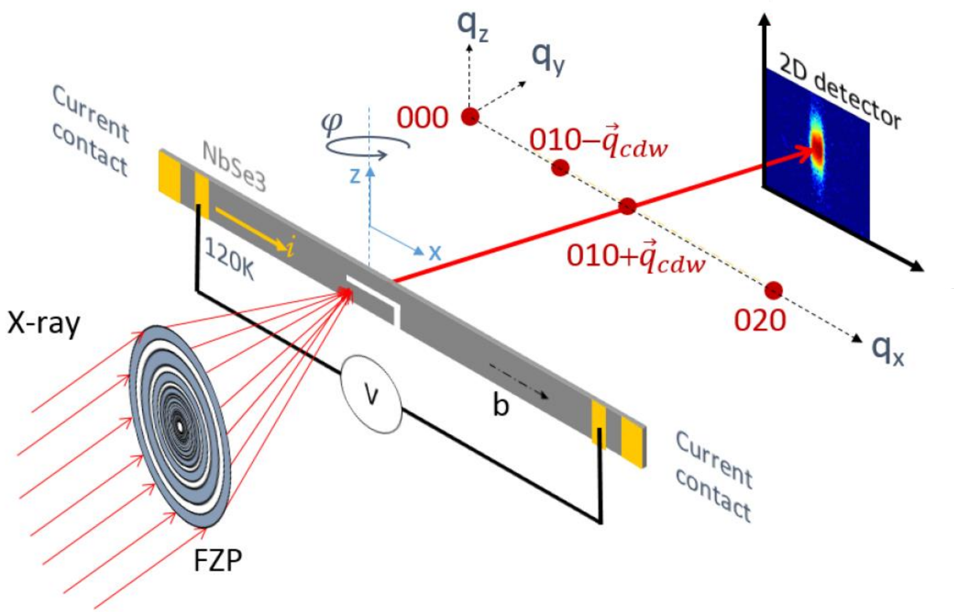
Workshop on Dark Field X-ray Microscopy

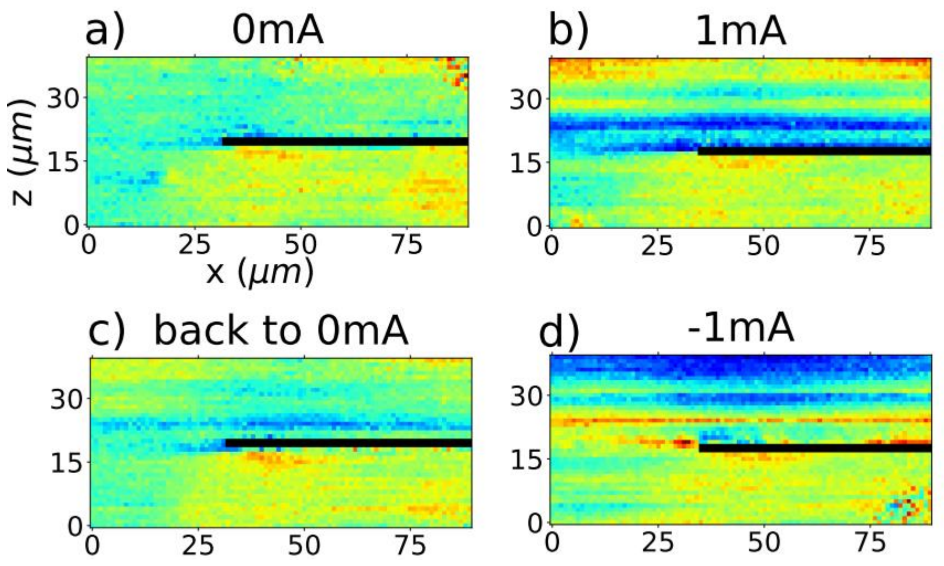
STREAMLINE

Study of charge density wave materials under current by X-ray diffraction

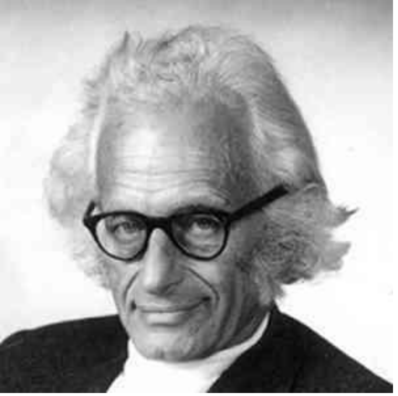


Presented by

Ewen Bellec



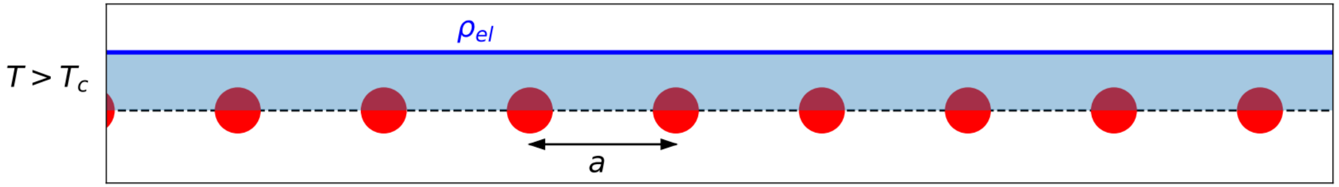
Charge density wave (CDW) transition



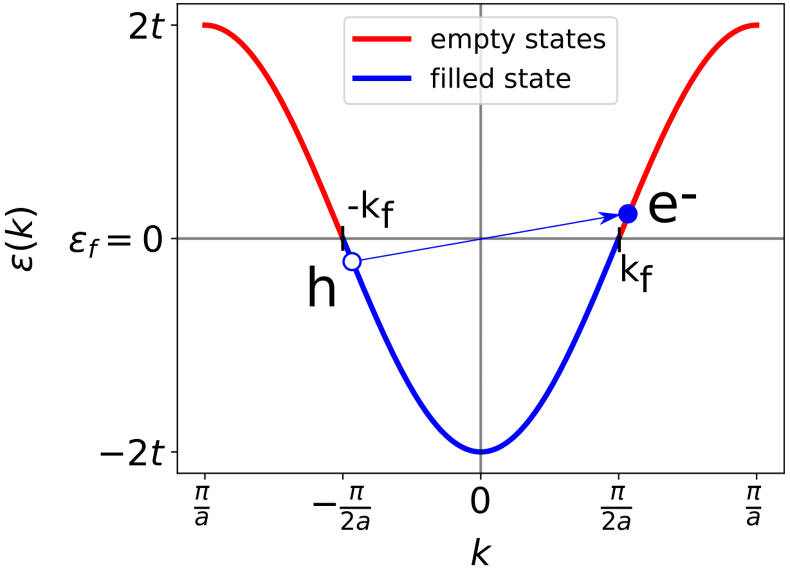
Herbert Fröhlich

Rudolf Peierls

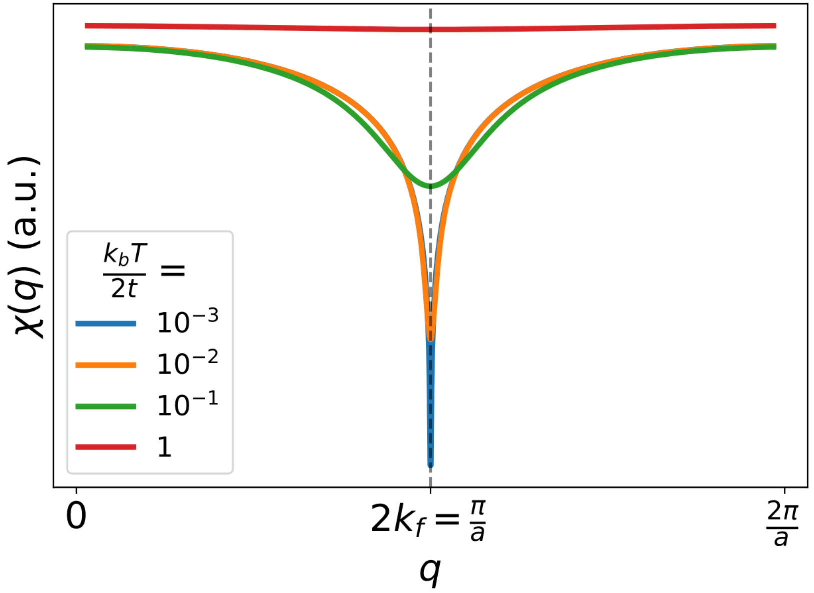
Model of a 1D atomic chain



$$H = -t \sum_{n=1}^{N} \left(c_{n+1}^{\dagger} c_n + c_n^{\dagger} c_{n+1} \right)$$

