International School on Aperiodic Crystals

26 September - 2 October 2010, Carqueiranne, France

Charge-density-wave crystals

Sander van Smaalen

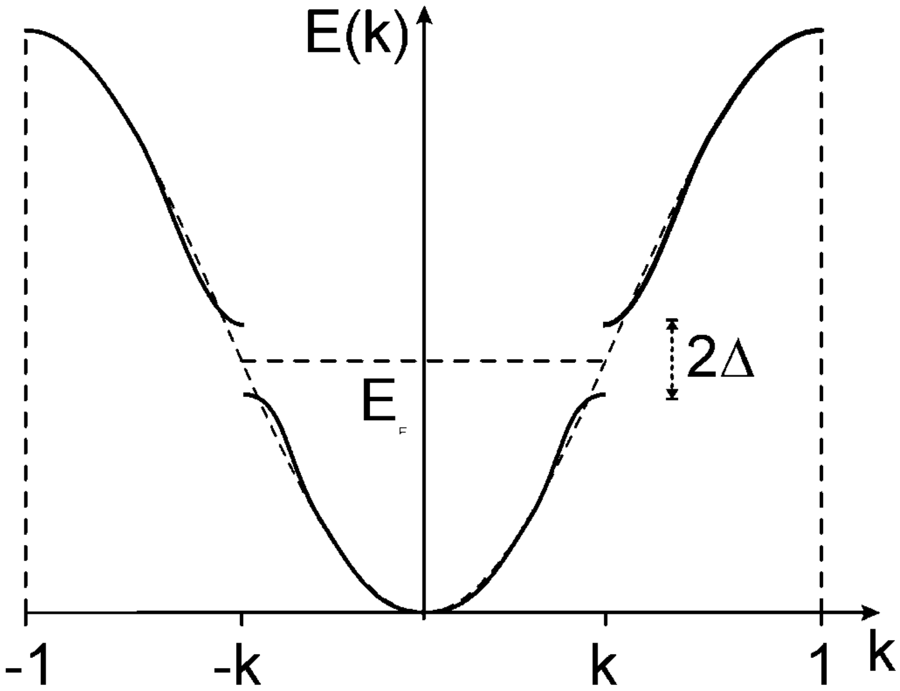
Laboratory for Crystallography

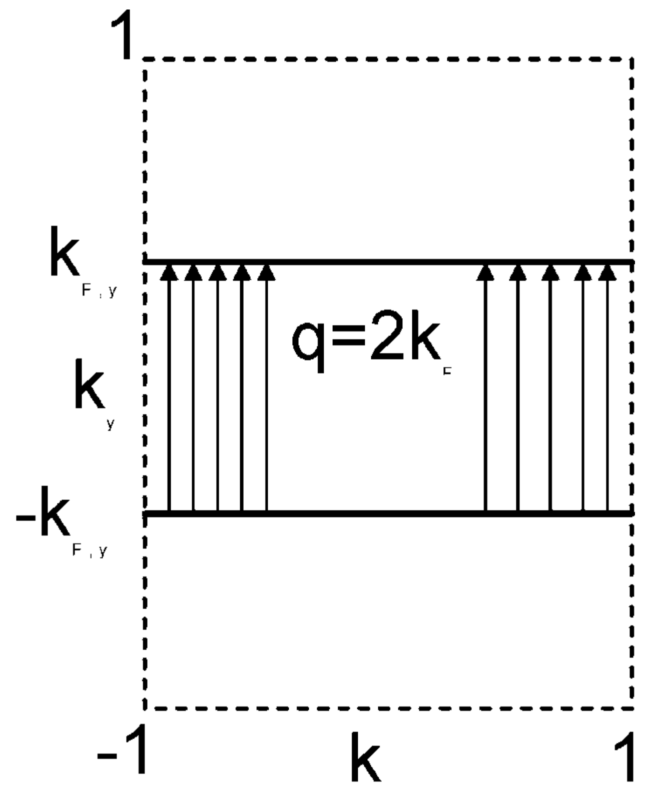
University of Bayreuth

Germany

Disclaimer and copyright notice

The charge-density-wave (CDW) instability

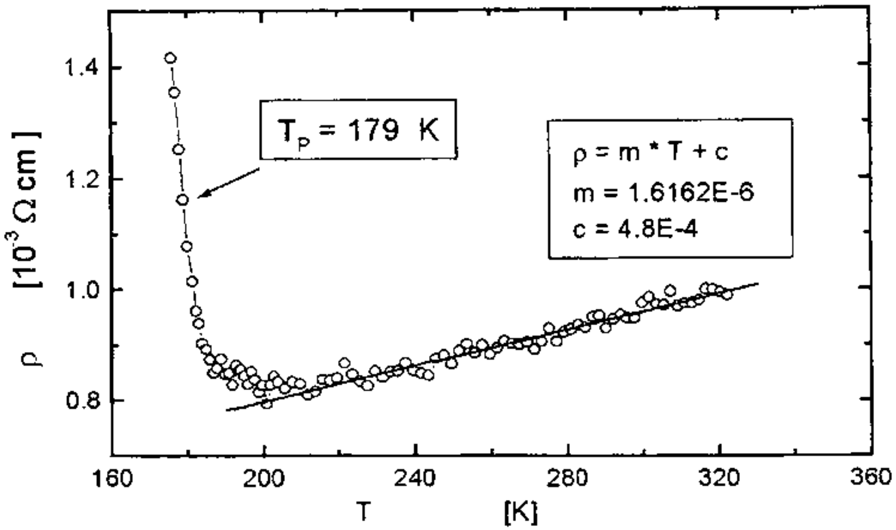


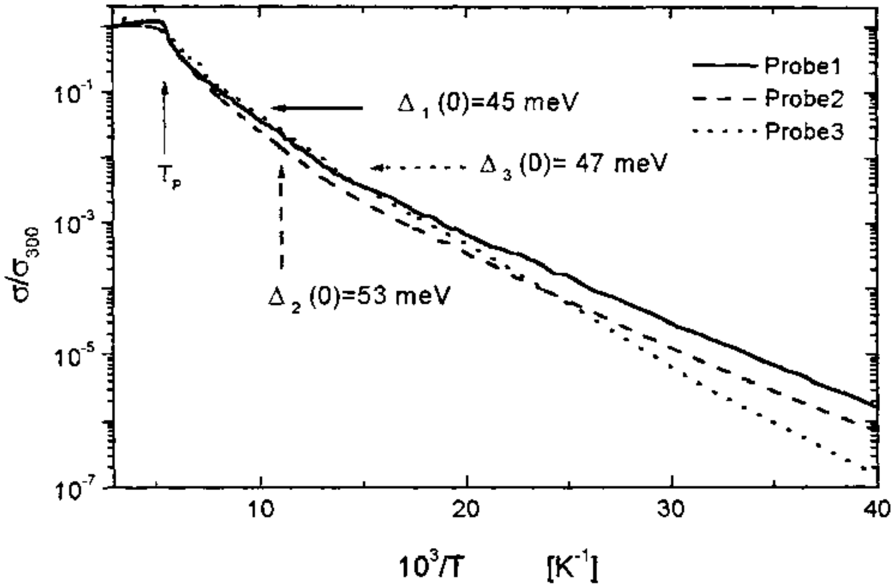


- Electron – phonon coupling
