Spatial studies of charge-density-wave deformations

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- Peierls transition, sliding CDW

- how to study, earlier studies

- X-ray diffraction on CDW deformation

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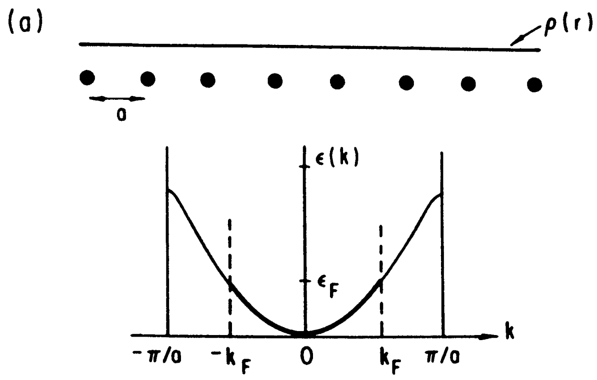
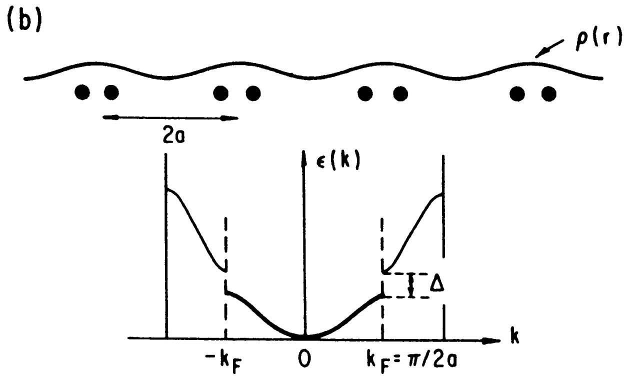
Peierls-model:





1D metallic chain with e^--phonon interaction:

unstable against modulation

=> charge-density-wave (CDW)

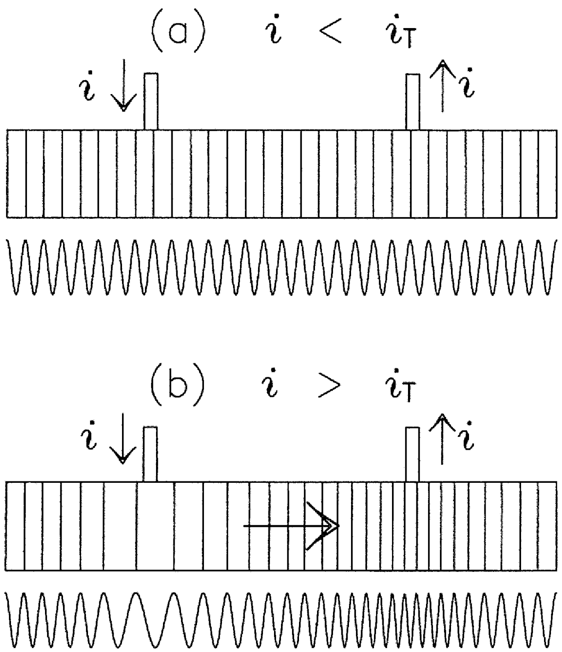
$$\rho(r) = \rho_0 + \Delta\rho \cdot \cos(2k_F r + \varphi)$$

defects: pinning of CDW phase φ

depinning by $E > E_T$

=> CDW slides, non-linear current

Sliding CDW:



(Fig.: Adelman et al., PRB **53** (1996) 1833)