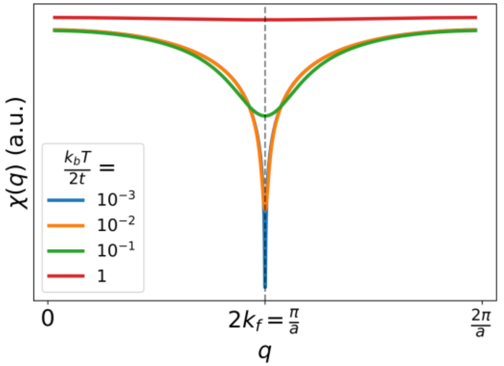


Electronic band above Tc



Electronic susceptibility

Charge density wave (CDW) transition

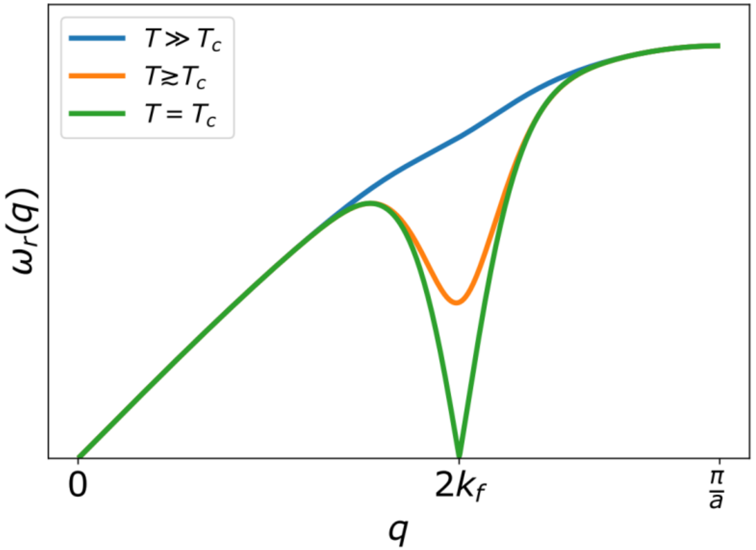


Electronic susceptibility

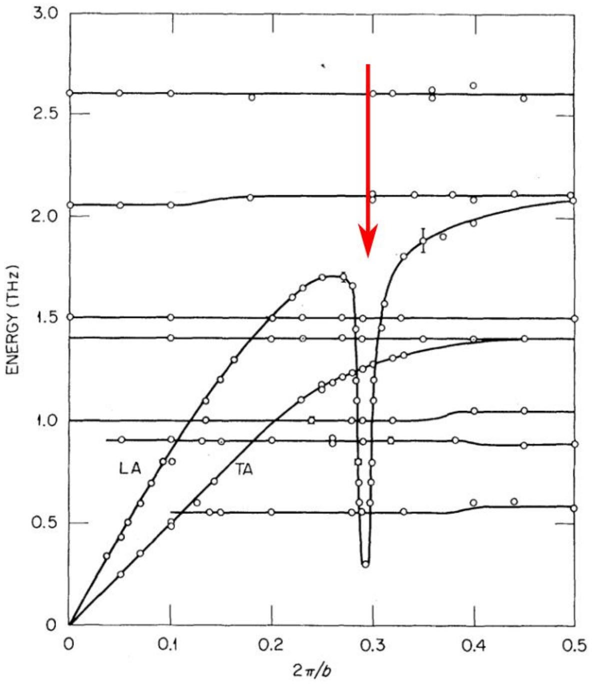
Kohn anomaly

$$\omega_r^2(q,T)=\omega^2(q)+\chi(q,T)\frac{2g(q)^2}{\hbar}\omega(q)$$

Renormalization of the phonon spectrum

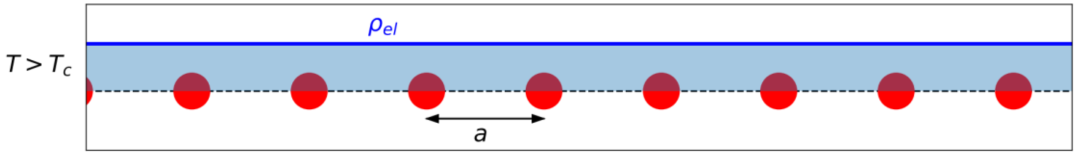


Schematic of the Kohn anomaly above, close to and at Tc



Phonon spectrum in TTF-TCNQ obtained by inelastic neutron scattering
H. A. Mook and Charles R. Watson PRL (1976)

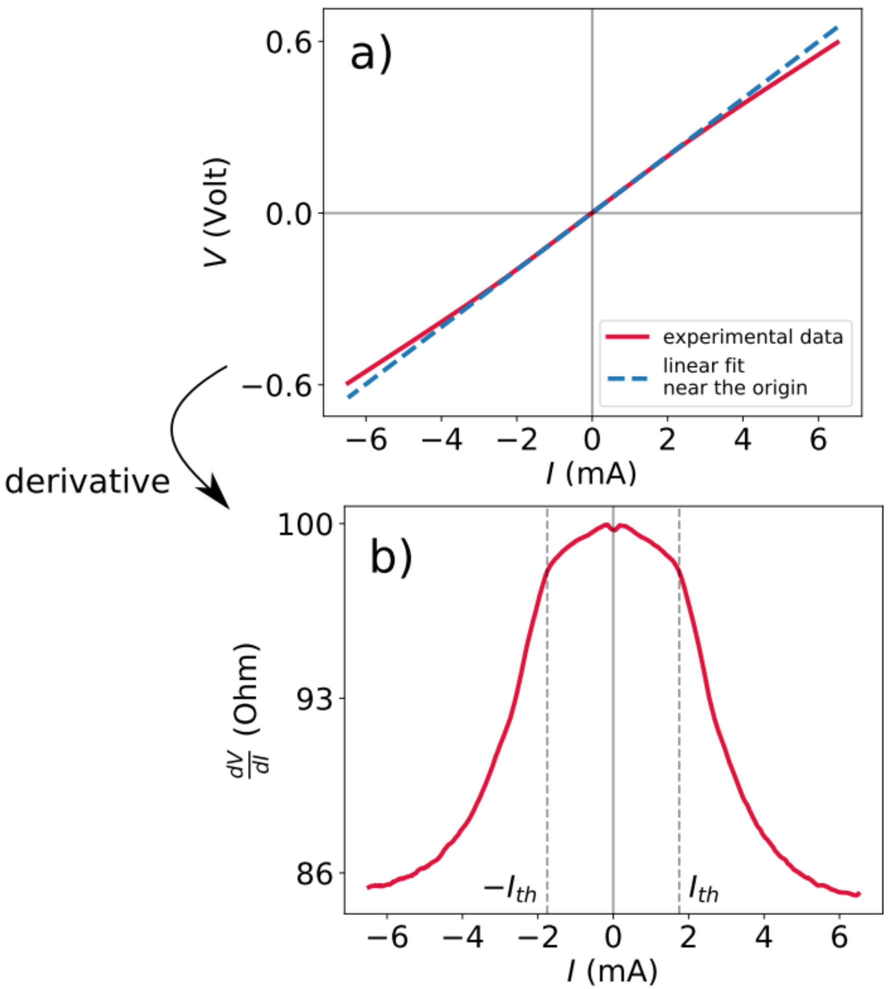
New periodicity in the ion lattice

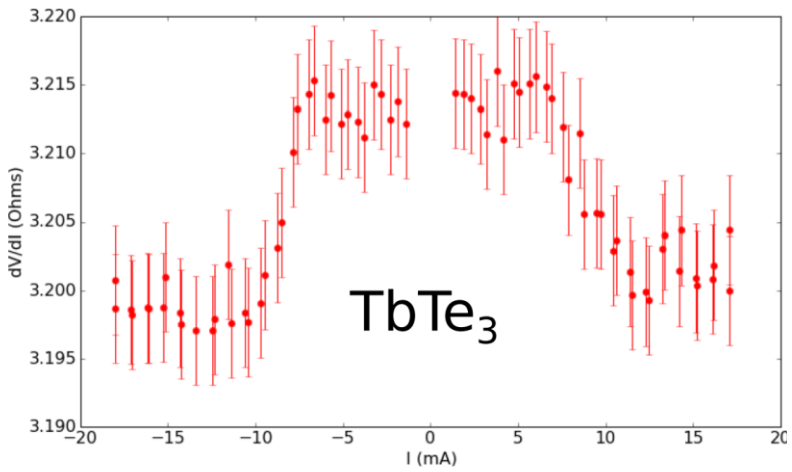


CDW under current

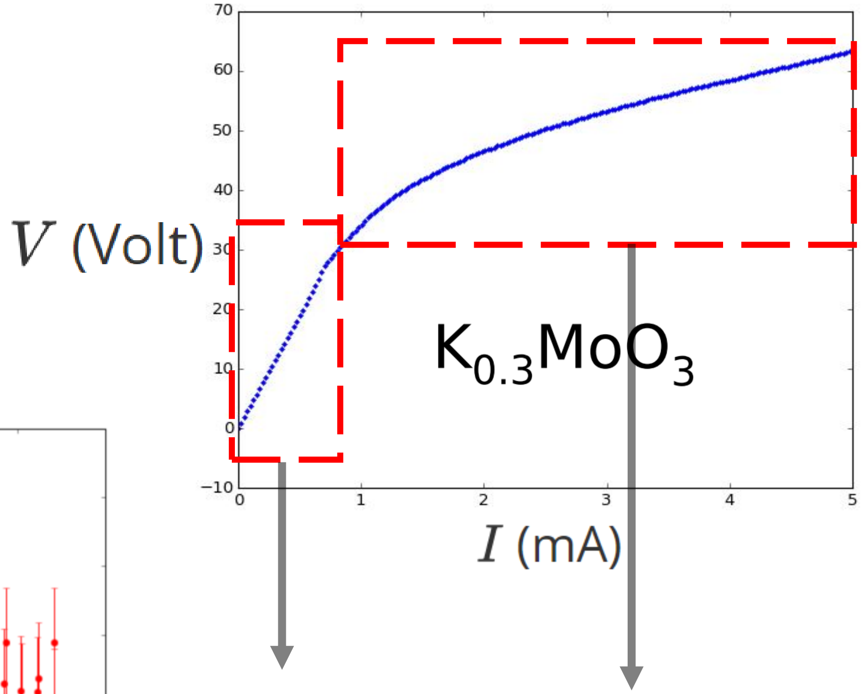
CDW collective current

Current-Voltage measurement in NbSe3 at 120K





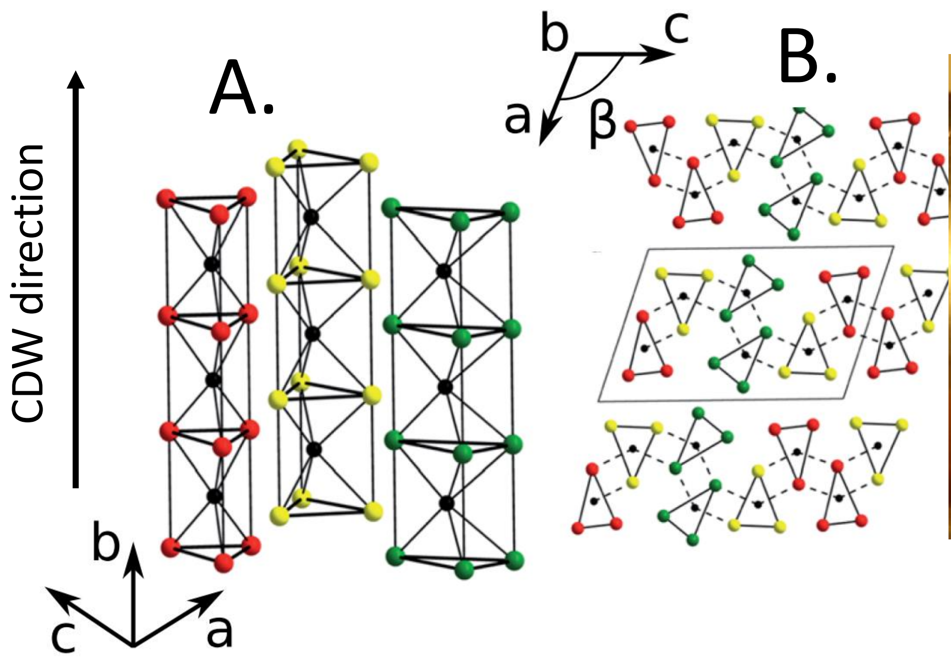
Current-voltage measurement in a $K_{0.3}MoO_3$

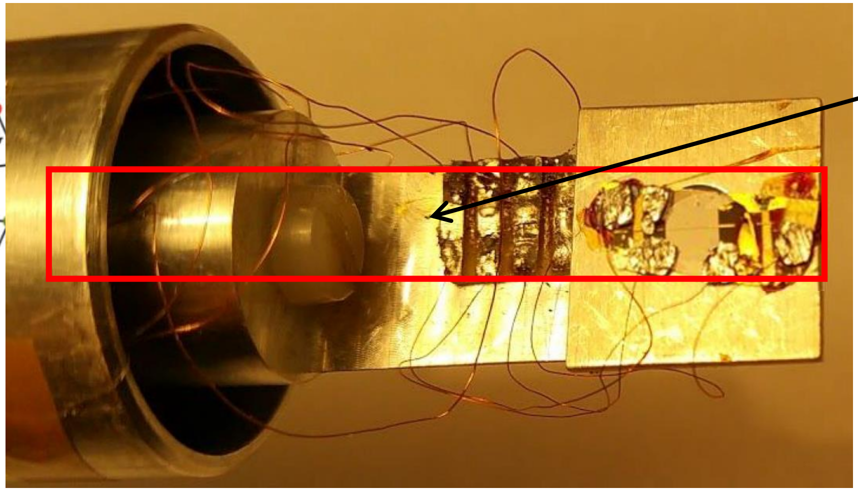


CDW doesn't contribute to the current

CDW contributes to the current but how ?

