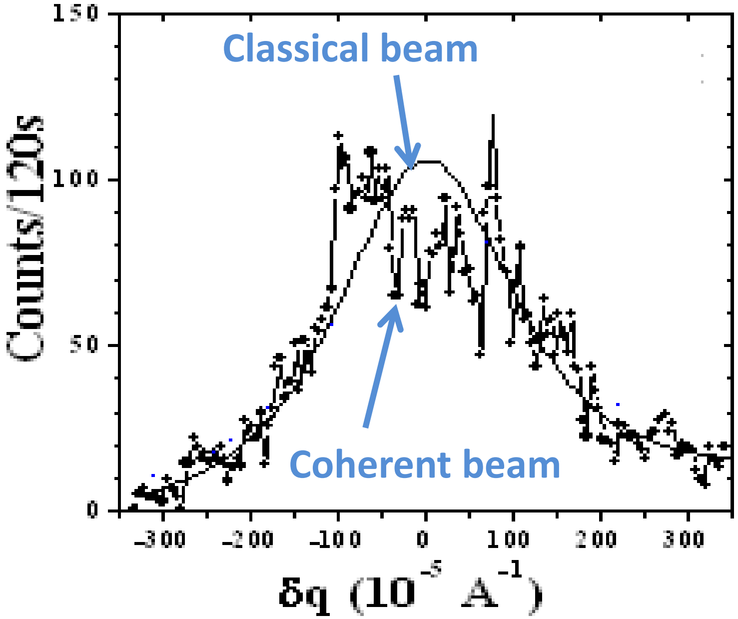
"coherent diffraction": pleonasm

$$2d\sin\theta = n\lambda$$



Typical scale of interfering objects:
Angstrom

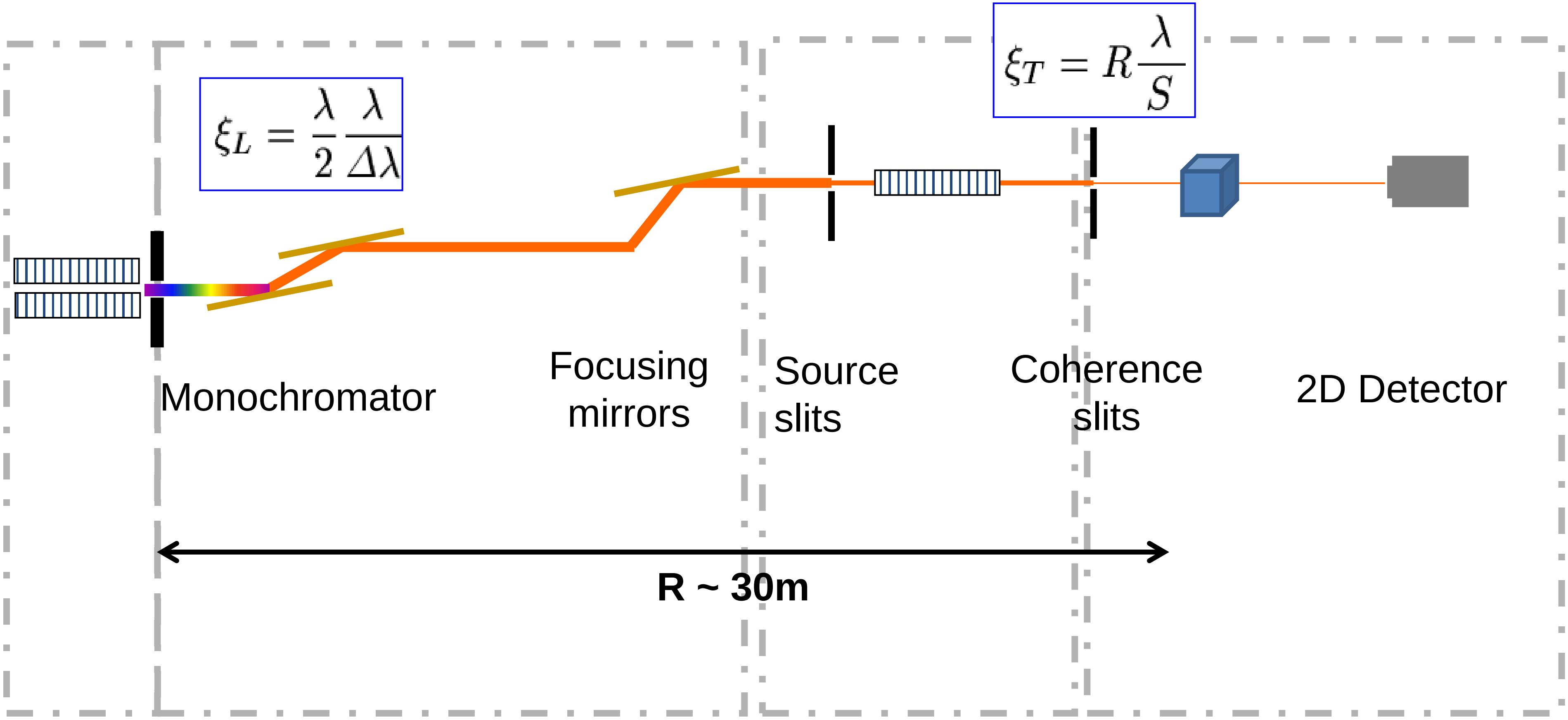
Bragg reflection of a sample with domains



Classical beam: poorly coherent beams (ξ_T ~ Å)
Coherent beam: ξ_T ~ µm
➔ interferences from domains (**speckles**)