- creation/annihilation of wavefronts at current contacts

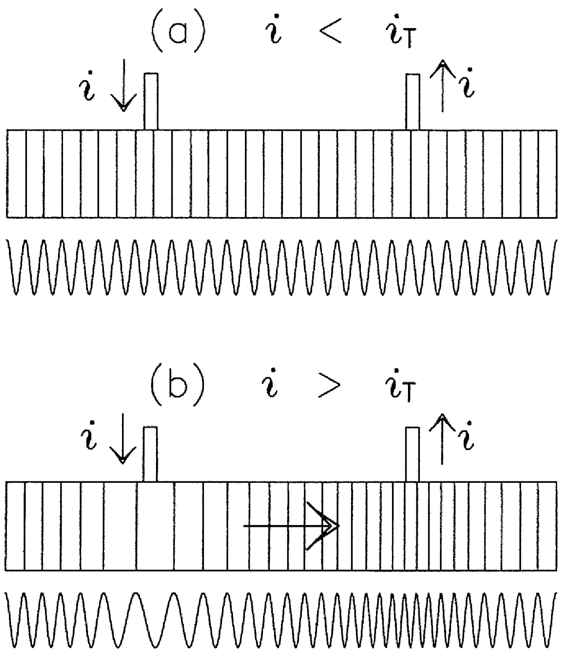
- conversion required:

normal current ⇔ condensed (CDW) current

=> phase slip

CDW elastically & plastically deformed

“How to study?”, “What to study?”



(Fig.: Adelman et al., PRB **53** (1996) 1833)

phase slip / current conversion located near current contacts

=> spatial dependence of CDW current:
$j_{CDW}(x)$

=> adding/removing CDW wavefronts:

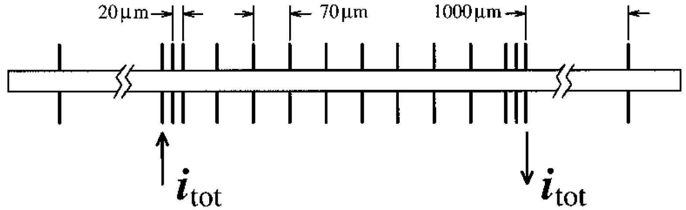
spatial dependence of CDW phase and

CDW wavelength:

$$Q_{CDW}(x) = Q_0 + q(x)$$

$$q(x) \propto \nabla\varphi$$

a) electrical (multi-contact):



(Fig.: Adelman et al., PRB **53** (1996) 1833)

Measurement: V(x) between neighboring contacts => E(x) and j_{CDW}(x)

examples:

j_{CDW}(x) in $NbSe_3$

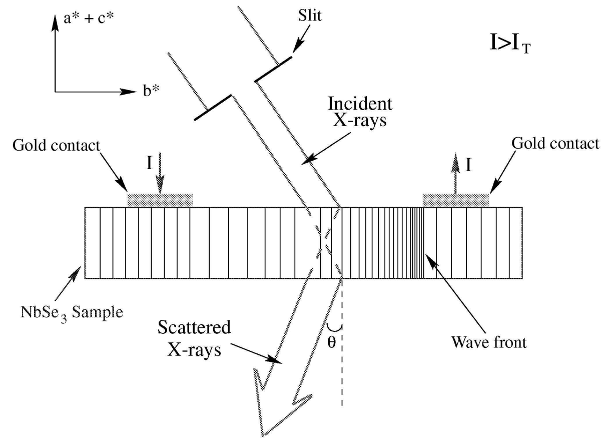
(Adelman et al., PRB **53** (1996) 1833)

E(x) in $K_{0.3}MoO_3$

(Itkis et al., J.Phys. Cond.Matter **5** (1993) 4631)

b) “radiation”:

X-ray diffraction



(Fig.: Rideau et al., EPL **56** (2001) 289)

Measurement: precise q(x) of CDW-satellite reflection using narrow beam

examples: $NbSe_3$ DiCarlo et al., PRL **70** (1993) 845

Requardt et al., PRL **80** (1998) 5631

but also: IR-transmission

Measurement: integral IR-transmission through sample using narrow beam (30µm)

example: $K_{0.3}MoO_3$

Itkis et al., PRB **52** (1995) R11545,

Synth. Metals **86** (1997) 1959

1^{st} example: IR-transmission, $K_{0.3}MoO_3$ (Itkis et al.)