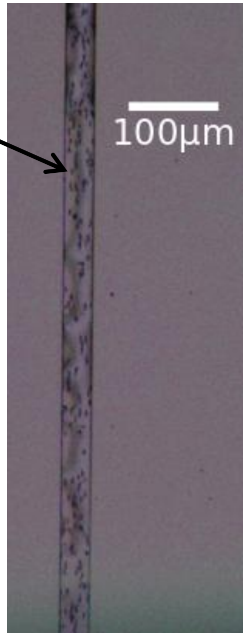
Quasi-1D Niobium Triselenide $NbSe_3$





NbSe$_3$

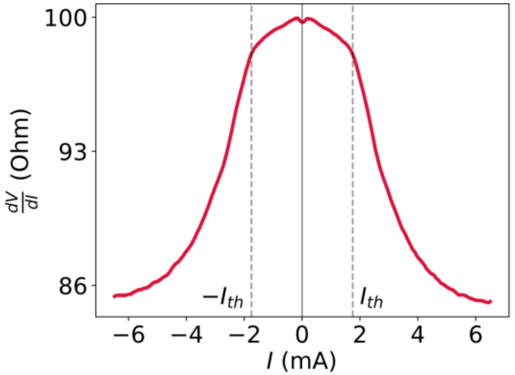
Picture on an optical microscope



CDW direction

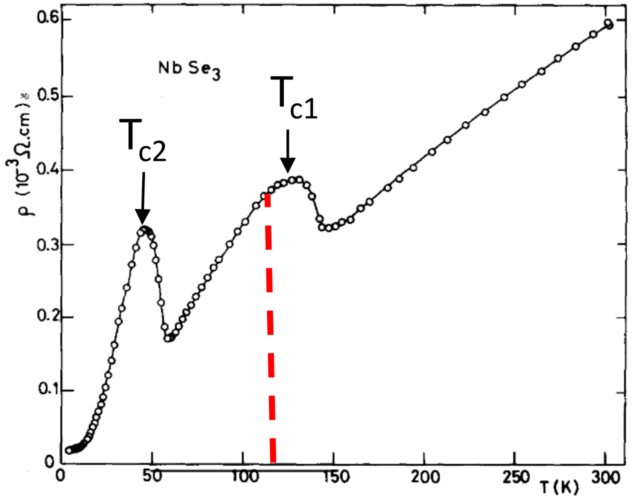
Typical sample size of 1mm x 40µm x 3µm

A. Crystal structure of Nobium Triselenide $NbSe_3$ showing the **quasi-1D chains** along the b direction. The CDW wavevector being Q = (0, $2k_f$, 0) in reciprocal lattice units.
B. The chains as seen from above.



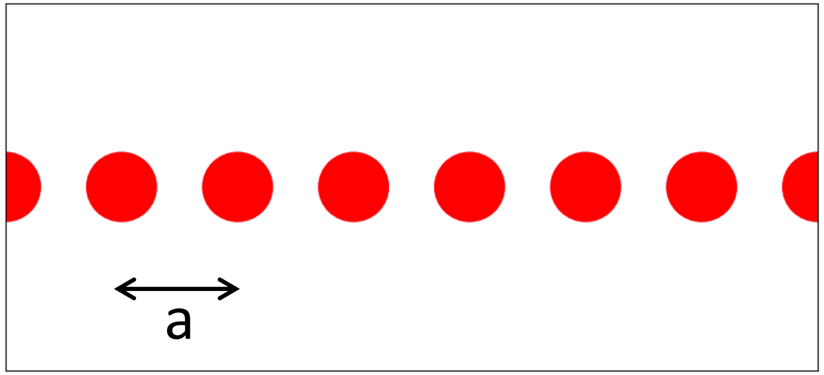
CDW collective current

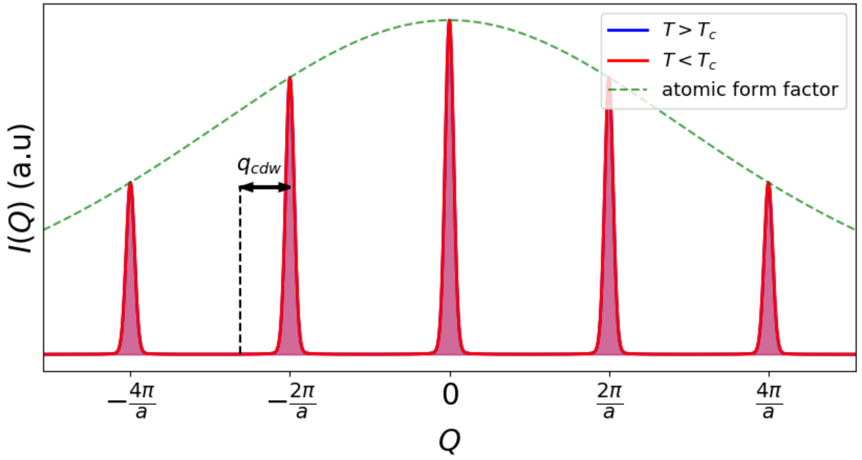
Resistivity measurement as function of temperature
J. Chaussy et al. Solid State Communications (1976)



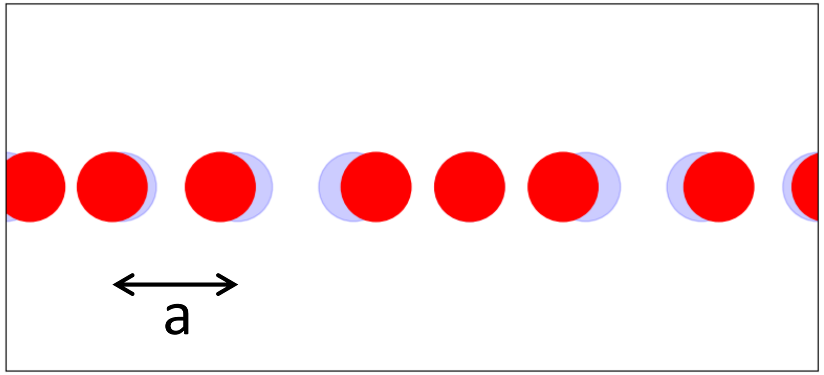
Two CDW transitions at Tc1 = 144K and Tc2 = 59K.
We studied only the first one.
All experiments presented here were made at T=120K>Tc2