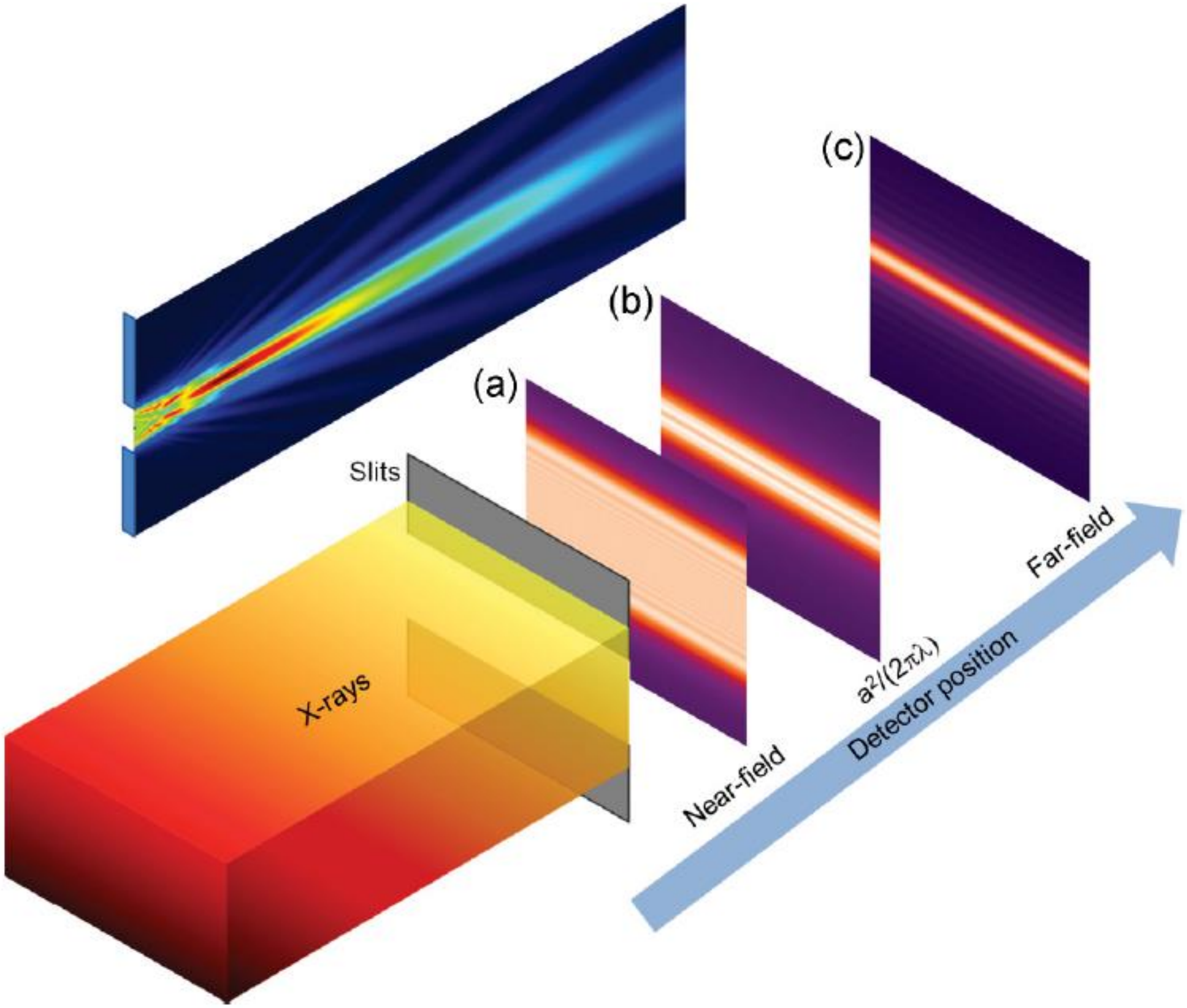
<u>Coherent diffraction</u>:
interference from µm-sized object +
gives information about phase-shifted domains (no spatial averaging)

How do we get coherent beams? CRISTAL setup (SOLEIL)



Coherent x-rays made possible thanks to ***3d generation synchrotrons***
that provide intense beams, ***small sources*** and ***large source-sample distances***.

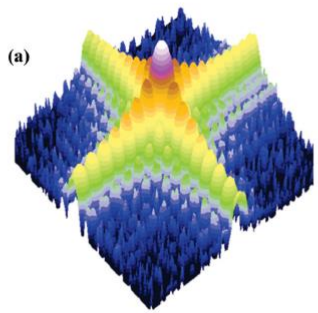
Testing coherence properties with slit diffraction

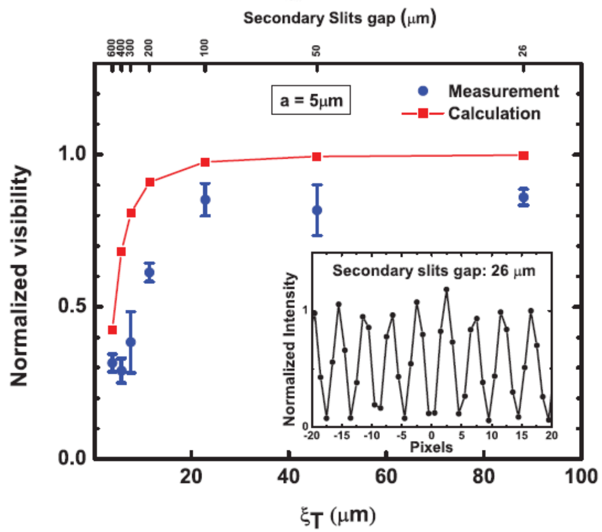


Interest: get the coherence properties of the x-ray beam by making slit diffraction!