- Metal – Insulator transition

- Fermi surface nesting
- $2k_F$ is incommensurate

The electrical conductivity against temperature





Metal-Insulator transition

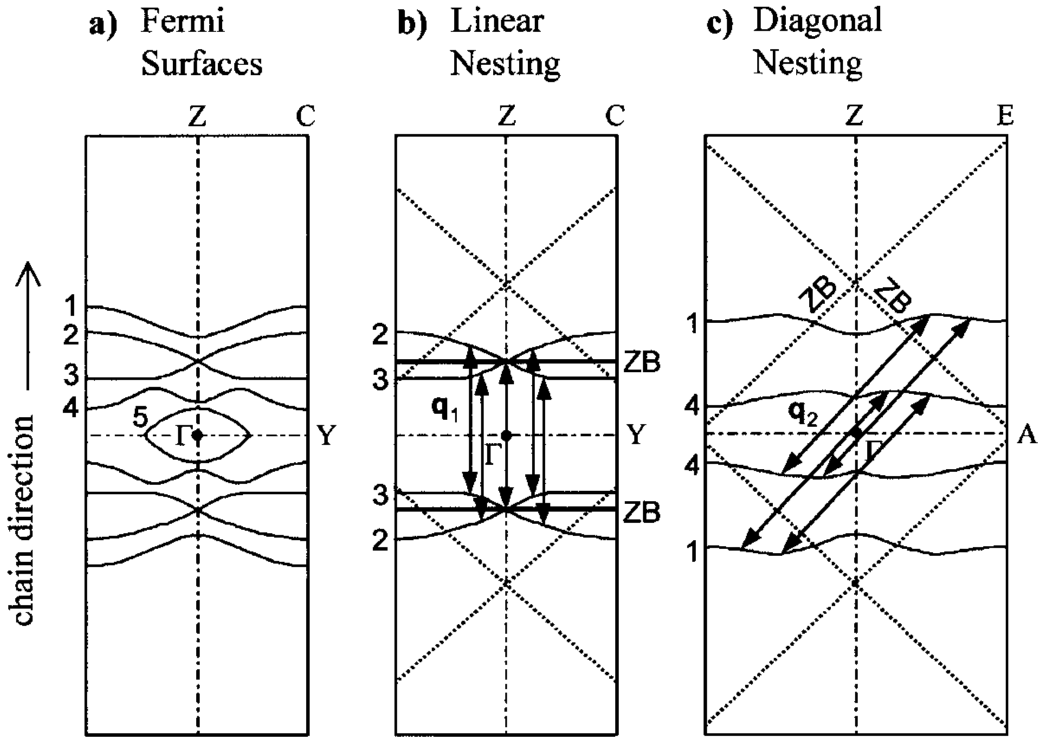
Gap at the Fermi surface

Semiconductor

$K_{0.3}MoO_3$ blue bronze

K. Hosseini (2000) Ph.D.-thesis, University of Bayreuth.

Nesting of Fermi surfaces in real compounds



$NbSe_3$

T_{c1} = 145 K

$\mathbf{q}^1 = (0, 0.241, 0)$

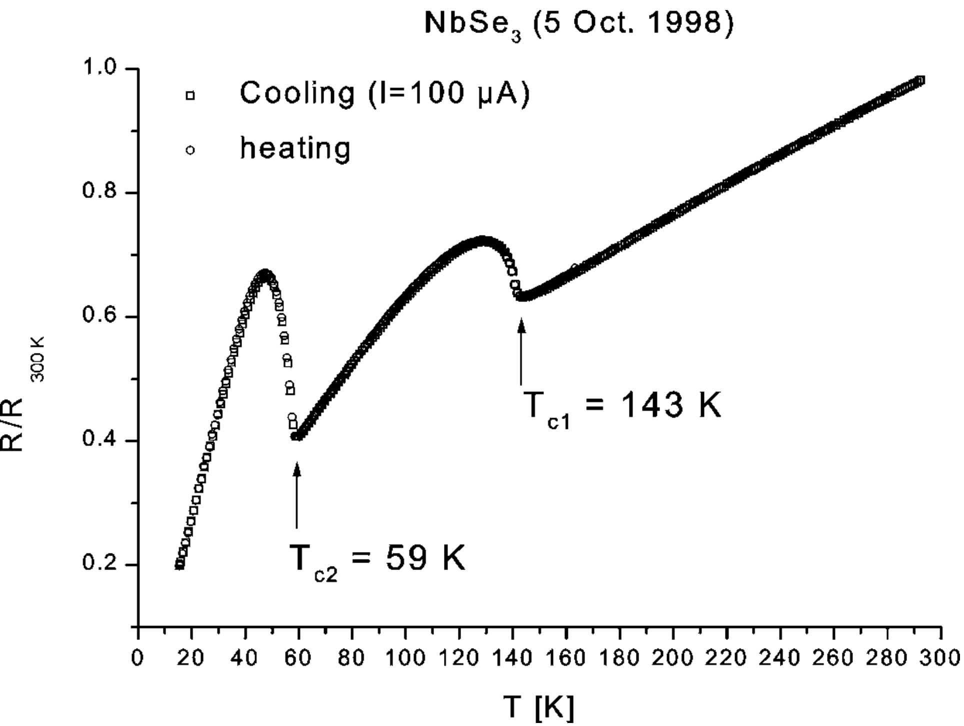