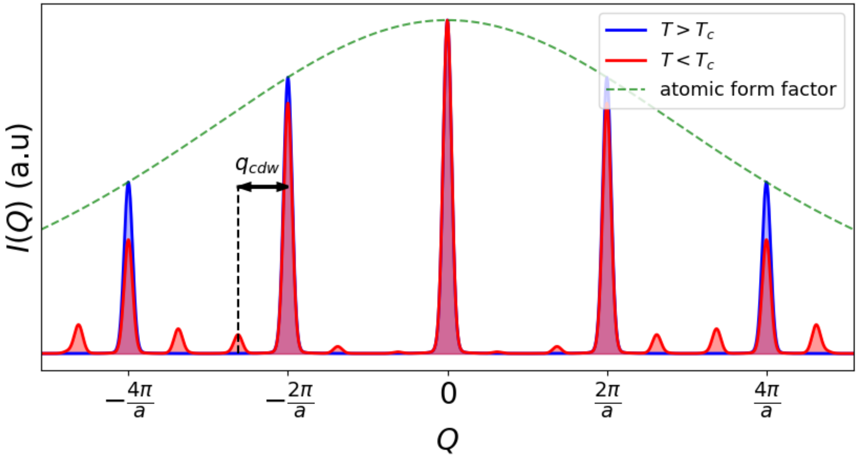
CDW X-ray diffraction



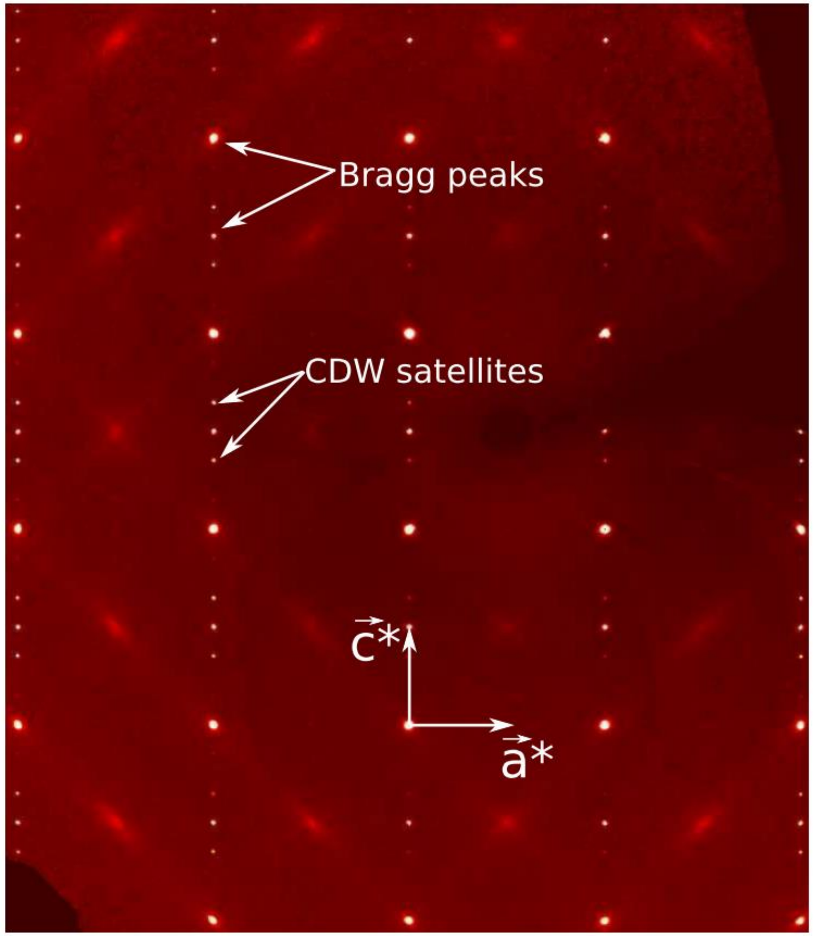


CDW X-ray diffraction



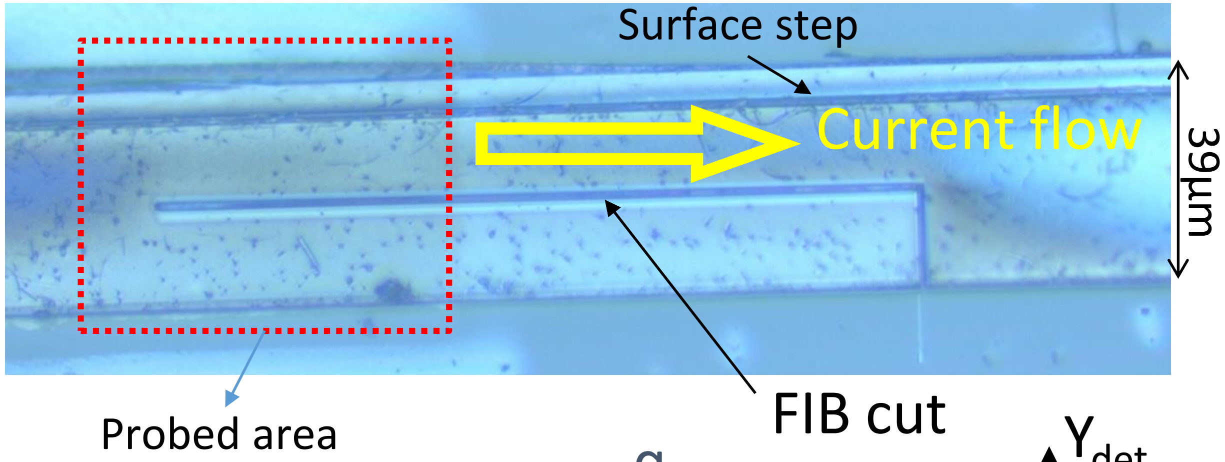


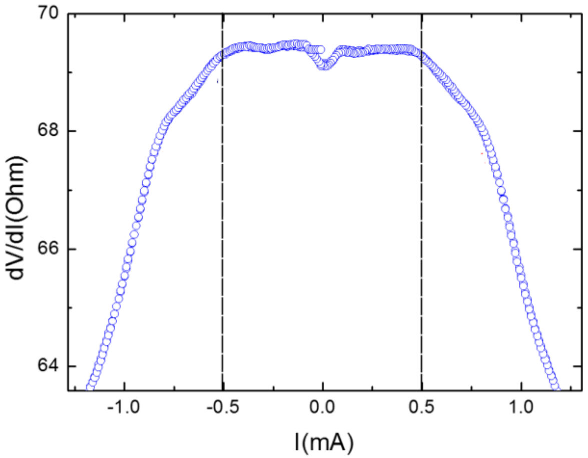
CDW satellite peaks appear on both side of the Bragg



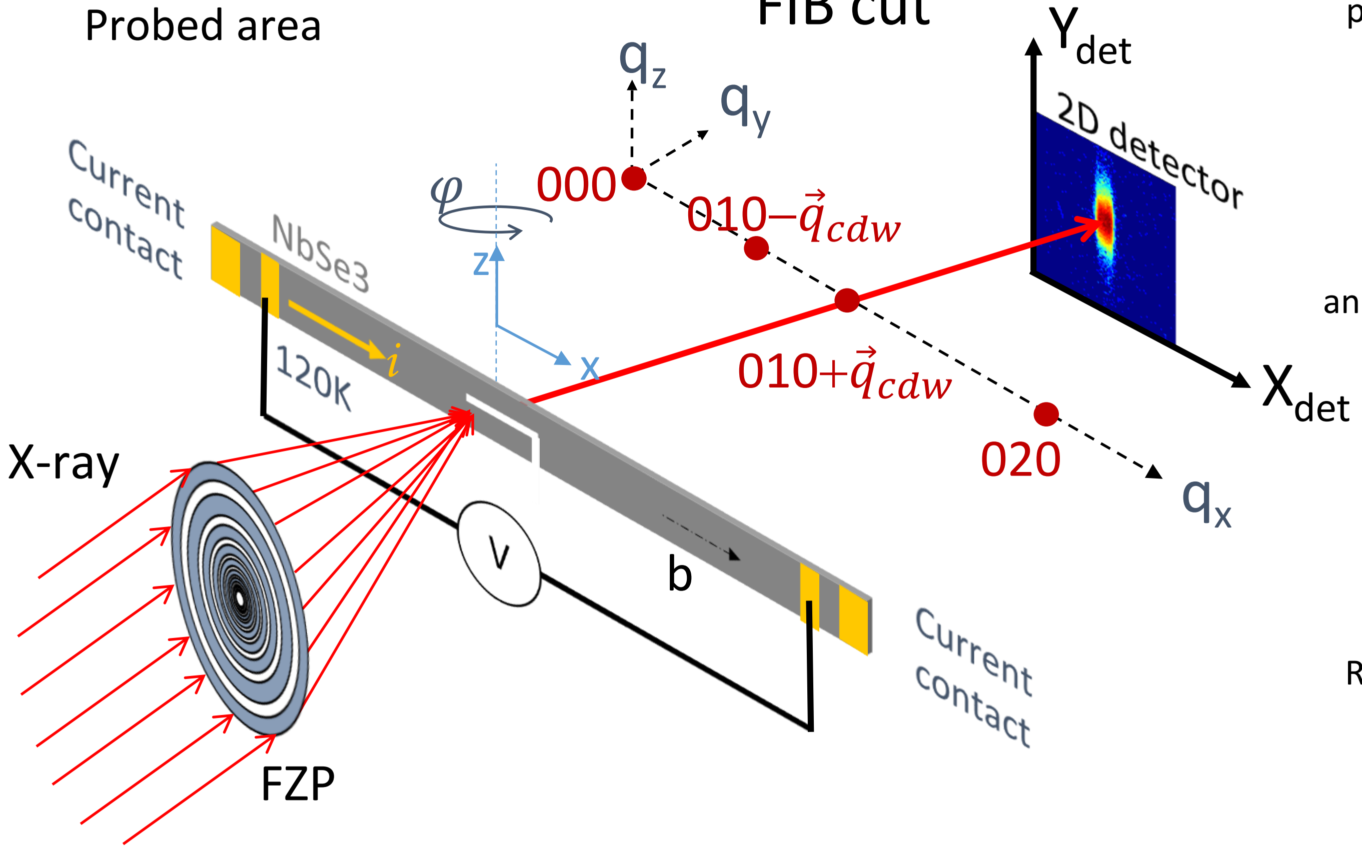
X-ray diffraction of TbTe3 at beamline Cristal (Soleil synchrotron)

X-ray micro-diffraction of the quasi-1D NbSe3





Differential resistivity at 120K
Ith = 0,5mA



Sample dimensions : 39µm × 3µm ×2.25mm

Current flows only in the upper regions of the sample

4-point gold contact to perform I-V measurements

Focalized X-ray beam area ≃ 200nm × 300nm

Measure Bragg (0 2 0) and CDW satellite (0 1 0)+q_{cdw}

Scan an area of 80µm × 50µm on the sample

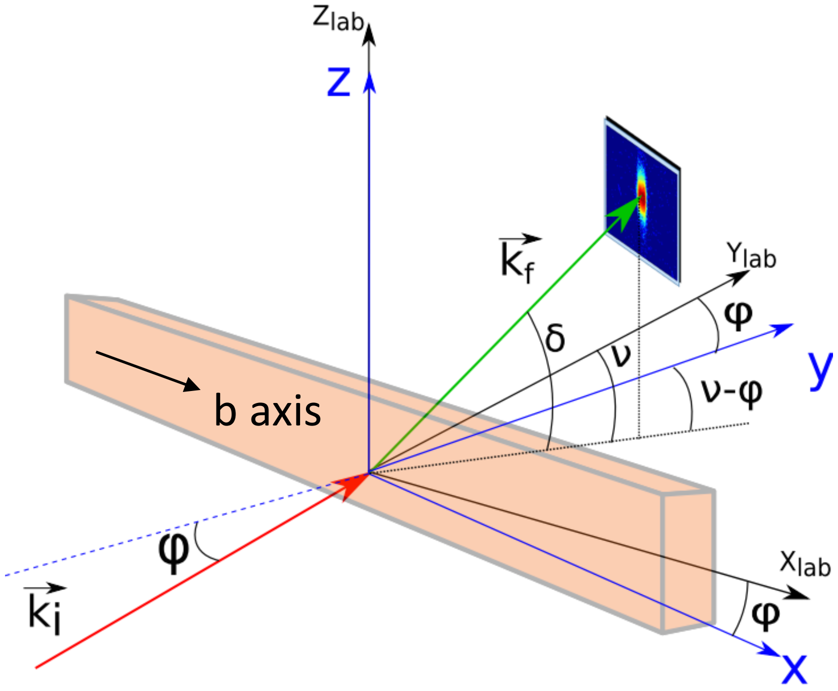
Rocking curve for each position of the beam on the sample

X-ray micro-diffraction of the quasi-1D NbSe3

What type of information can we extract?