Testing coherence properties with slit diffraction – CRISTAL, SOLEIL

In the far field

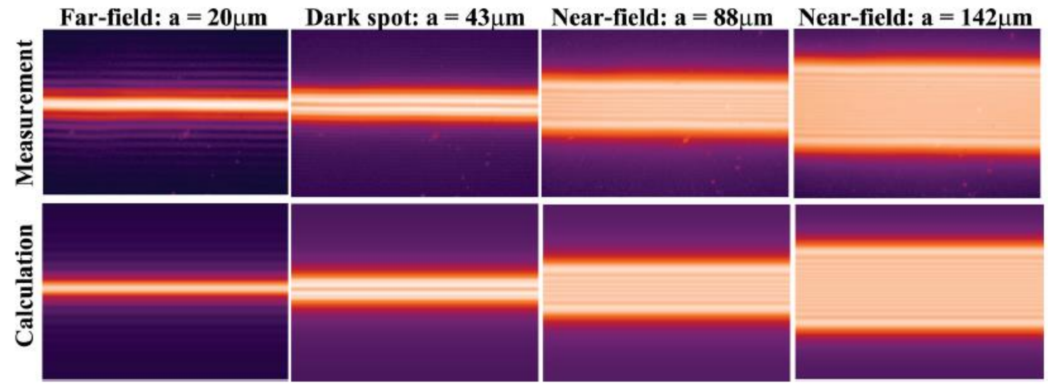


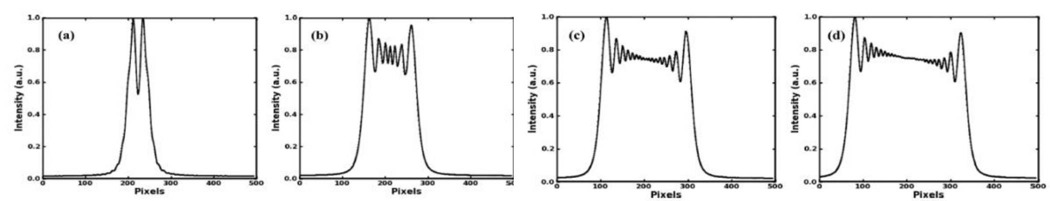


$$V = \beta \frac{\sin\left(\frac{\pi b}{\eta}\right)}{\frac{\pi b}{\eta}}$$

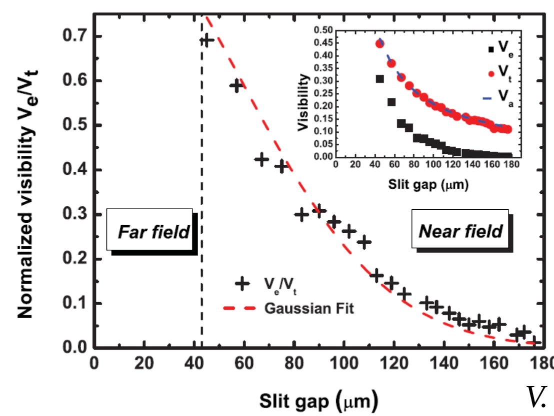
Finite pixel size lowers measured visibility by ~10%

In the near field





a = 43µm *a = 88µm* *a = 142µm* *a = 182µm*

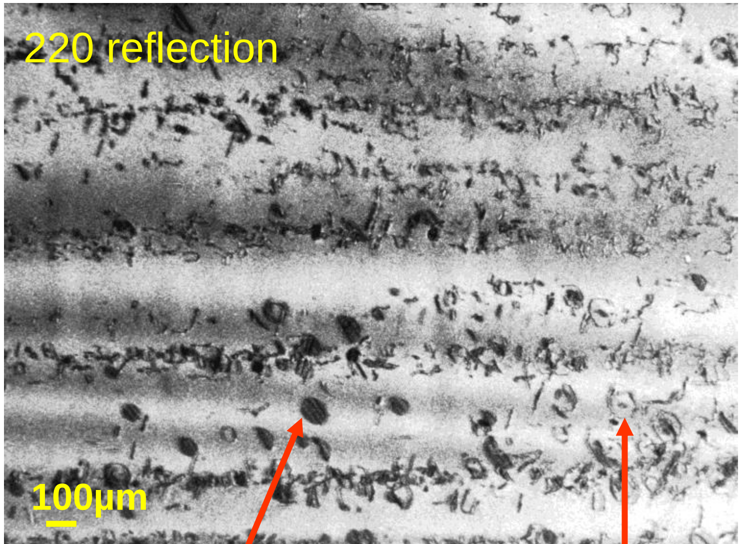


$$\frac{V_e}{V_t}(a) = e^{-\frac{a^2}{2\xi_{TF}^2}}$$

- Measured ξ_T = 64±2µm
- Calculated one: 70 µm

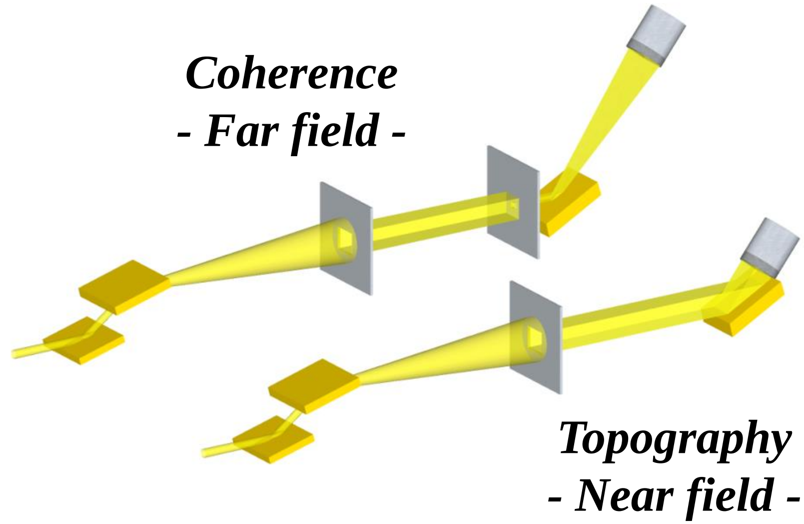
*V. Jacques et al., PRB **86**, 144117 (2012)*

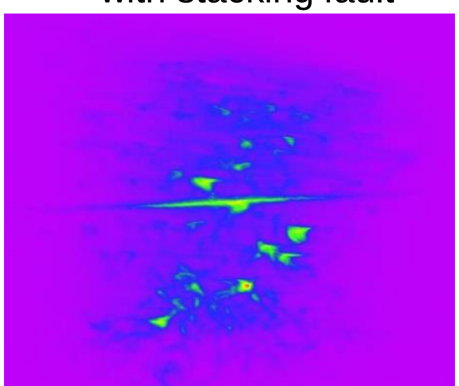
Dislocation loops in silicon (CRISTAL , SOLEIL)