T_{c2} = 59 K

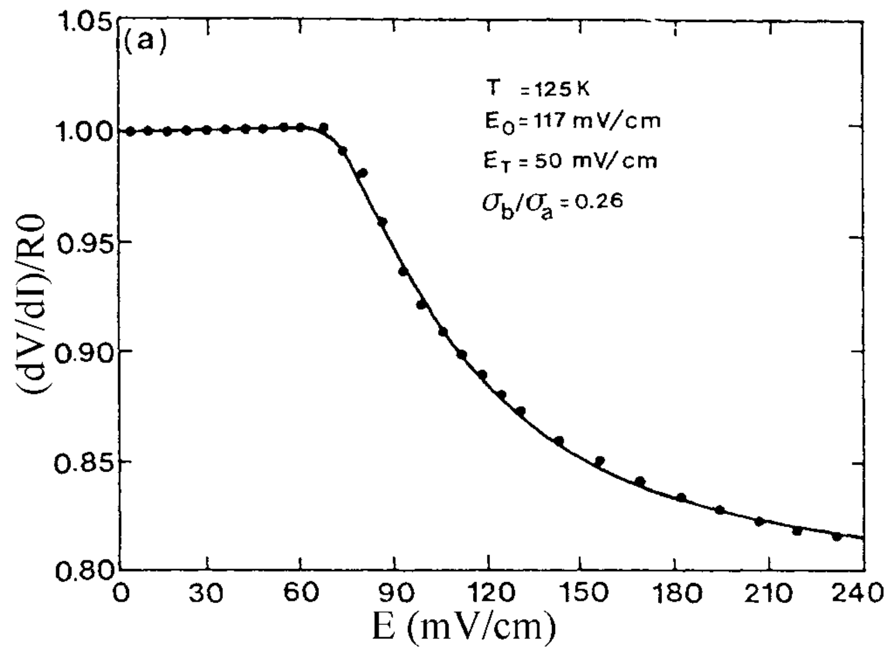
$\mathbf{q}^2 = (0.5, 0.261, 0.5)$

Lowering of electronic energy requires atomic modulations

J. Schafer *et al.*, Phys. Rev. Lett. **87**, 196403 (2001)

Anisotropic and non-linear conductivities





$NbSe_3$ — R(**b**) : R(**c**) = 1 : 14

CDW is incommensurate along **b**

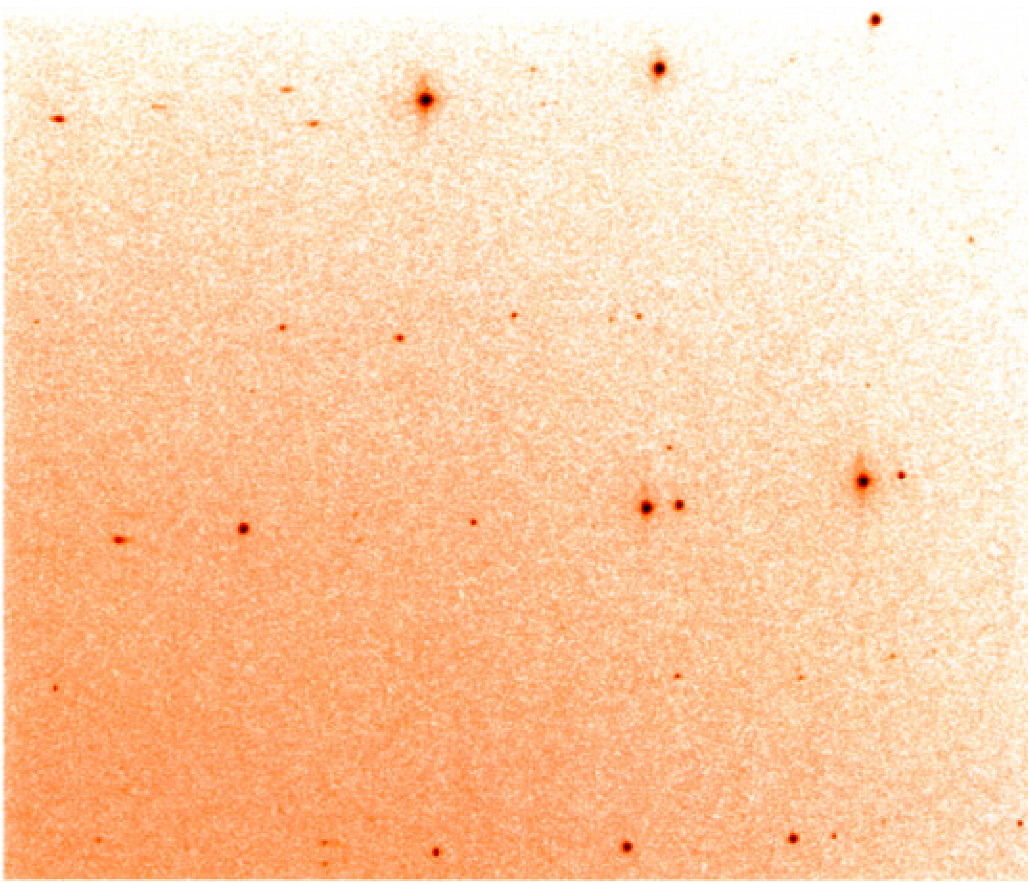
Sliding of pinned CDW

compare phason

N.P. Ong & J.W. Brill, Phys. Rev. B **18**, 5265 (1978)