Looking only at the centroid of the beam, one can get the wavevector as function of position on sample

$$\vec{Q}(x, z)$$



$$\vec{Q} = \frac{2\pi}{\lambda}\begin{pmatrix} \cos(\delta)\sin(\nu-\varphi)+\sin(\varphi) \\ \cos(\delta)\cos(\nu-\varphi)-\cos(\varphi) \\ \sin(\nu) \end{pmatrix}$$

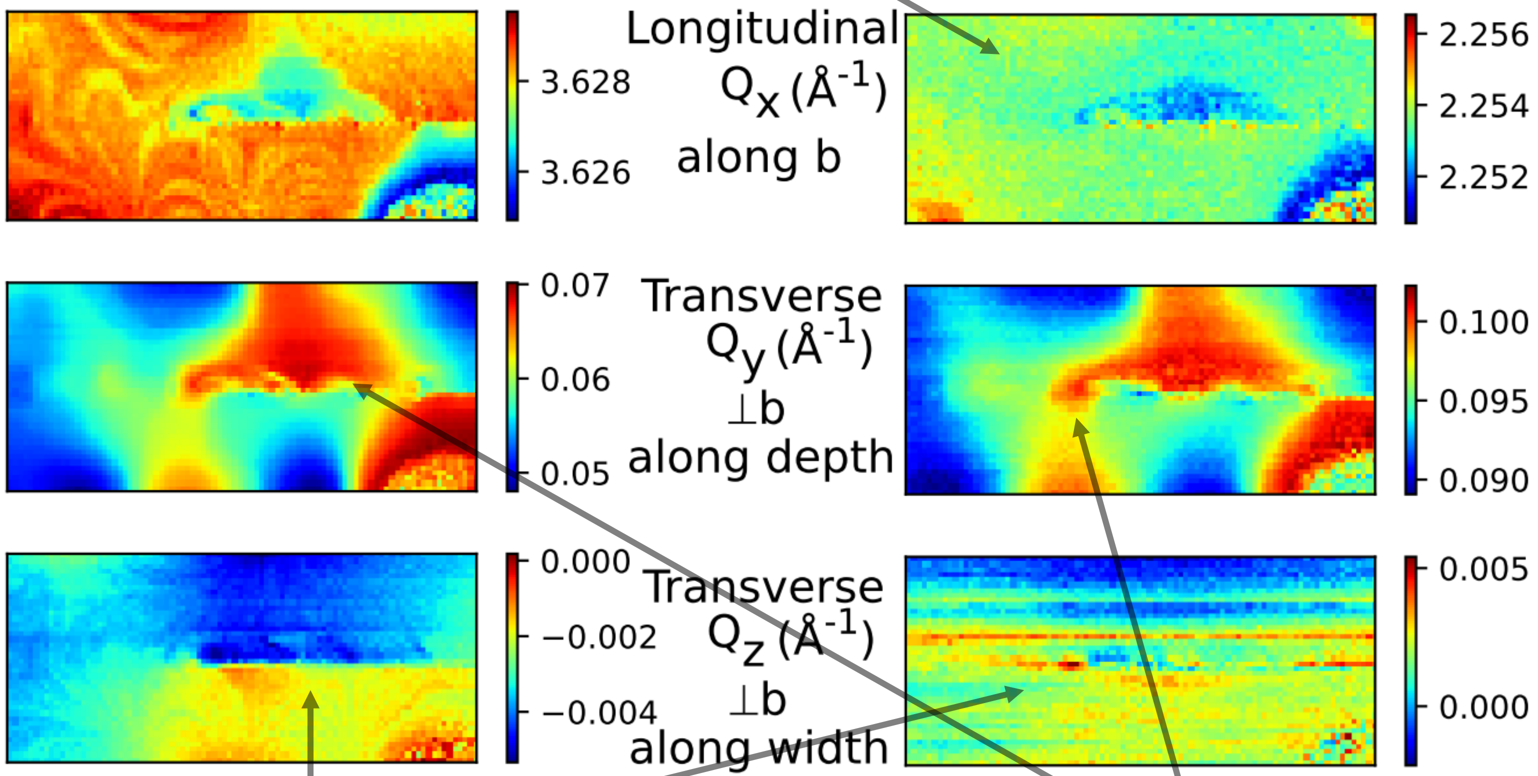
CDW direction at equilibrium

Bragg

$\vec{Q}_B$=(0 2 0)

CDW satellite

$\vec{Q}_S$=(0 1 0)+$\vec{q}_{cdw}$



Very different maps along z !

Crystal deformation along y (visible on Bragg and CDW satellite)

X-ray micro-diffraction of the quasi-1D NbSe3

What we expect to see under currents?

We measure the CDW satellite peak wavevector variation under current

$$\delta\vec{q} = \vec{Q}_S(I) - \vec{Q}_S(0\,\mathrm{mA})$$

CDW charge density

$$\rho_{cdw}(\vec{r}) = A\cos[2k_f x + \boxed{\phi(\vec{r})}]$$

$2k_f$ is the CDW wavevector at equilibrium (no applied electric field)

The charge density wave can deformation can be described by a phase degree of freedom

which is related to the phase via

$$\delta\vec{q}(x,z) = \begin{pmatrix} \frac{\partial\phi}{\partial x}(x,z) \\ \frac{\partial\phi}{\partial y}(x,z) \\ \frac{\partial\phi}{\partial z}(x,z) \end{pmatrix}$$

The free energy expression is

$$F[\phi] \propto \int \left[c_x^2\left(\frac{\partial\phi}{\partial x}\right)^2 + c_y^2\left(\frac{\partial\phi}{\partial y}\right)^2 + c_z^2\left(\frac{\partial\phi}{\partial z}\right)^2 + \eta E x \frac{\partial\phi}{\partial x} \right]$$

E being the constant electric field applied to the sample

X-ray micro-diffraction of the quasi-1D NbSe3

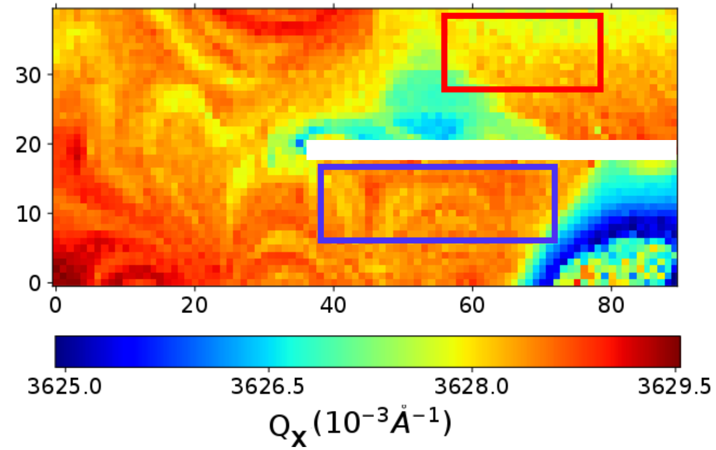
Longitudinal CDW deformation

$$F[\phi] \propto \int \left[\boxed{c_x^2 \left(\frac{\partial \phi}{\partial x}\right)^2} + c_y^2 \left(\frac{\partial \phi}{\partial y}\right)^2 + c_z^2 \left(\frac{\partial \phi}{\partial z}\right)^2 \boxed{+ \eta E x \frac{\partial \phi}{\partial x}} \right]$$

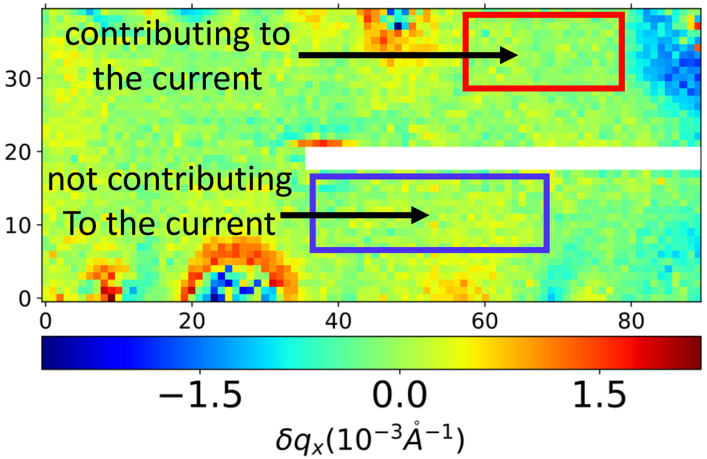
Deformation along x cost elastic energy

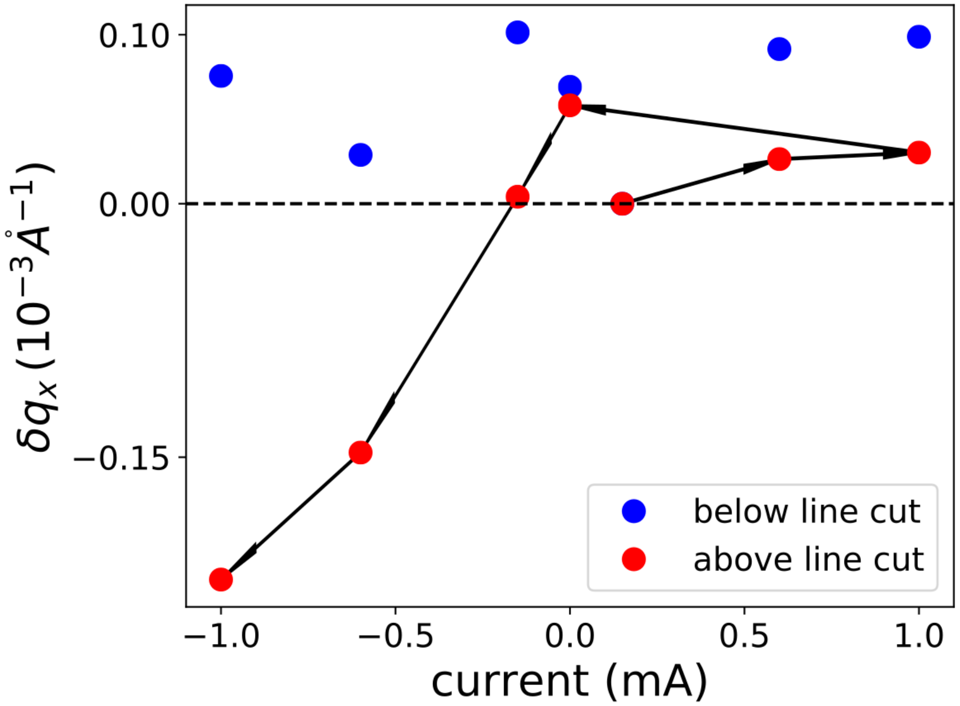
But can decrease it under applied electric field