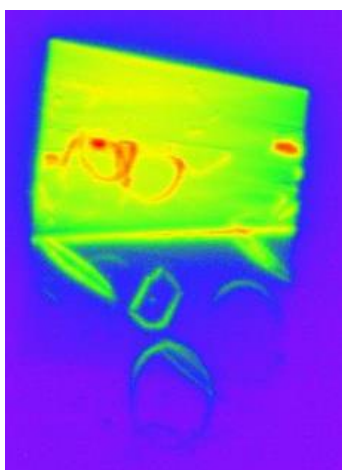


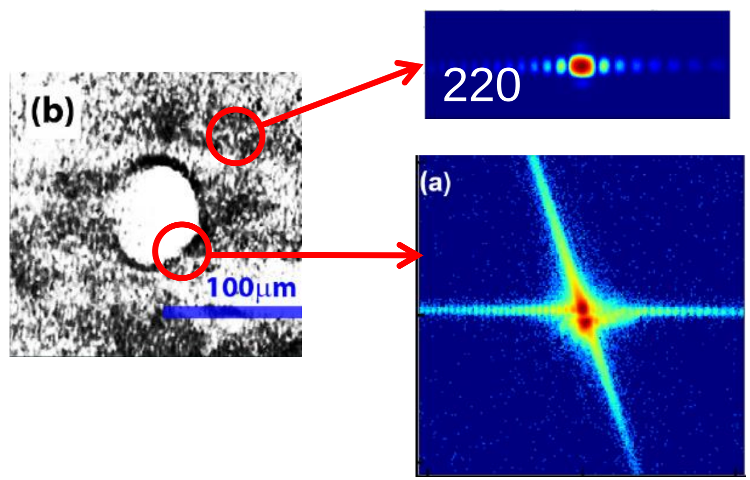
Partial dislocation
with stacking fault

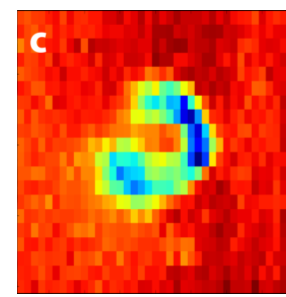
Prismatic loop









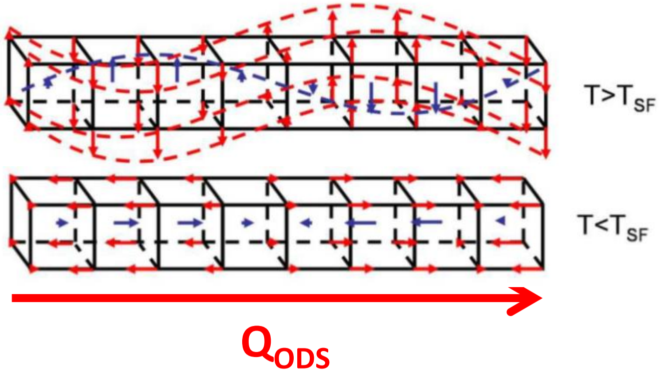


Resolution
=
beam size

V. Jacques et al., PRL **106**, 065502 (2011)

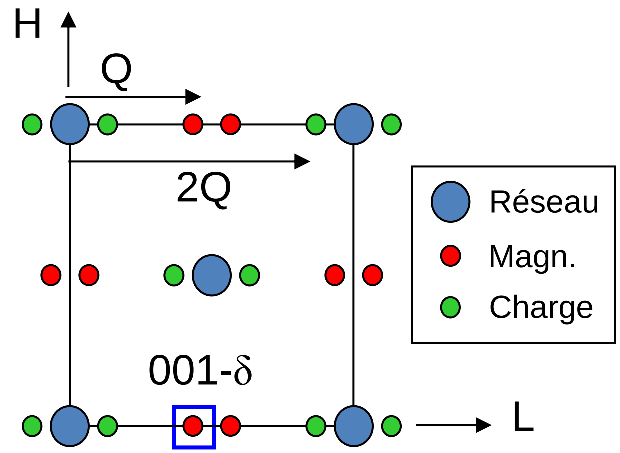
Back to chromium: SDW dislocations

Chromium structure



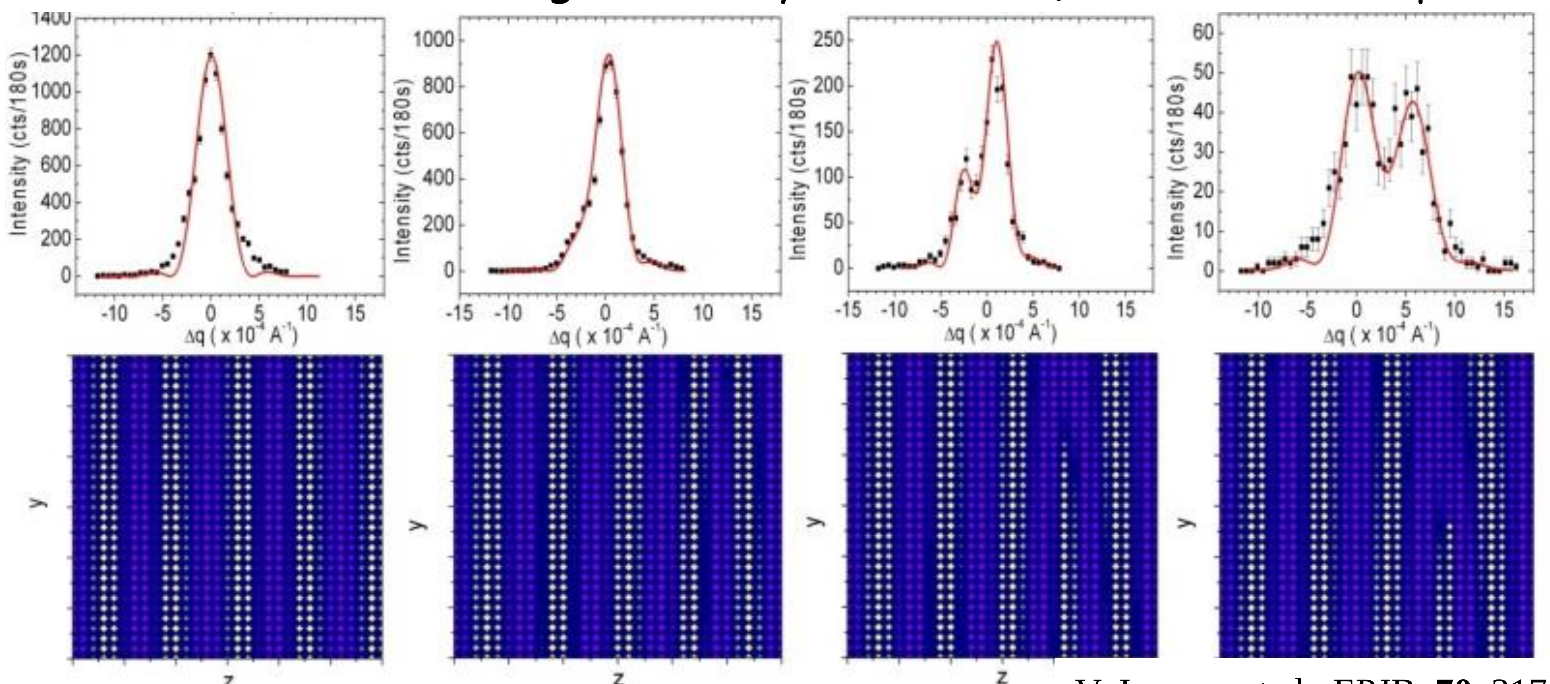
+ CDW

ID20, ESRF



T = 140K; E = 5.95keV

Coherent and **non-resonant magnetic** x-ray diffraction (Transverse SDW polarization)