R. M. Fleming, Phys. Rev. B **22**, 5606 (1980)

X-ray diffraction by the CDW of $NiTa_2Se_7$



$(h\ 3\ l)$

$(h\ 2{+}1/2\ l)$

$(h\ 2\ l)$

$(h\ 1{+}1/2\ l)$

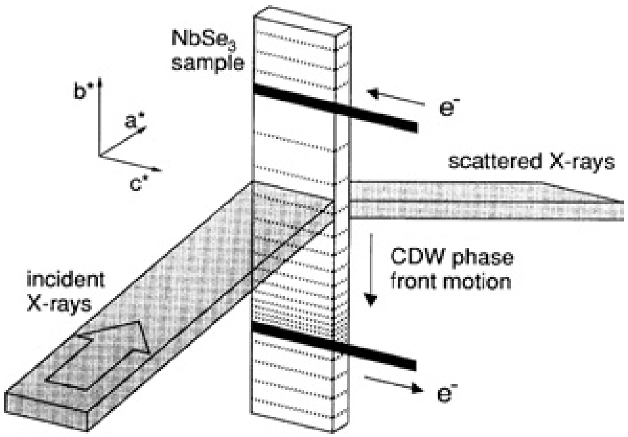
$(h\ 1\ l)$

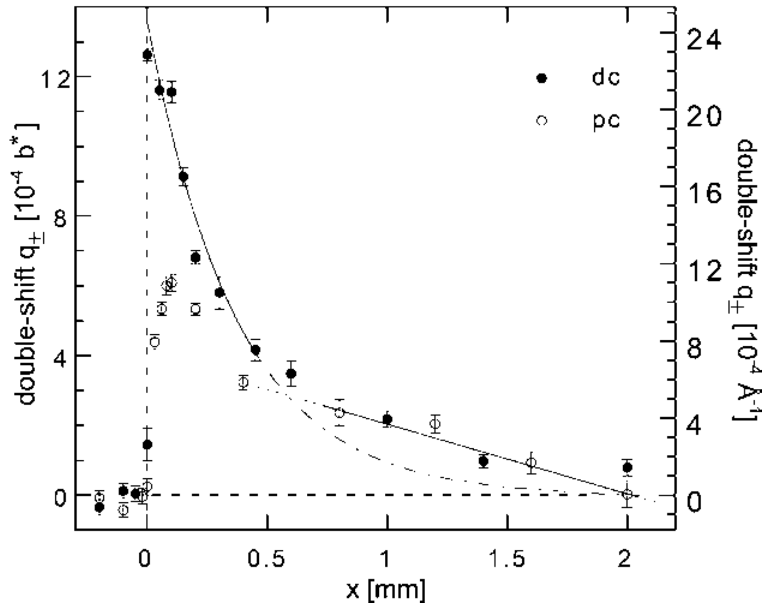
$$\mathbf{S} = h\,\mathbf{a}^* + k\,\mathbf{b}^* + l\,\mathbf{c}^* + m_1\,\mathbf{q}^1 + m_2\,\mathbf{q}^2 + \cdots$$

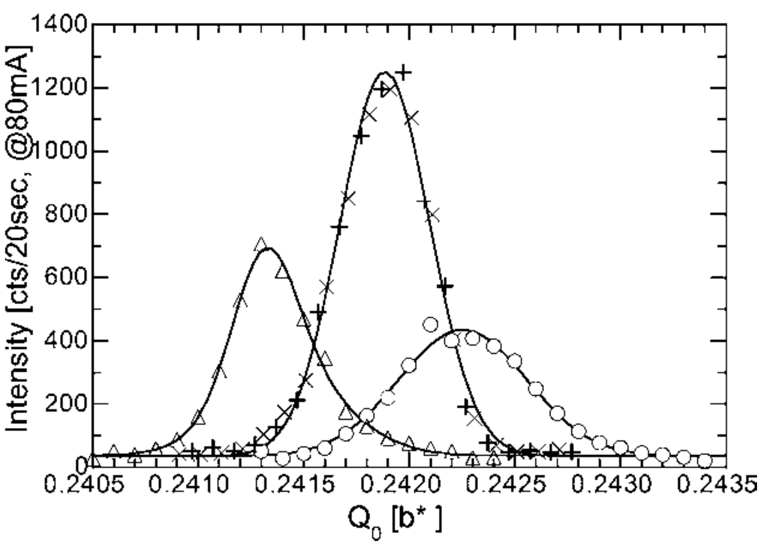
$$\mathbf{q} = \sigma_1\mathbf{a}^* + \sigma_2\mathbf{b}^* + \sigma_3\mathbf{c}^* \qquad \mathbf{q} = 0.483\,\mathbf{b}^*$$