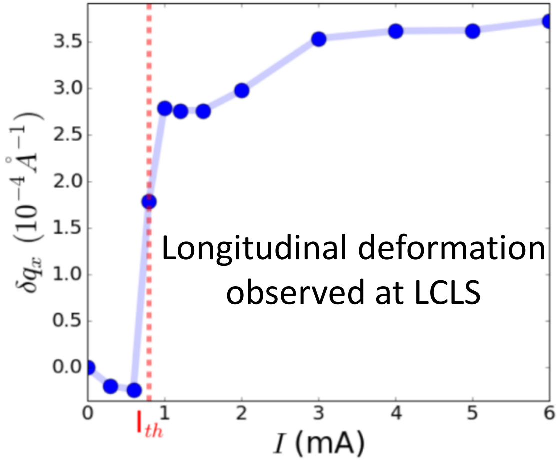
Bragg (0 2 0) at -1 mA

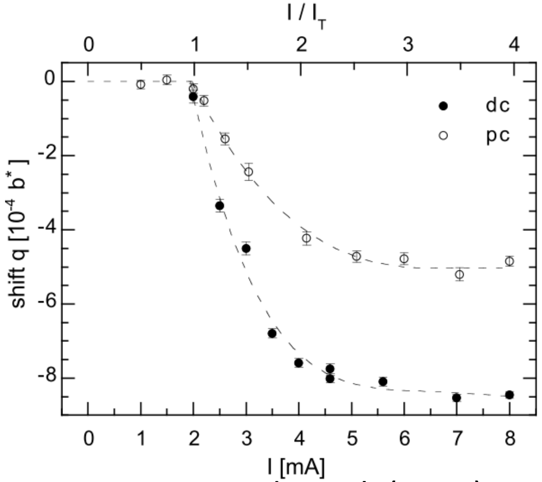


Satellite (0 1 0)+$\vec{q}_{cdw}$ at -1 mA



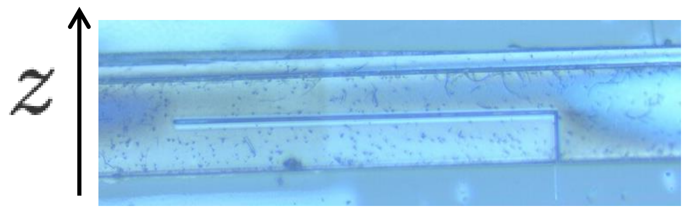






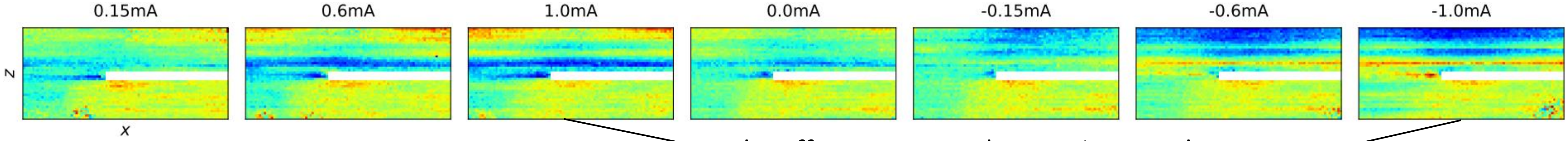
H. Requardt et al. (1998)

X-ray micro-diffraction of the quasi-1D NbSe3

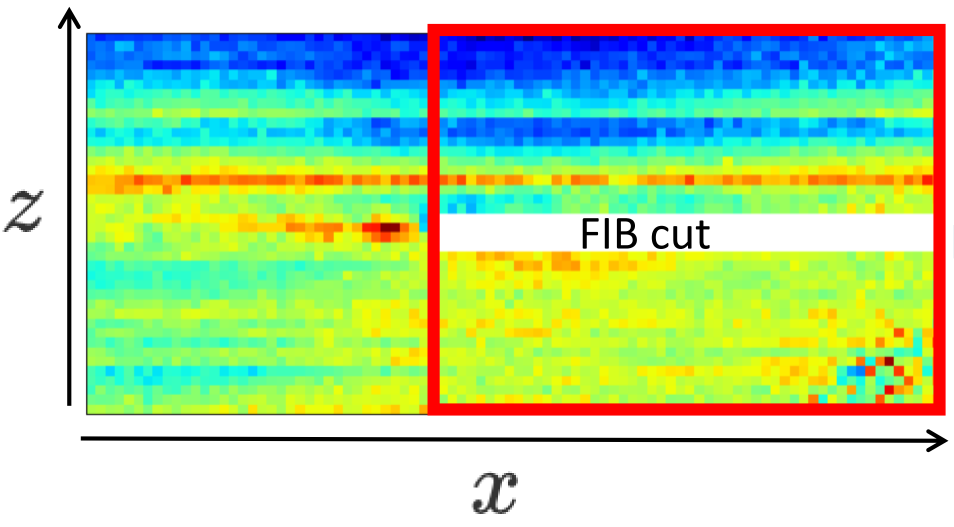


Transverse CDW deformation

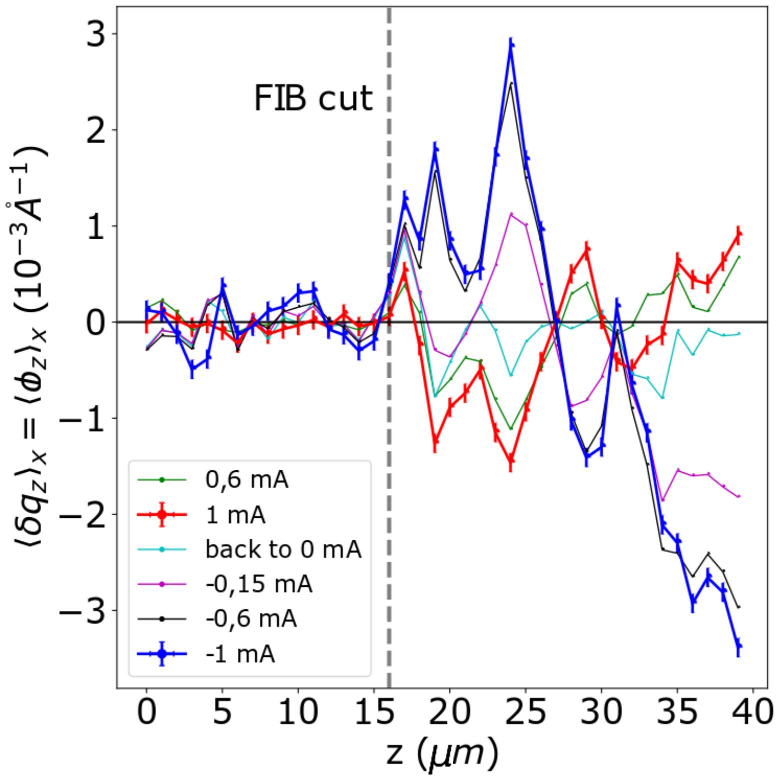
maps of $\delta q_z = \frac{\partial \phi}{\partial z}$ at different currents



The effect reverses when we inverse the current

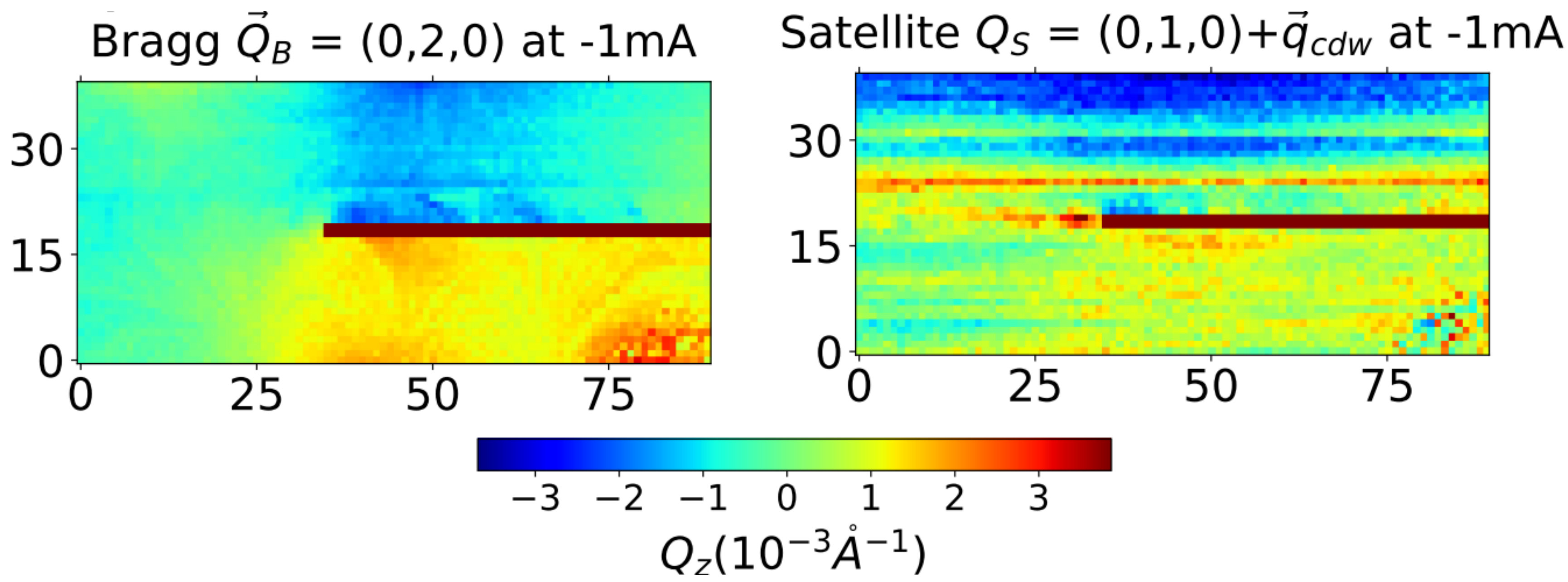


Average over x in the red region



X-ray micro-diffraction of the quasi-1D NbSe3

Transverse CDW deformation, why?



The same deformations are not observed on the Bragg.
Therefore, this is an evolution of the CDW only.