integral IR-transmission $\tau(x)$, T=98K
changes by $\Delta\tau$ (x) when CDW is sliding

$$(\Delta\tau / \tau) \propto \nabla\varphi$$

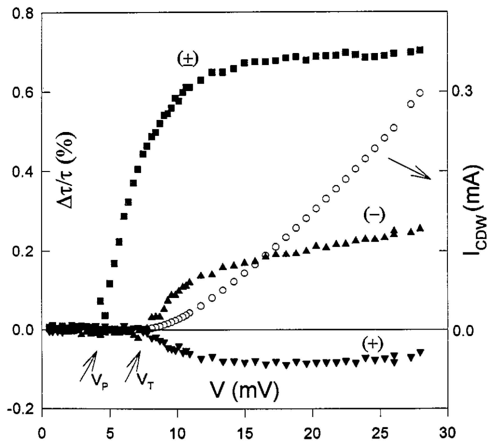
$\Delta\tau / \tau$ changes strongest near contacts

applying unipolar (+,-) and bipolar (±) pulses:

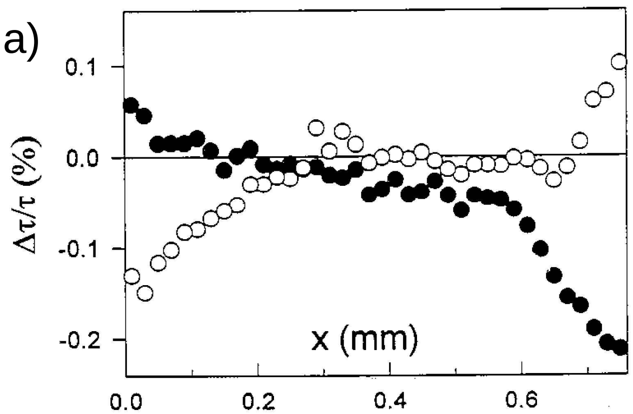
unipolar (a,b) => CDW slides when depinning at contacts

bipolar (b,c) => CDW depins first in bulk (V_P), then at contacts (V_T) and slides

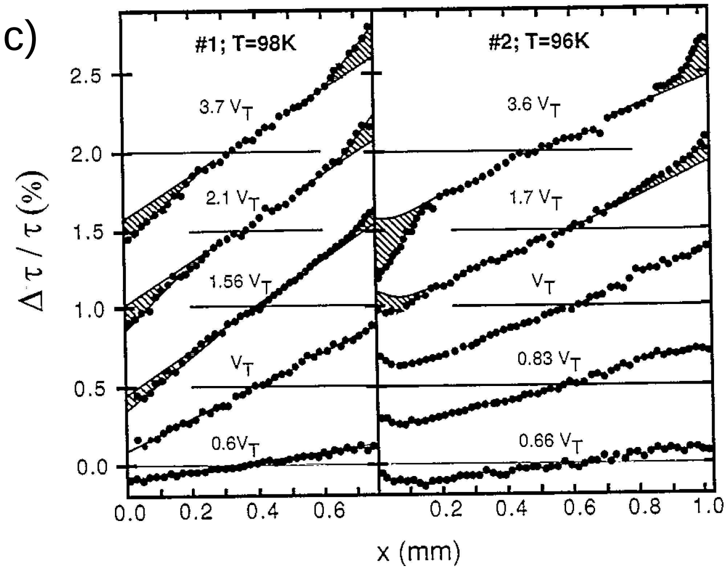
b)



a)