A. Spijkerman *et al.*, Phys. Rev. B **52**, 3892 (1995)

Deformation of the sliding CDW in $NbSe_3$







Conversion from electronic to sliding-CDW current

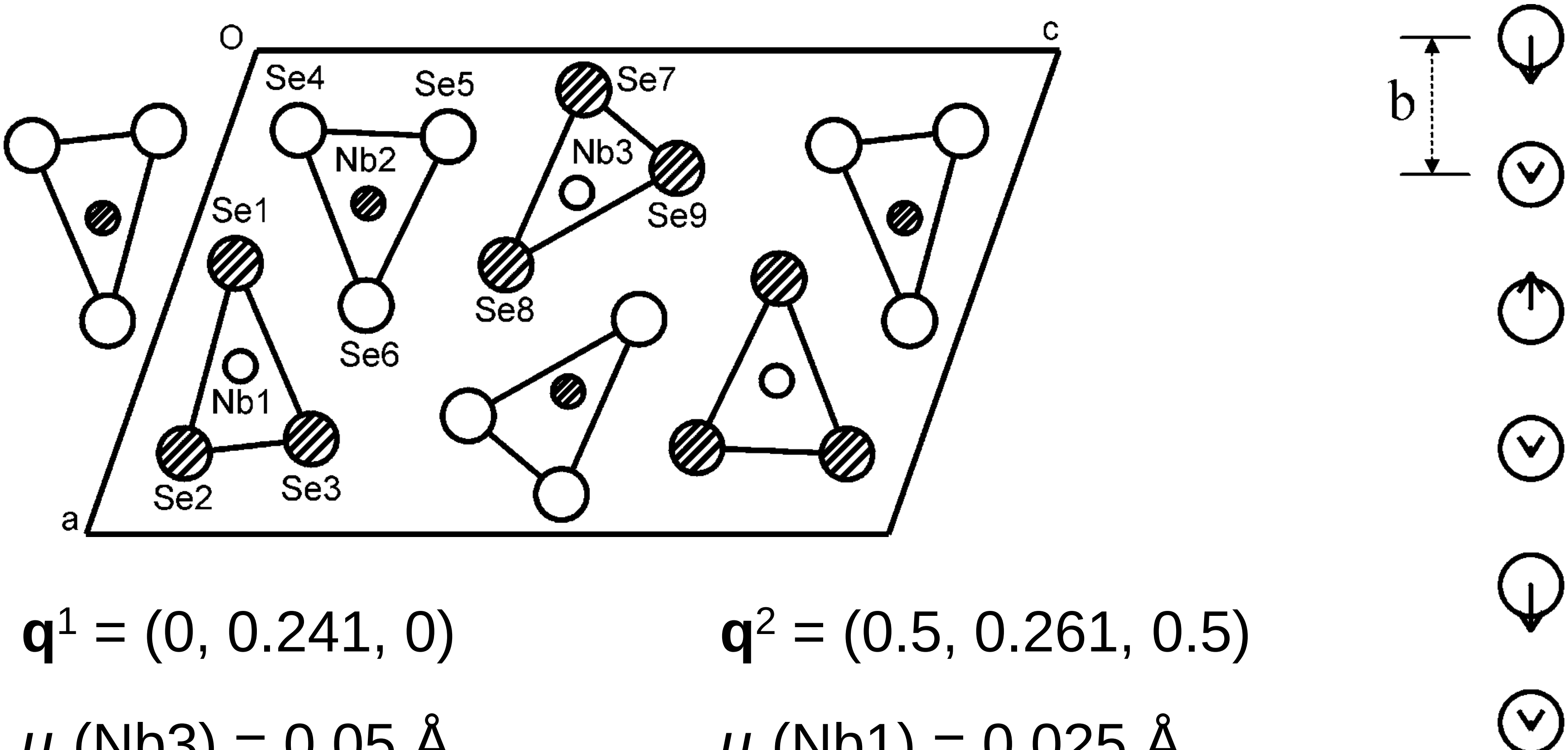
$$j_{tot} = j_e + j_i + j_{CDW}$$

$$\rho_{CDW} + \rho_i = 1$$

D. DiCarlo *et al.*, Phys. Rev. Lett. **70**, 845 (1993)

H. Requardt *et al.*, Phys. Rev. Lett. **80**, 5631 (1998)

Incommensurately modulated structure of $NbSe_3$



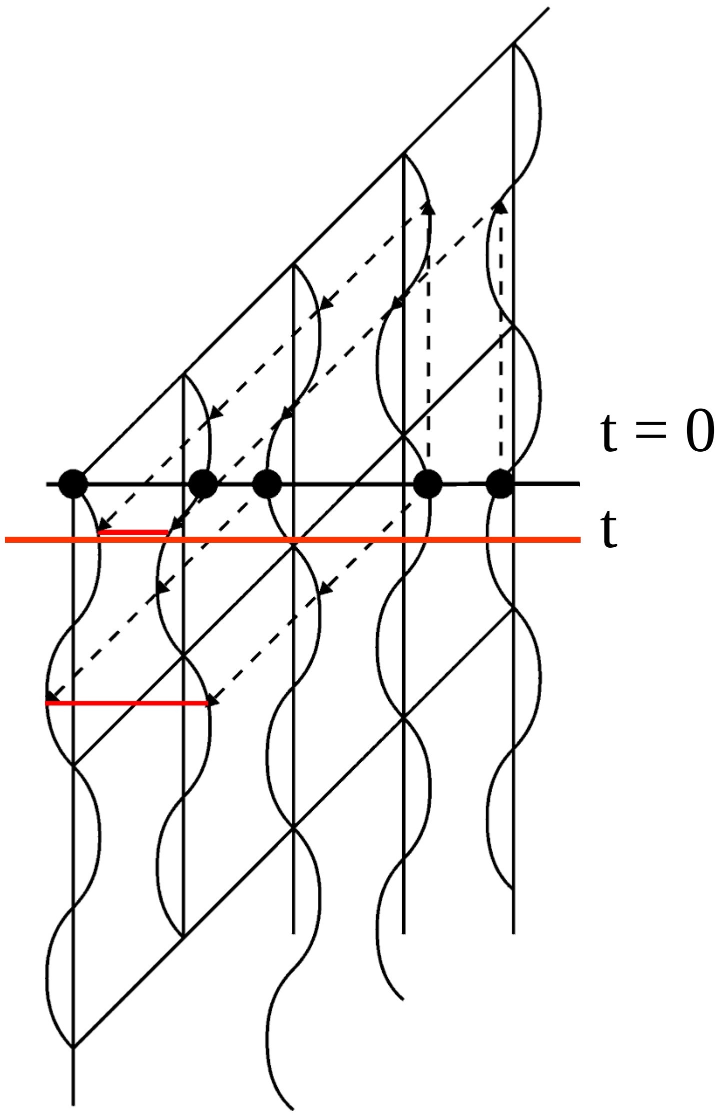
$\mathbf{q}^1 = (0, 0.241, 0)$ $\mathbf{q}^2 = (0.5, 0.261, 0.5)$