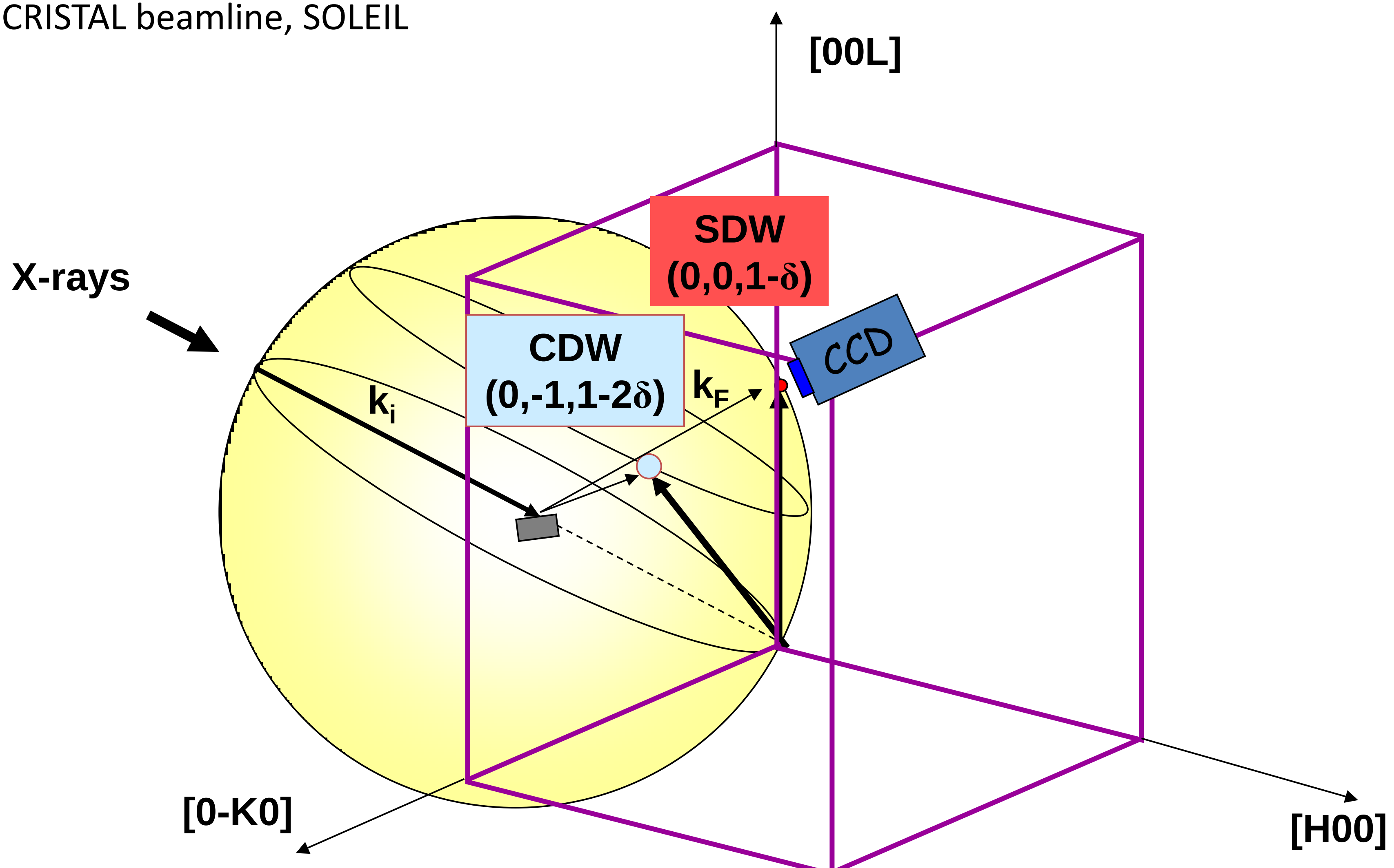


V. Jacques et al., EPJB **70**, 317 (2009)

Comparison between CDW and SDW modulations in chromium

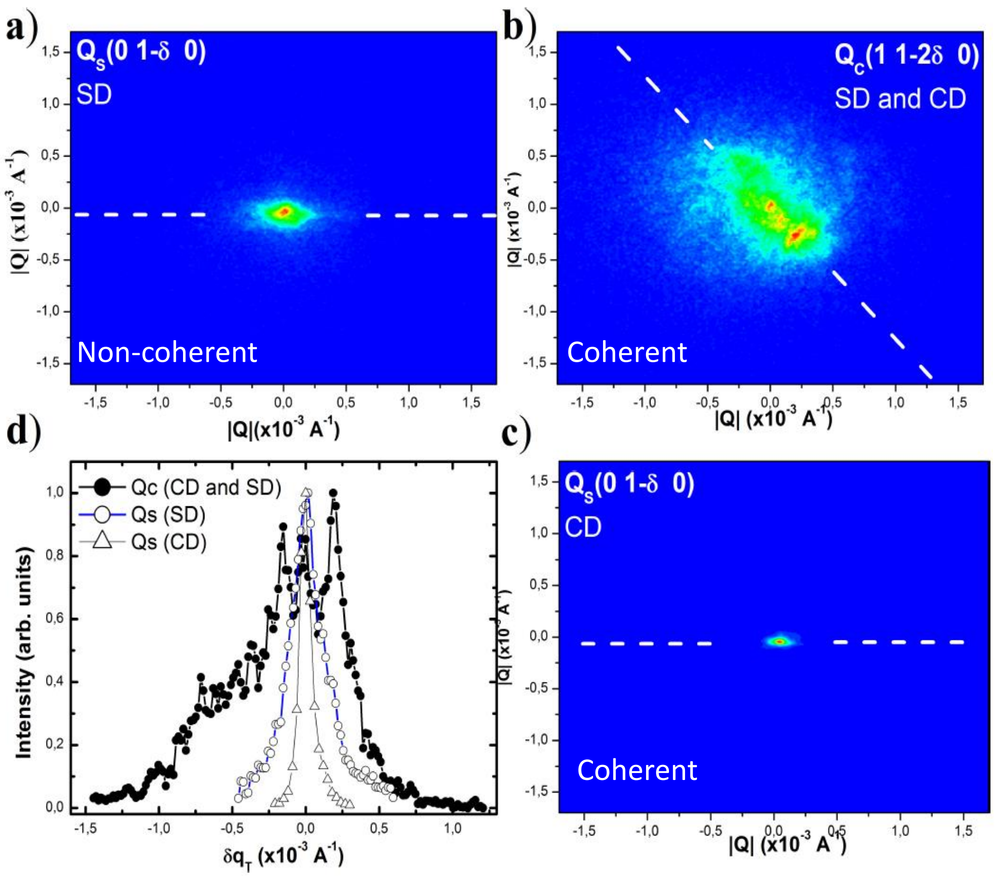
Coherent, **magnetic** and **simultaneous** x-ray diffraction on CDW and SDW reflections