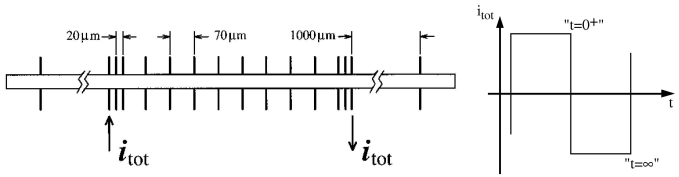


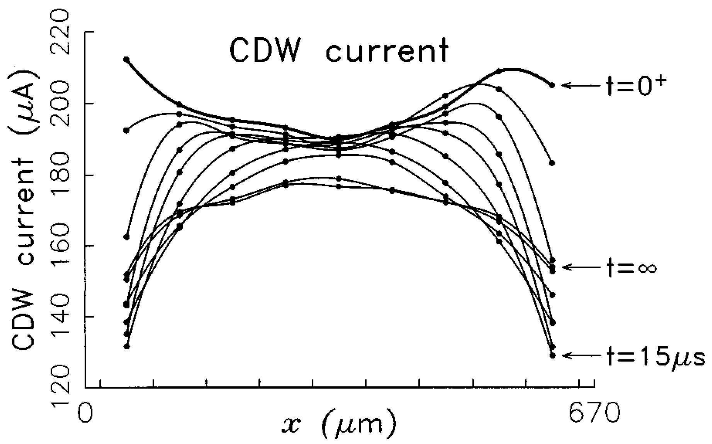
c)



Figs.: Itkis et al., Synth. Metals **86** (1997) 1959

2^{nd} example: CDW-current j_{CDW}, $NbSe_3$ (Adelman et al.)





Spatially dependend voltage and resistivity measurements, T=90K

=> CDW current $j_C(x)$ and CDW-deformation $\nabla\varphi(x)$

equations start with:

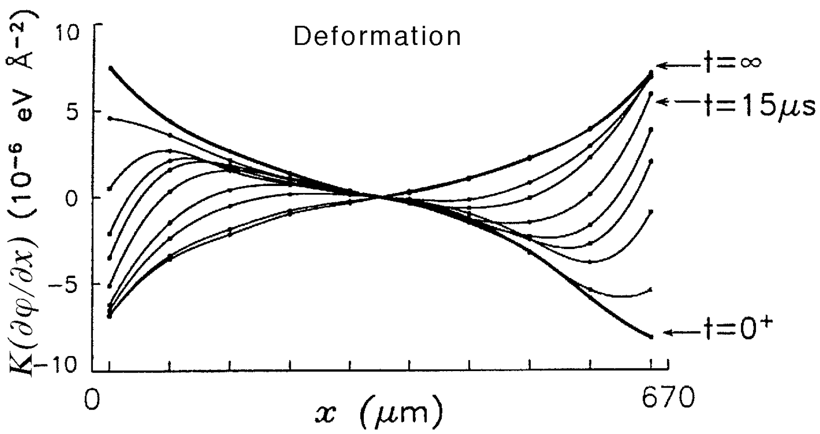
Forces: $$\gamma\frac{\partial\varphi}{\partial t}=\left(\frac{en_C}{Q}\right)\cdot(E-E_P)+K\cdot\left(\frac{\partial^2\varphi}{\partial x^2}\right)$$

Strain: $$\varepsilon=\frac{1}{Q}\cdot\frac{\partial\varphi}{\partial x}$$

Phase slip rate (homogeneous nucleation):

$$r_{PS}(x)=r_0\cdot\exp\left(-\frac{en_C}{Q}\cdot\frac{V_a}{2QK\varepsilon(x)}\right)$$

$$\boxed{i_C=\frac{1}{\rho_C+\rho_S}\cdot\left(\rho_S i_{tot}-E_P(i_C)+\left(\frac{en_C}{Q}\right)^{-1}K\frac{\partial^2\varphi}{\partial x^2}\right)}$$