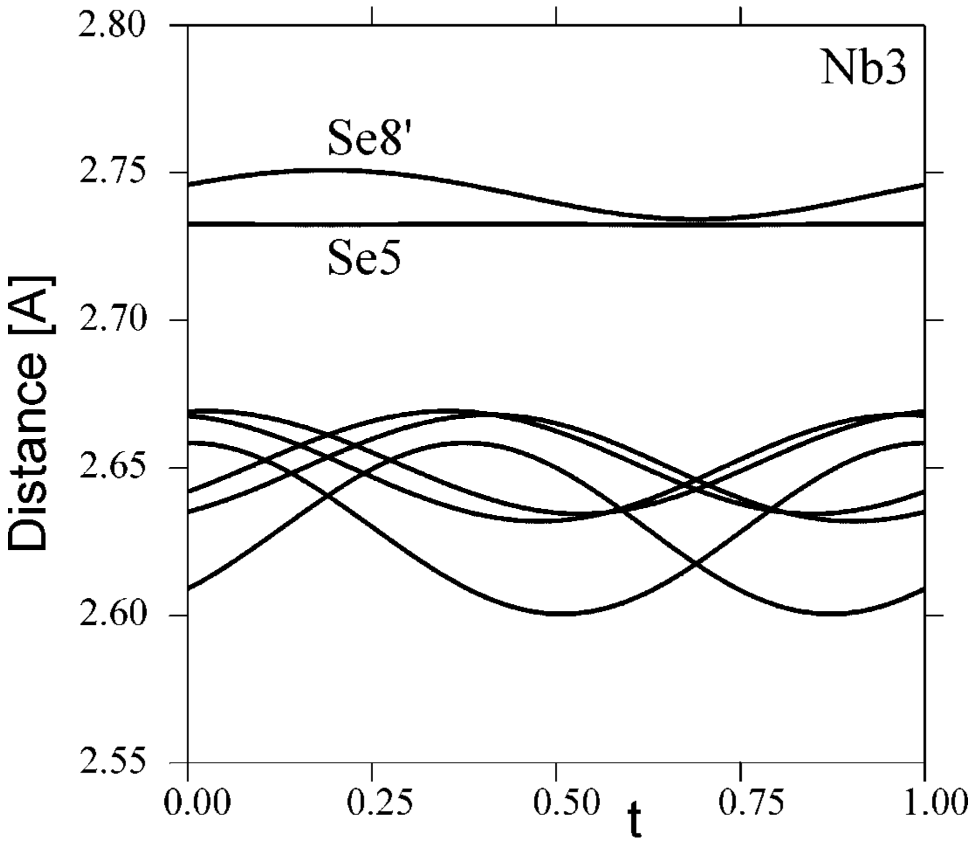
u_y(Nb3) = 0.05 Å u_y(Nb1) = 0.025 Å

SSG 11.2.6.4: $P2_1/m(0, 0.241, 0)s0\,(1/2, 0.260, 1/2)00$

S. van Smaalen *et al.*, Phys. Rev. B **45**, 3103 (1992)

Elastic coupling and Residual strain

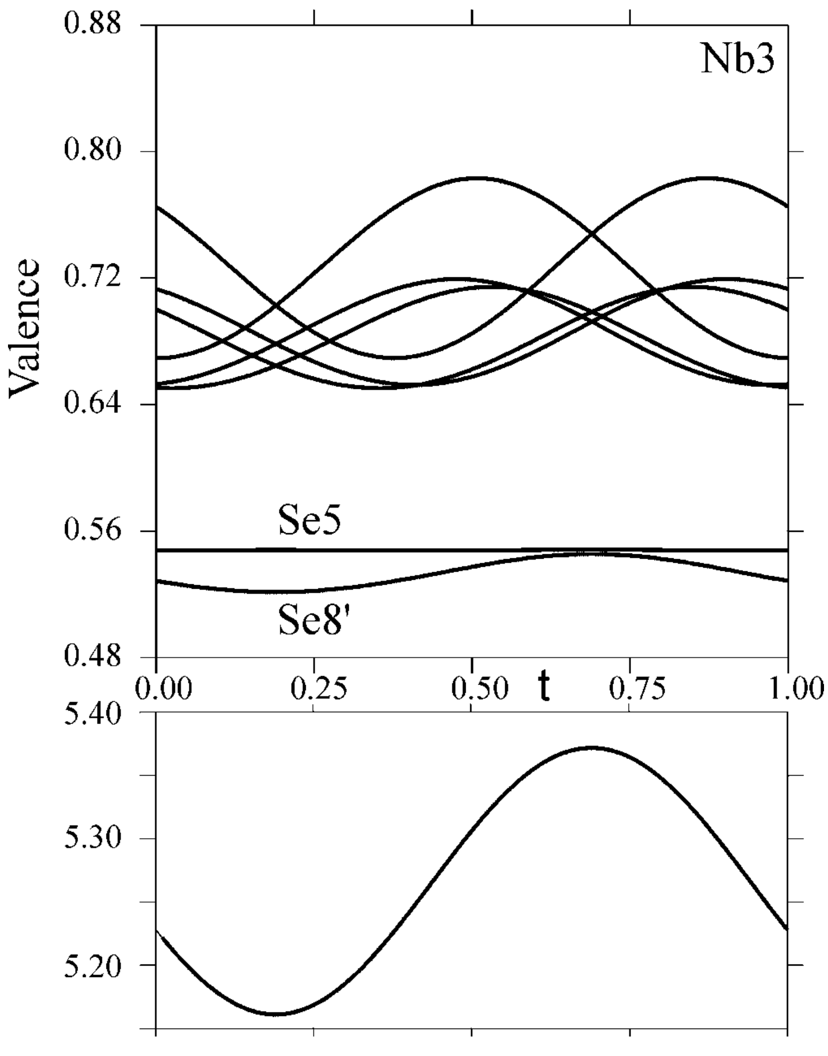




Experiment $\Delta d = 0.06$ Å

Maximum possible $\Delta d = 0.16$ Å

Atomic valences by the Bond-valence method