But why this happens?

$$F[\phi] \propto \int \left[c_x^2 \left(\frac{\partial \phi}{\partial x}\right)^2 + c_y^2 \left(\frac{\partial \phi}{\partial y}\right)^2 \boxed{+ c_z^2 \left(\frac{\partial \phi}{\partial z}\right)^2} + \eta E x \frac{\partial \phi}{\partial x} \right]$$

Transverse CDW deformations only increase the free energy

X-ray micro-diffraction of the quasi-1D NbSe3

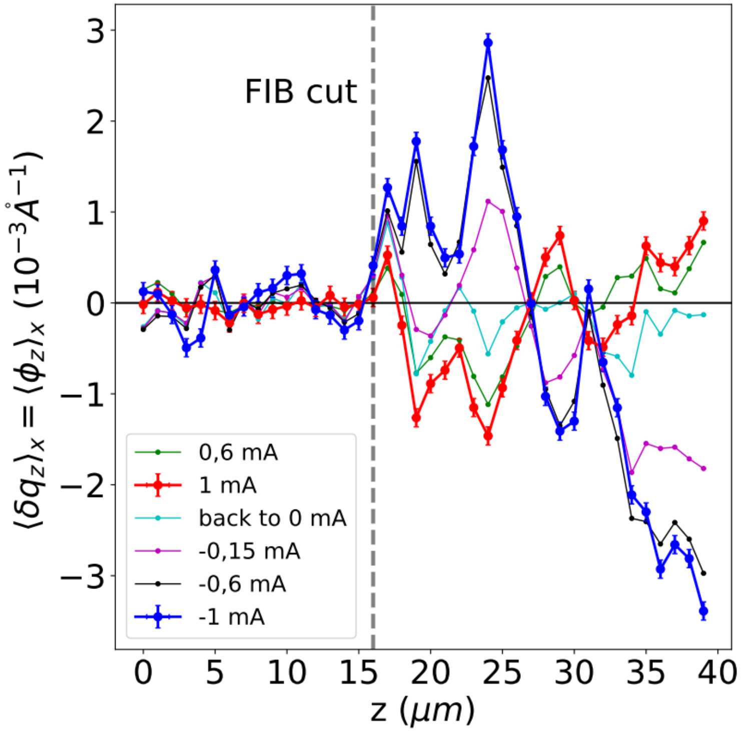
Discrete integration

$$\phi(z) = \sum_{z'<z} \frac{\partial \phi}{\partial z}(z')$$

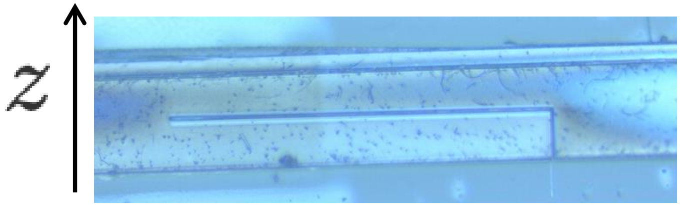
$$\phi(0) = 0$$

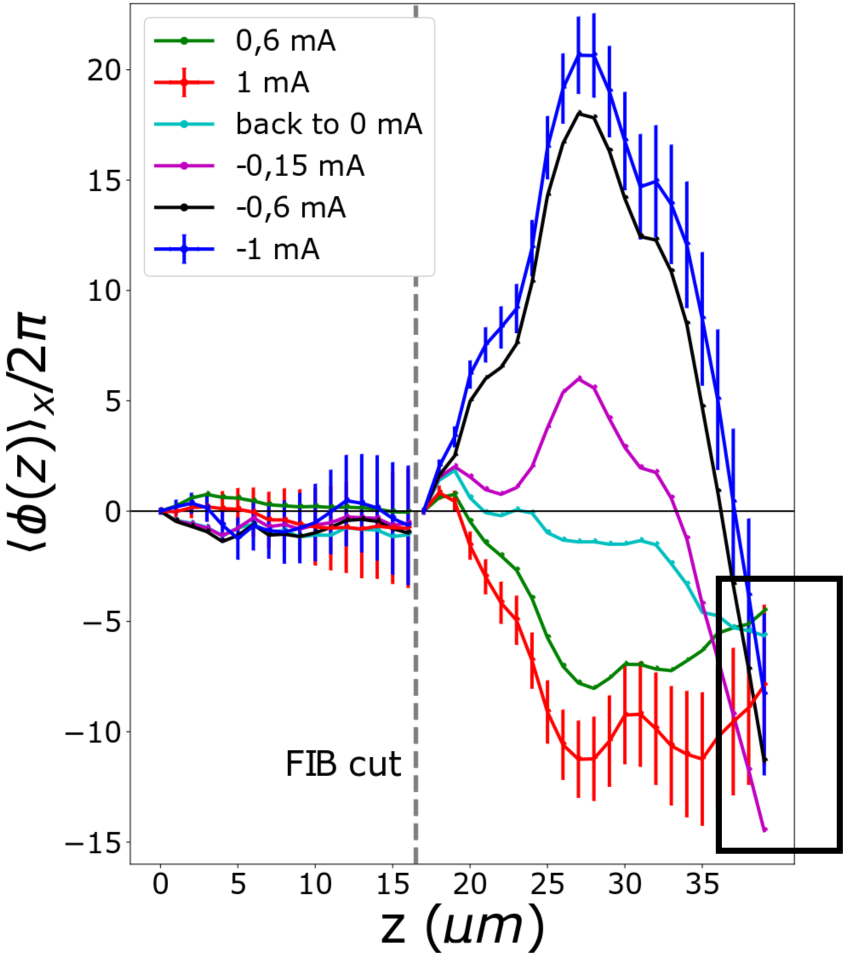
$$\phi(\text{upper border of the FIB cut}) = 0$$