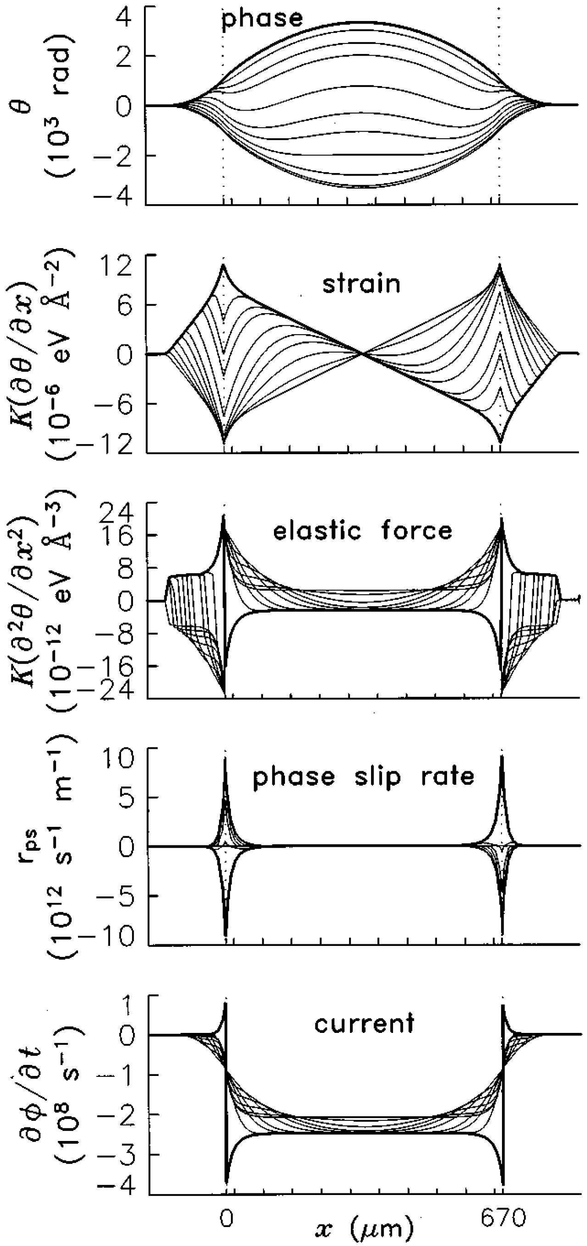
Figs.: Adelman et al., PRB **53** (1996) 1833

Adelman et al.:

taking parameters from experimental data $i_C(t,x)$ and equations

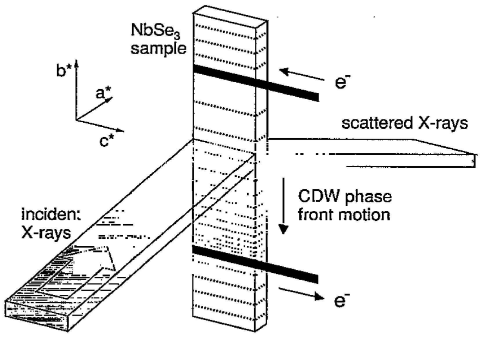
=> **Simulation of $i_C(t,x)$, $r_{PS}(t,x)$, Ñj (t,x) and j (t,x)**

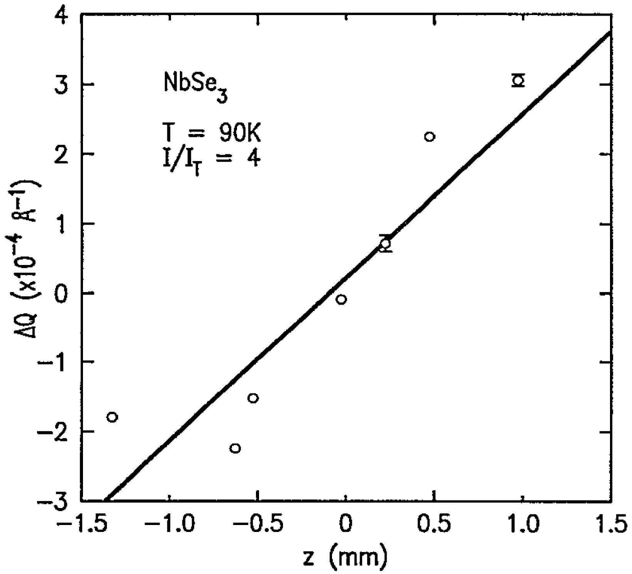
=> CDW deformation essentially linear between current contacts with small nonlinear contribution due to phase slip; phase slip takes place in a very narrow section around current contacts