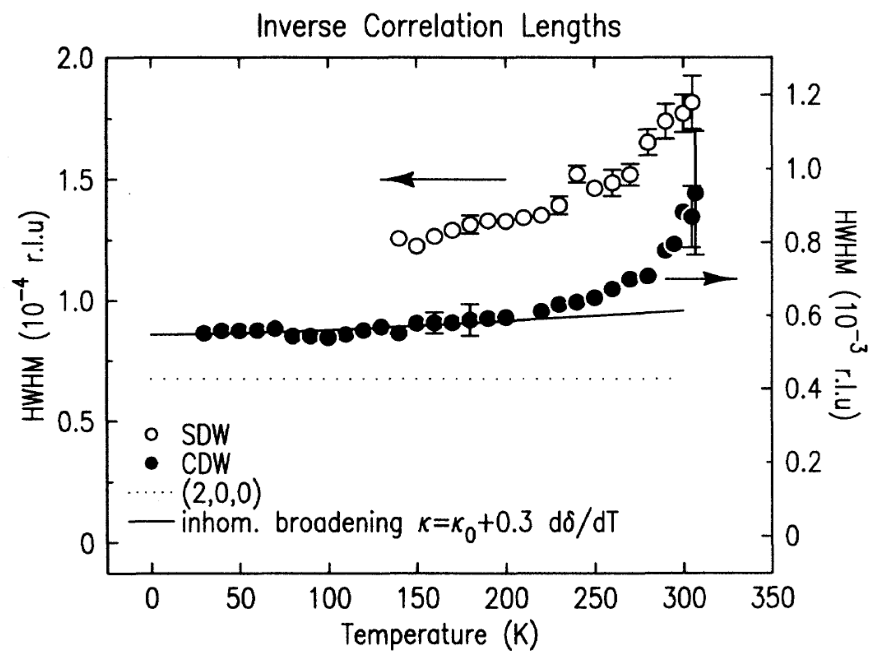
CRISTAL beamline, SOLEIL



No need to move the sample ➔ same volume is probed for the two reflections

Results





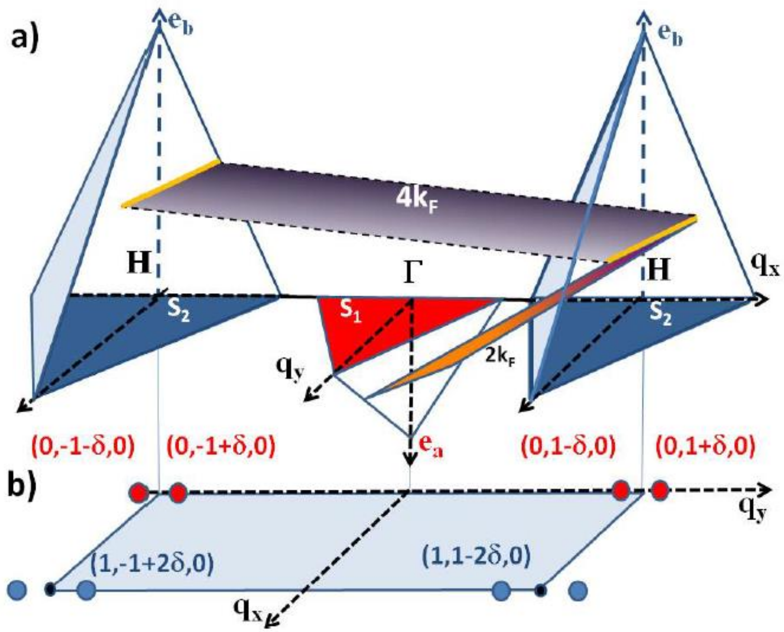
Hill, Helgesen & Gibbs, PRB ***51****, 10336 (1995)*

Longitudinal directions
Not same volumes probed
Role of charged point defects

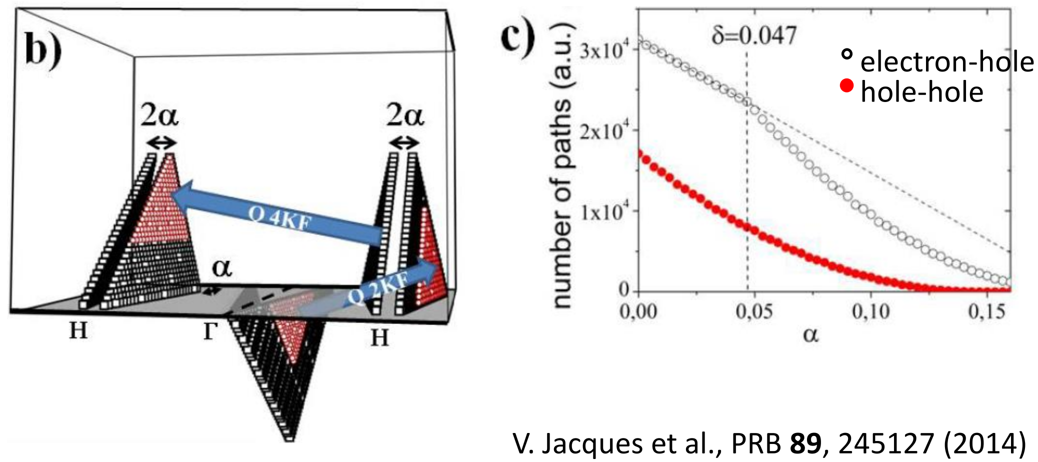
- No defect AT ALL on the SDW within the probed volume
- Many defects on CDW: not in agreement with CDW formation through magnetoelastic coupling

What about the 3 bands model to account for the CDW behaviour?