Corresponding to $\dfrac{\partial \phi}{\partial z}$



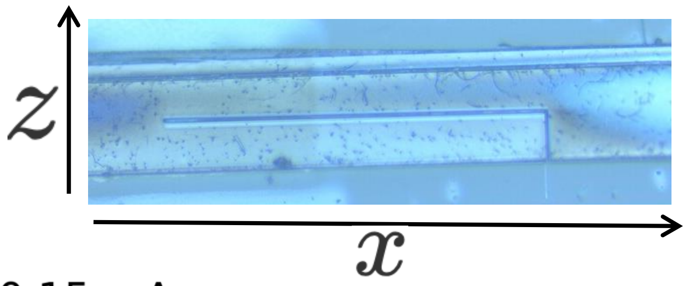
Phase reconstruction





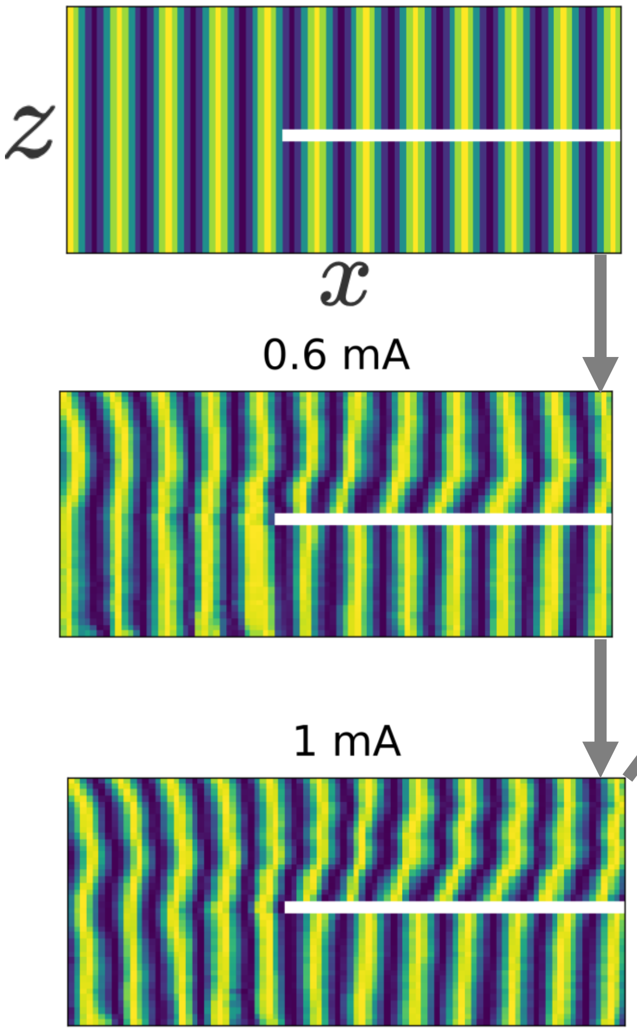
Surface pinning

X-ray micro-diffraction of the quasi-1D NbSe3

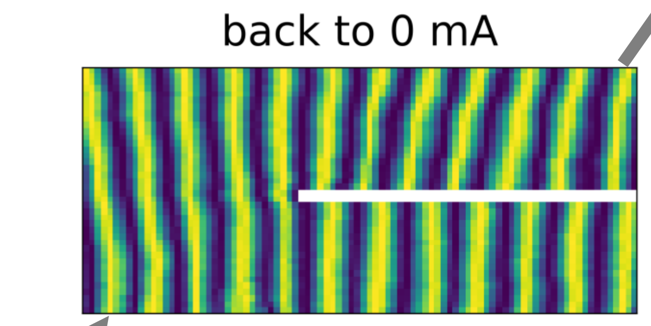


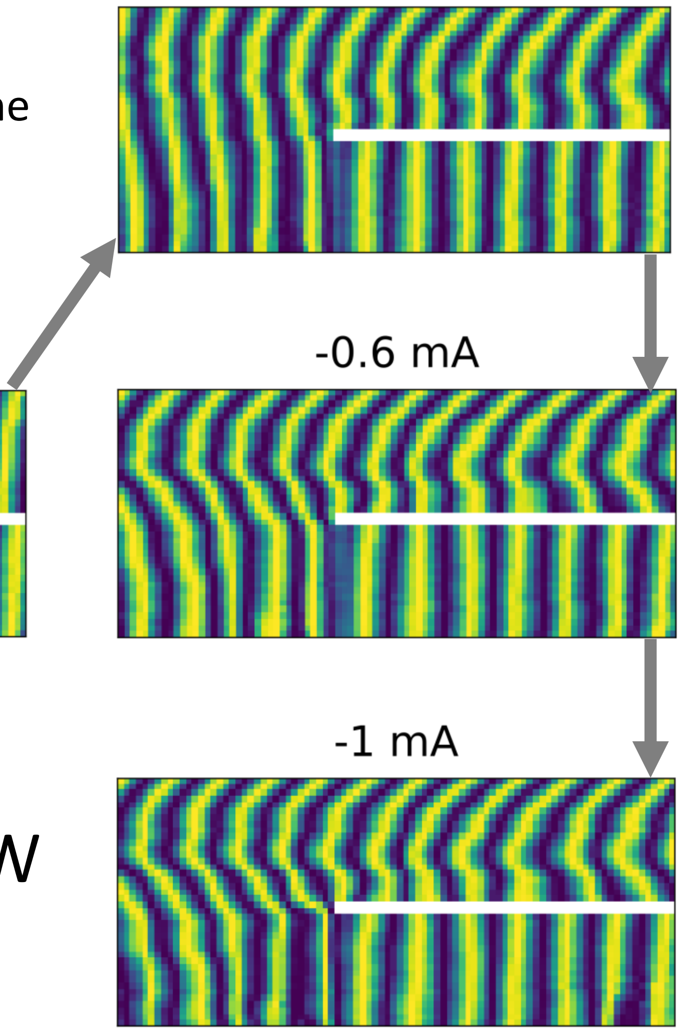
2D Phase reconstruction

$$\rho(x,z) = \cos\left[\frac{2\pi}{\lambda_{cdw}}x + \phi(x,z)\right]$$



Increased to observe the CDW deformation



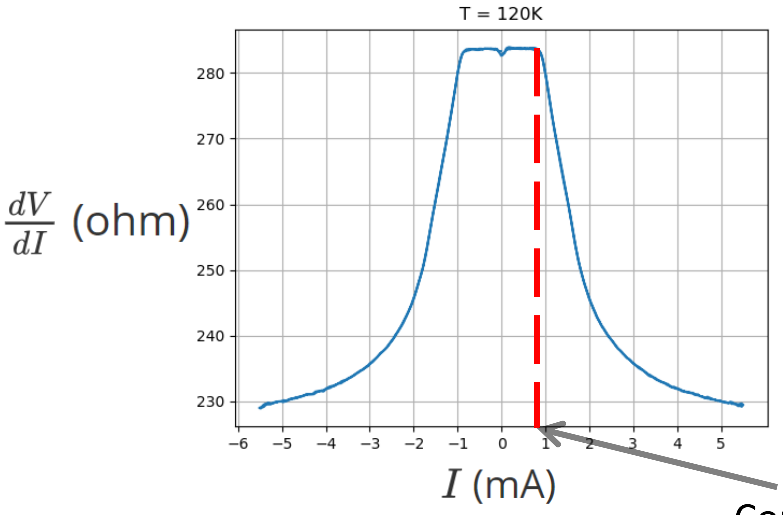


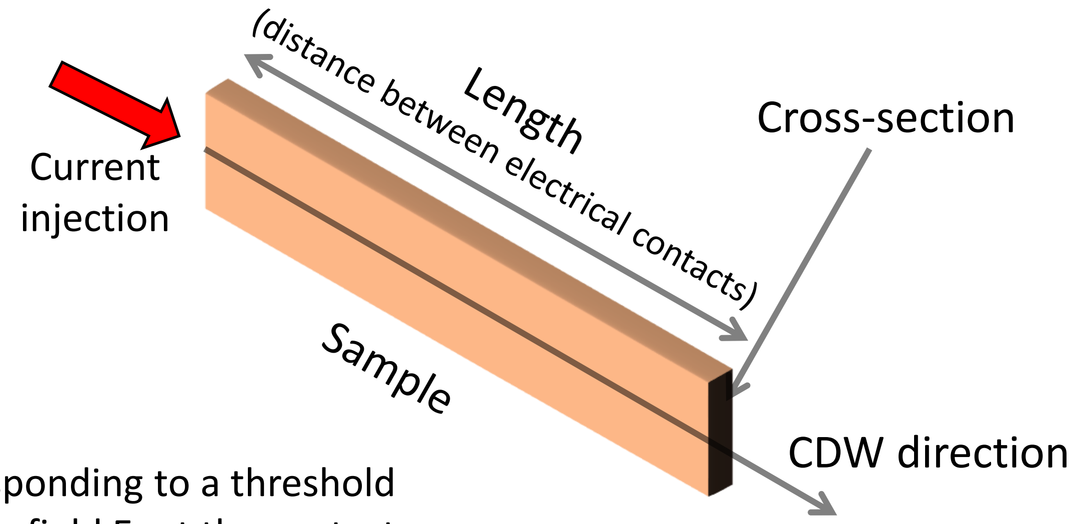
Sketch of the CDW under currents

Evidence of charge density wave transverse pinning by x-ray microdiffraction, E. Bellec et al., PRB (2020)

Solving the phase equation with surface pinning

Differential resistivity as function of current in $NbSe_3$





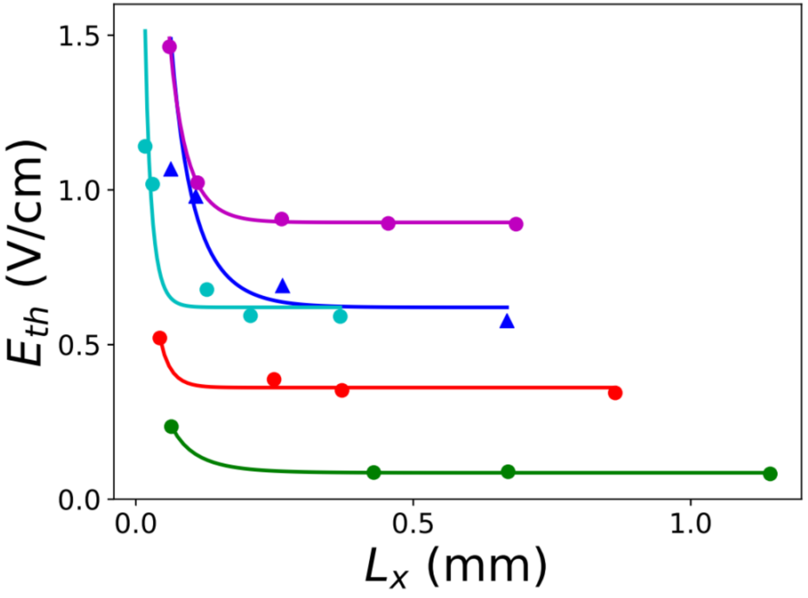
Corresponding to a threshold electric field E_T at the contact

Solve the CDW phase equation

$$\left(\Delta - \omega^2\right)\phi(\vec{r}) = E$$

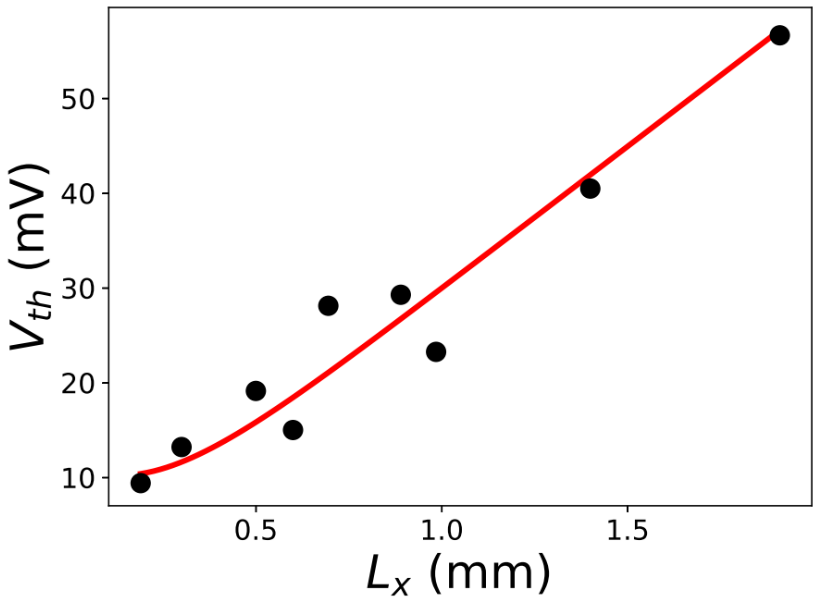
+

Surface pinning

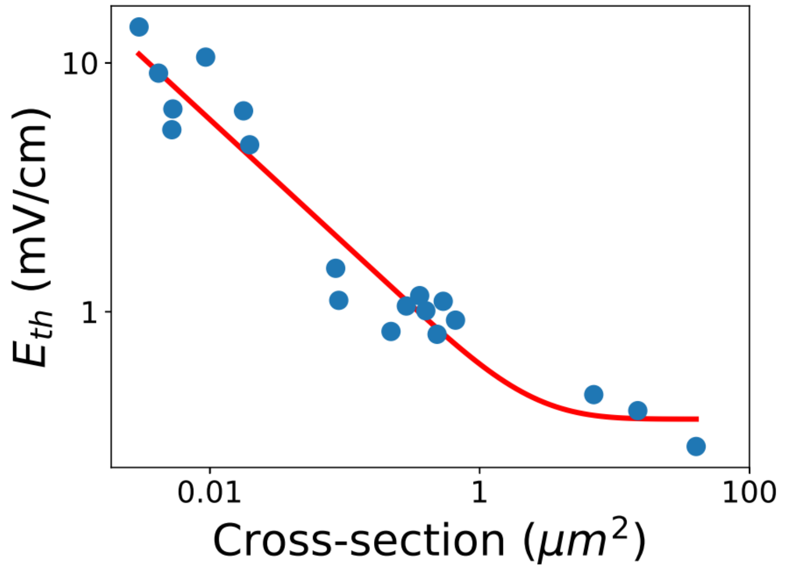


Dots : Prester PRB (1985) ($NbSe_3$)

Triangles : Mihaly et al. Solid State Communication (1983) (TaS_3)



Zettl and Gruner PRB (1984) ($NbSe_3$)



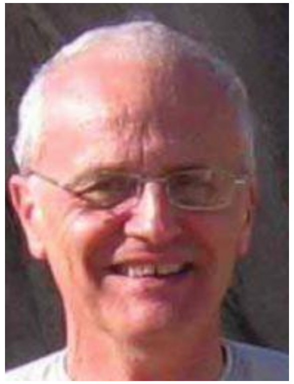
Borodin Physica B+C (1986) (TaS_3)

Aknowledgments

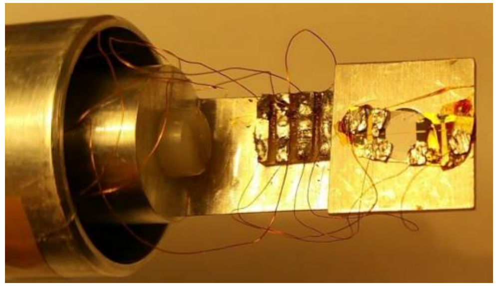
David Le Bolloc'h

Vincent Jacques

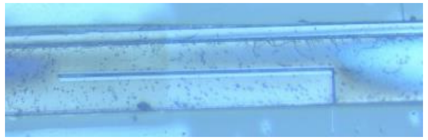
Isabel González Vallejo



Pierre Monceau

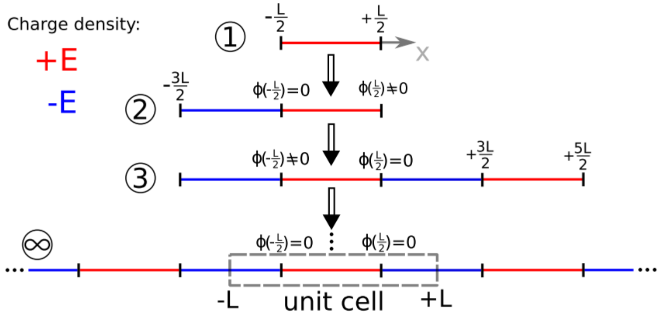


Alexander Sinchenko



Andrey P. Orlov

team LUTECE and PULS



Jonathan Caillaux
Gilles Abramovici

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Tobias Schulli
Steven Leake
Tao Zhou
Gilbert Chahine

Evidence of charge density wave transverse pinning by x-ray microdiffraction, E. Bellec et al., PRB (2020)

The essential role of surface pinning in the dynamics of charge density waves submitted to external dc fields, E. Bellec et al., Eur. Phys. J. B (2020)