3rd example: X-ray diffraction, $NbSe_3$

1st study by DiCarlo et al. (PRL **70** (1993) 845) :





monitor shift ΔQ of CDW-satellite position Q along z (|| **b***) applying depinning pulsed current

beam width: 800μm

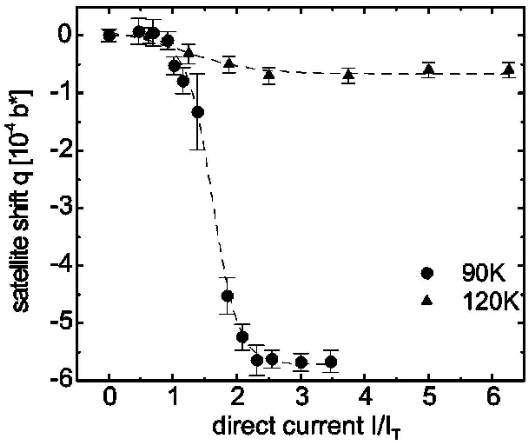
no data very close to current contacts

compare data with linear model by Ramakrishna et al. (PRL **68** (1992) 2066):

$$\Delta q(z) = \frac{\partial \varphi}{\partial x} = \frac{e\rho_C}{QK_Z} \cdot V_{PS} \cdot \frac{z}{L}$$

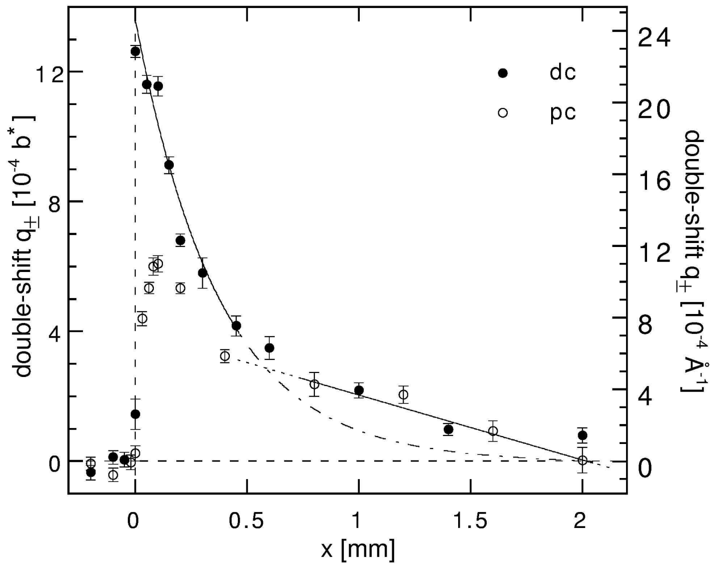
2^{nd} study by Requardt et al. (PRL **80** (1998) 5631) :

- applying *dc* signal for steady state measurements on $NbSe_3$
- pulsed current (*pc*) data for comparison
- beam width 30-100µm
- data from sample centre to beyond contact boundary



CDW satellite shift $q = Q_{CDW}-Q_0$

x=100µm from contact boundary



90K, $I = 2.13 \cdot I_T$, $q_\pm = Q_{CDW}(I>0)-Q_{CDW}(I<0)$

2 regimes in *dc* q(x)-profile:

- exponential decay from contact boundary to $x \approx 0.5$

length scale: 375±50µm

- linear decrease for $x > 0.7$

Brazovskii-model (PRB **61** (2000) 10640) , interpretation of results from Requardt et al.

considers disbalance between:

- condensed (CDW-) charge carriers (density n_{CDW}=(1-ρ_i(T))n_i) and
- non-condensed, "normal" charge carriers (density n_e)

μ_n = chem. potential of normal carriers

$$U = \left(\frac{1}{\pi}\nabla\varphi\right) \Big/ N_F^i + \Phi$$ stress of CDW

(Φ = potential from external electrical field,

N_F^i = DOS of "condensible" charge carriers)