$$\nu_{ij} = \exp\left[\left(R_0 - r_{ij}\right)/b\right]$$

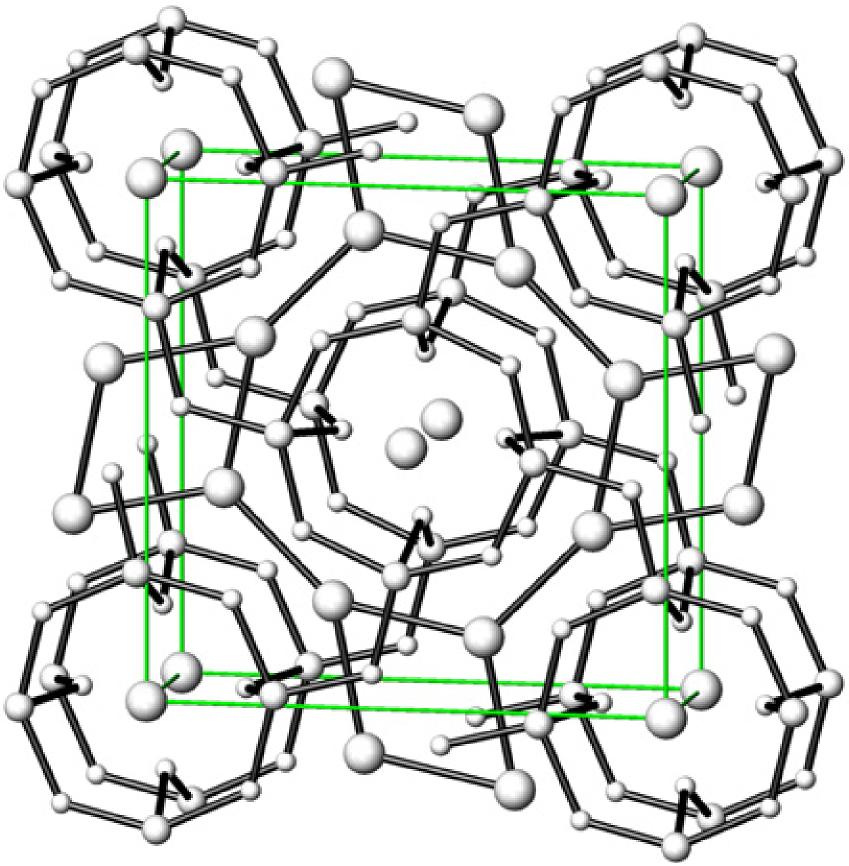
$$V_i = \sum_{j=1}^{\text{neighbors}} \nu_{ij}$$

$$b = 0.37\ \text{Å}$$

R_0 from good structures

Towards a constant valence

Strongly coupled CDW in $R_5Ir_4Si_{10}$



$R_5Ir_4Si_{10}$, R = Er, Lu,...

$Sc_5Co_4Si_{10}$ structure type

P4/mbm (Z = 2)