Interpretation through elctron-hole and hole-hole pairing



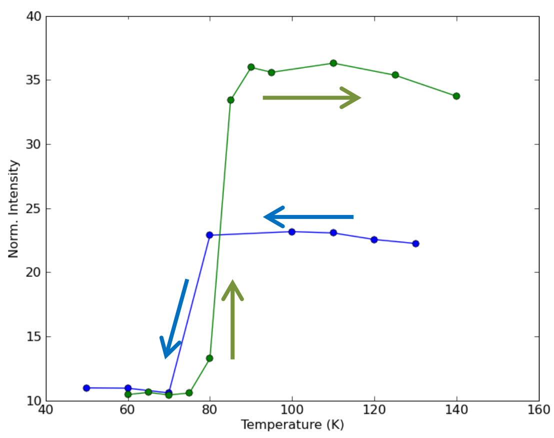
We introduce point defects by removing states at the border of the Brillouin zone



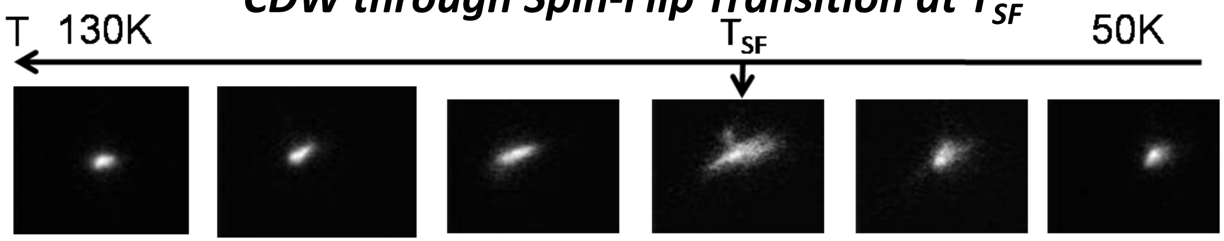
V. Jacques et al., PRB **89**, 245127 (2014)

Just by counting the number of possible states we see that the SDW is more stable with respect to point defects.

Cristal, Soleil



CDW through Spin-Flip Transition at T_{SF}

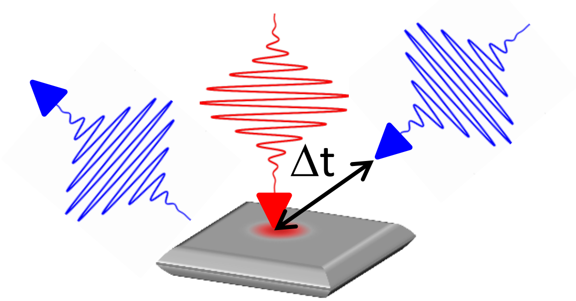


ID01, ESRF

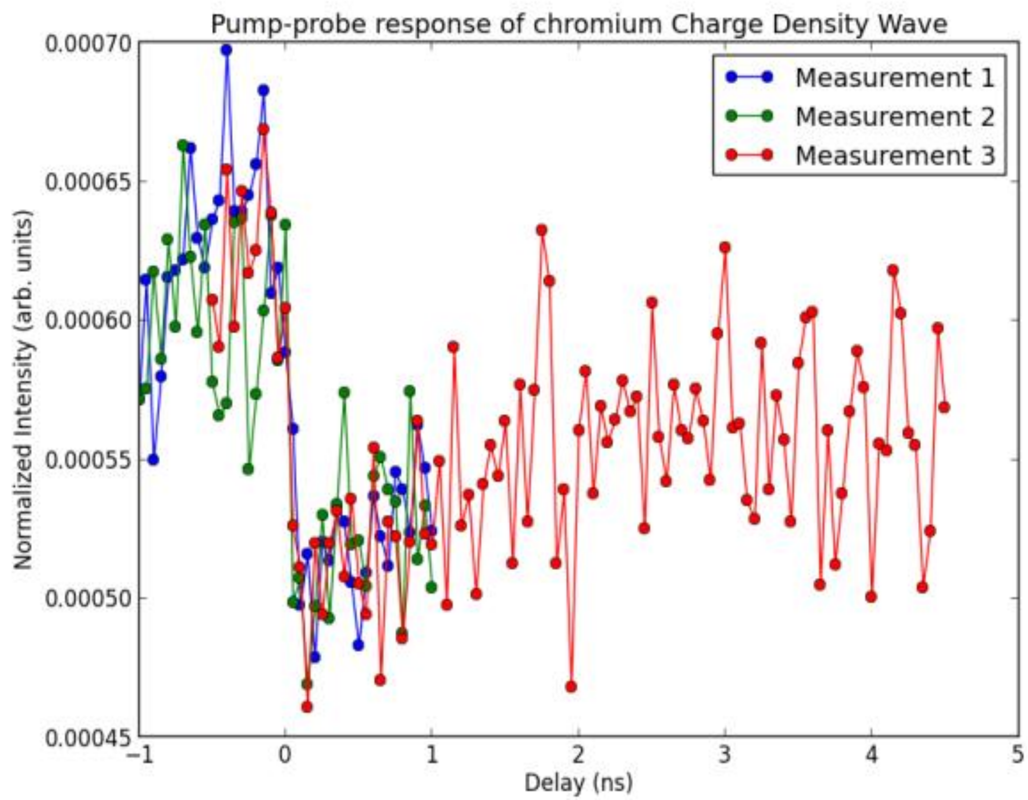
➔ Charge density wave is affected by spin-flip transition

Time-resolved x-ray diffraction – CRISTAL beamline (SOLEIL Synchrotron)

Aim: understand role of lattice in the CDW formation



T=140K (He blower)