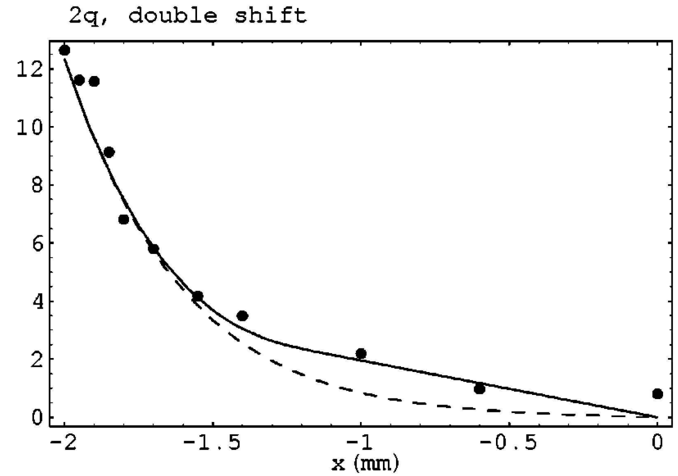
$$\boxed{\eta = \mu_n - U \propto q}$$

further "ingredient" of model:
carrier conversion $r_{PS}(\eta) = \nabla j_{CDW}$

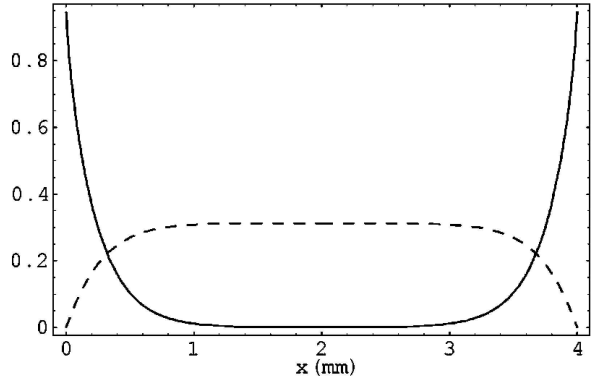
- homogeneous: $r_{PS} \propto \exp(-\eta_0/|\eta|)$
- heterogeneous: e.g. $r_{PS} \propto \eta$
- "active": $r_{PS} \propto j_{CDW}$

assuming heterogeneous and active conversion:

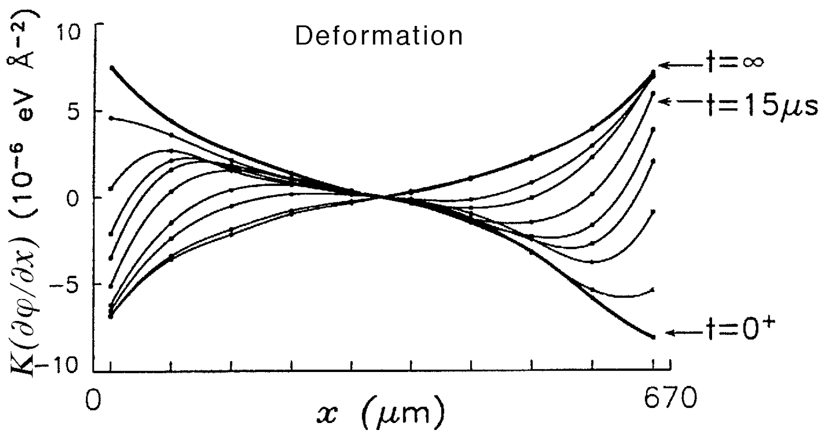
linear regime: assuming piining of lateral growth of CDW wavefronts/dislocation loops

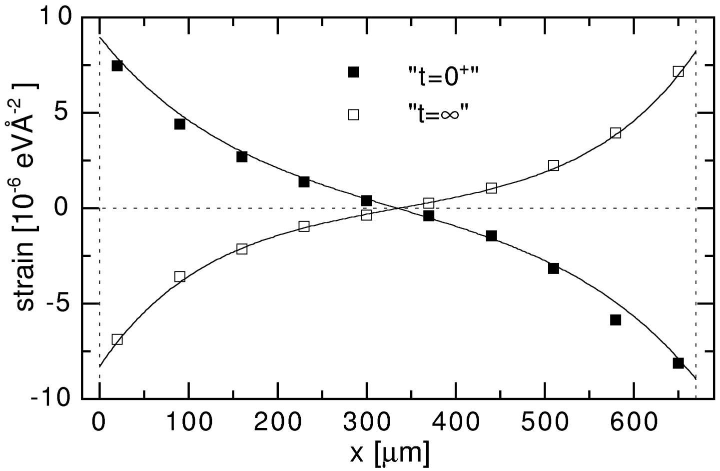


CDW current- and electrical field profile:



Brazovskii-model, application to multi-contact data by Adelman et al.:





“short sample”

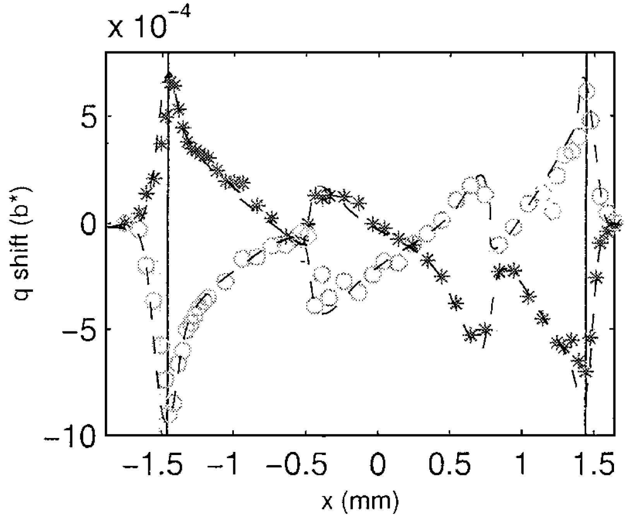
overlap of the two exponential decays coming from the two current contacts

$$\nabla\varphi \propto \exp\left(-\frac{x}{l}\right) - \exp\left(-\frac{L-x}{l}\right)$$

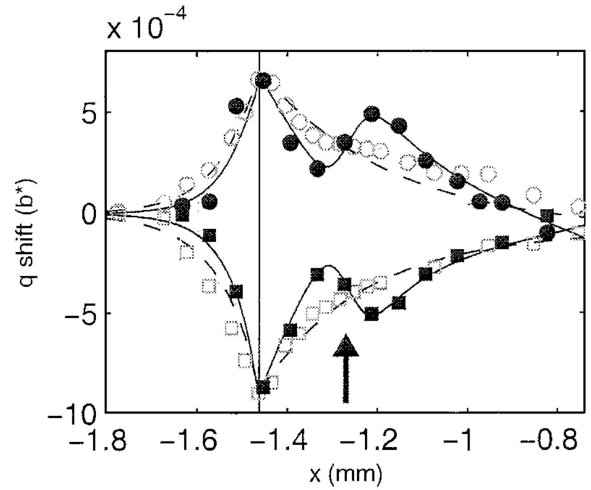
length scale: l = 140±20μm

study by Rideau et al. (EPL **56** (2001) 289: CDW-deformation near defects

$NbSe_3$, T=90K, beam width: 20µm



- current contact very narrow (15µm): region beyond contact not "shunted" but with observable deformation q $(\nabla\varphi)$
- very steep decay of CDW deformation away from contact towards sample centre
- but at x ≈ –0.5 and ≈ 0.85 significant deformation: sign of resumed current conversion to maintain charge transport across defect



- X-ray irradiation (30µm beam width) induced defect (arrow) gives rise to additional CDW deformation

=> additional current conversion centre

length scale of effect on deformation: 75µm

Conclusion

- spatial dependences in CDW observed by various methods:

CDW-current profile, IR-transmission = indirect methods for CDW-strain measurements

high-resolution X-ray diffraction = direct observation of CDW-strain

- $NbSe_3$: current injection/extraction gives rise to CDW-deformation, decaying exponentially with distance from contact

- $NbSe_3$: CDW-deformation seems to be well described by Brazovskii-model

CDW-deformation due to charge disbalance

heterogeneous phase slip/current conversion

- defects and current contacts play similar role:

centres of current conversion, charge disbalance