Measured reflection: 0,1,1-2δ

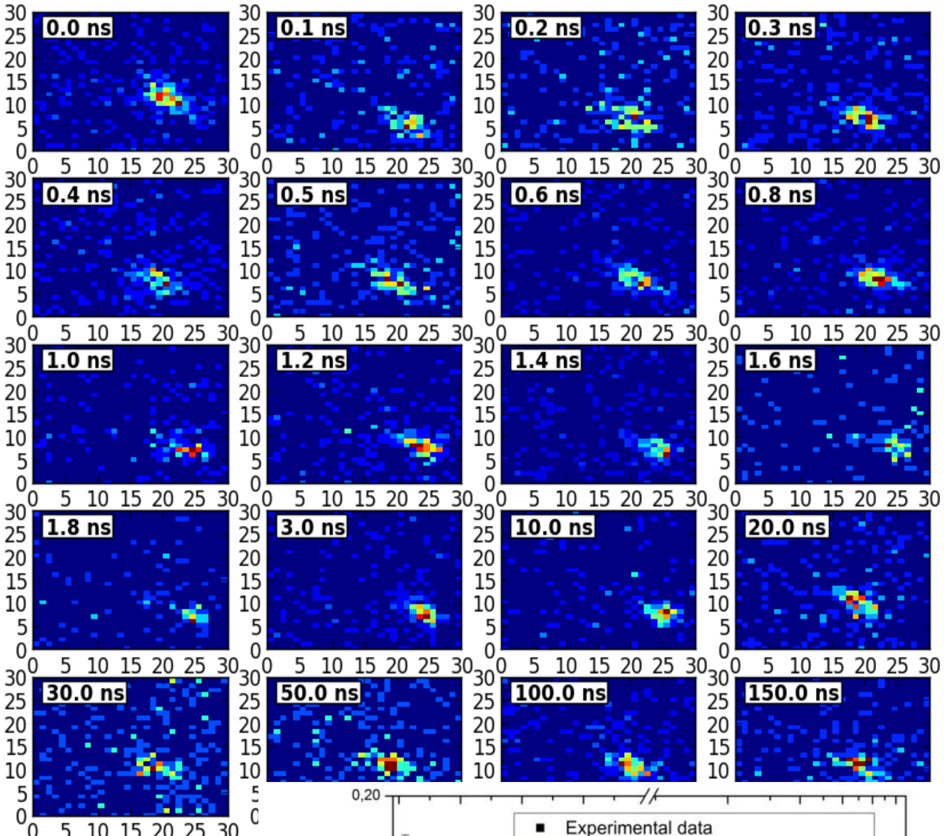
<u>Laser pump:</u>
800nm
25fs pulse duration
~1kHz repetition rate

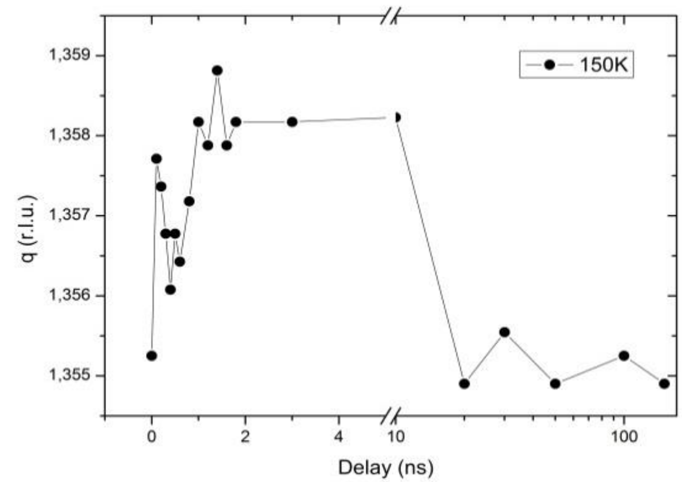
<u>X-ray pulse</u>:
7.1keV
70ps pulse duration

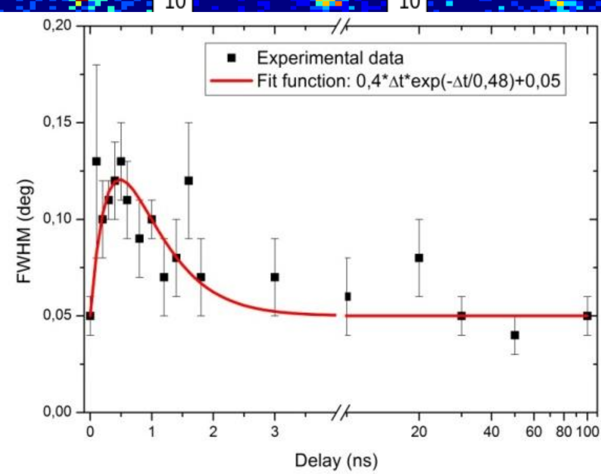
<u>Grazing incidence x-rays:</u> 1,5°

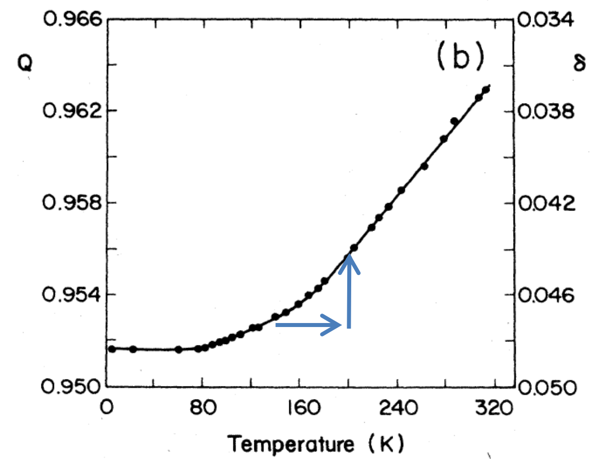
Time-resolved x-ray diffraction – CRISTAL beamline (SOLEIL Synchrotron)

CDW reflection at rocking curve maximum:









Mostly driven by thermal effects
but the CDW correlation length
is back before the CDW amplitude.

Conclusion and perspectives

- The new techniques used here allow getting a new vision of the physics of chromium:

Coherent x-ray diffraction: very efficient to study spatial arrangements of any modulation
Time-resolved diffraction: should help understand the role of the lattice in the CDW formation mechanism

- *From coherent x-ray diffraction measurements of CDW and SDW reflections*:
  the 3 bands model seems more appropriate

- *From coherent x-ray diffraction at spin-flip transition*: coupling between the two is obvious

- *From time-resolved experiment*: system is back to initial state within 10ns: very long ➔ thermal effect

PERSPECTIVE:
Perform time-resolved experiments with femtosecond time resolution to see the dynamics of CDW formation
(slicing at SOLEIL / XFEL)

Special thanks to:
D. Le Bolloc’h, S. Ravy, E. Pinsolle, C. Laulhé

Thank you for your attention!