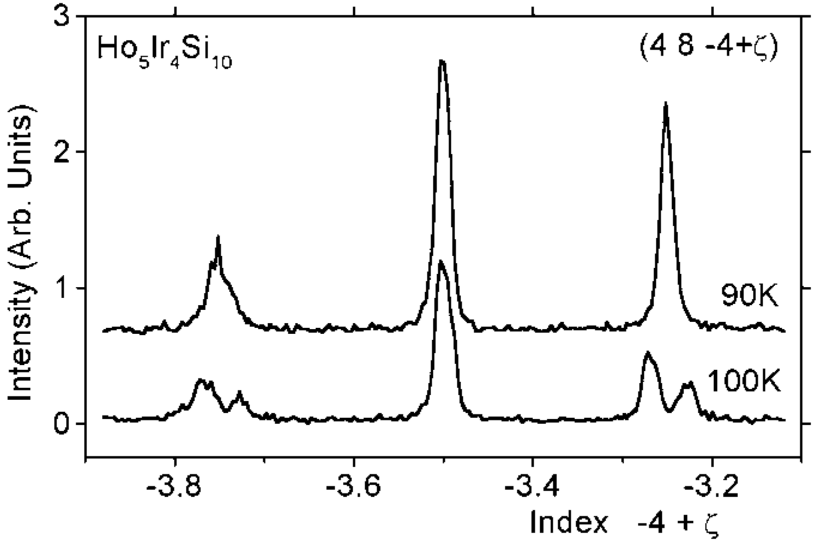
a = 12.53 Å, c = 4.21 Å

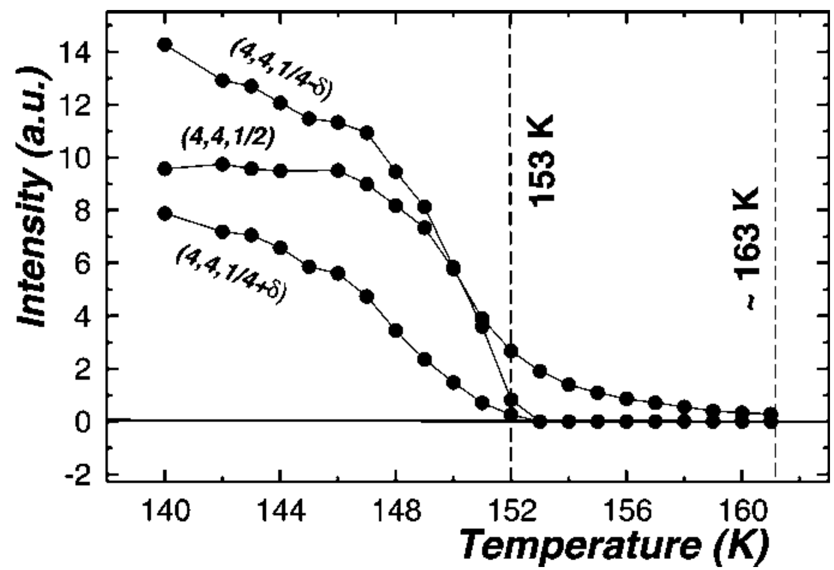
No obvious 1D features

Shelton *et al.* (1986): CDW

H.F. Braun, K. Yvon & R. Braun, Acta Crystallogr. B **36**, 2397 (1980)

Combined incommensurate/commensurate CDW transition in $Er_5Ir_4Si_{10}$ at T_{CDW} = 151 K



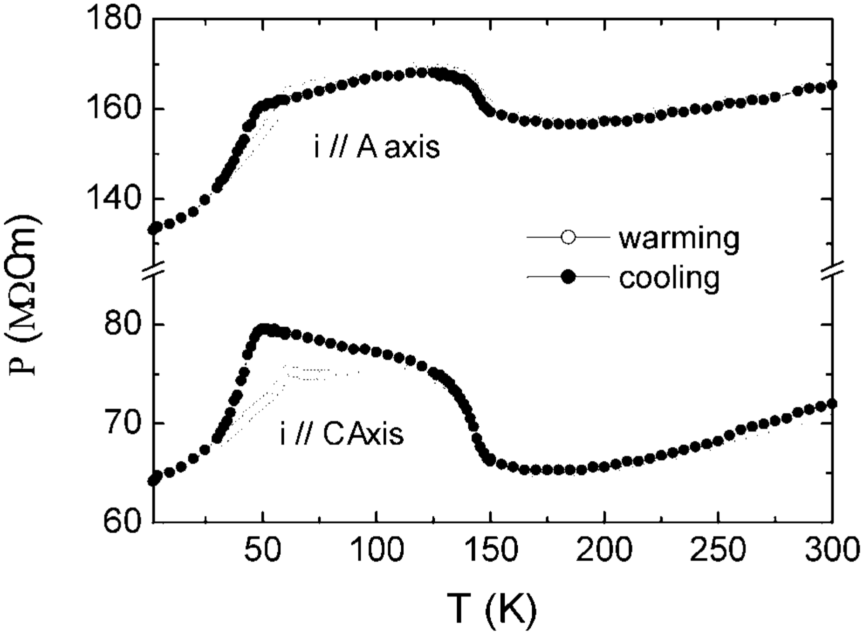


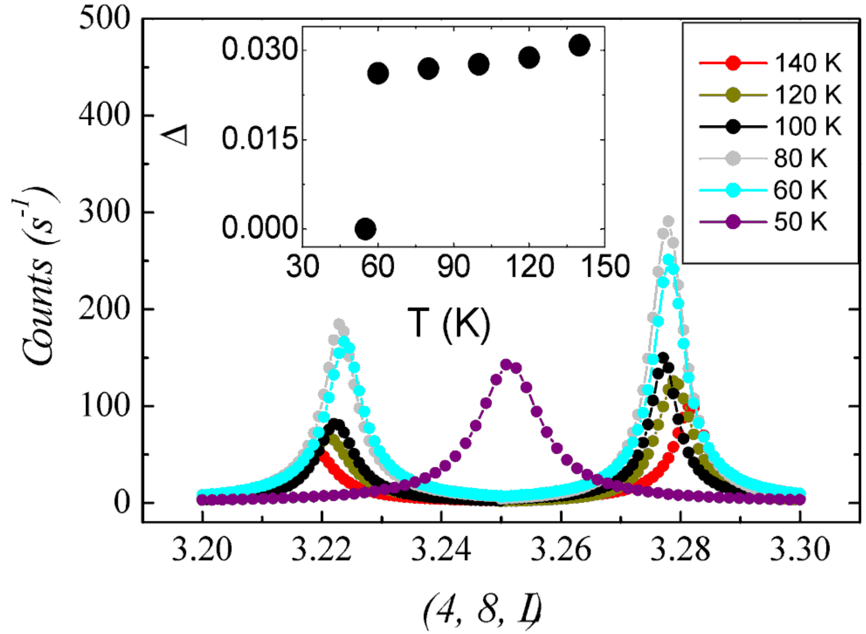
Primary order parameter: $\mathbf{q}^1 = (1/2)\,\mathbf{c}^*$

Modified band-structure provides nesting condition for the incommensurate CDW: $\mathbf{q}^2 = (1/4\pm\delta)\,\mathbf{c}^*$

Galli *et al.,* Phys. Rev. Lett. **85**, 158 (2000) & J. Phys.: Condens. Matter **14**, 5067 (2002)

Lock-in transition in $Er_5Ir_4Si_{10}$





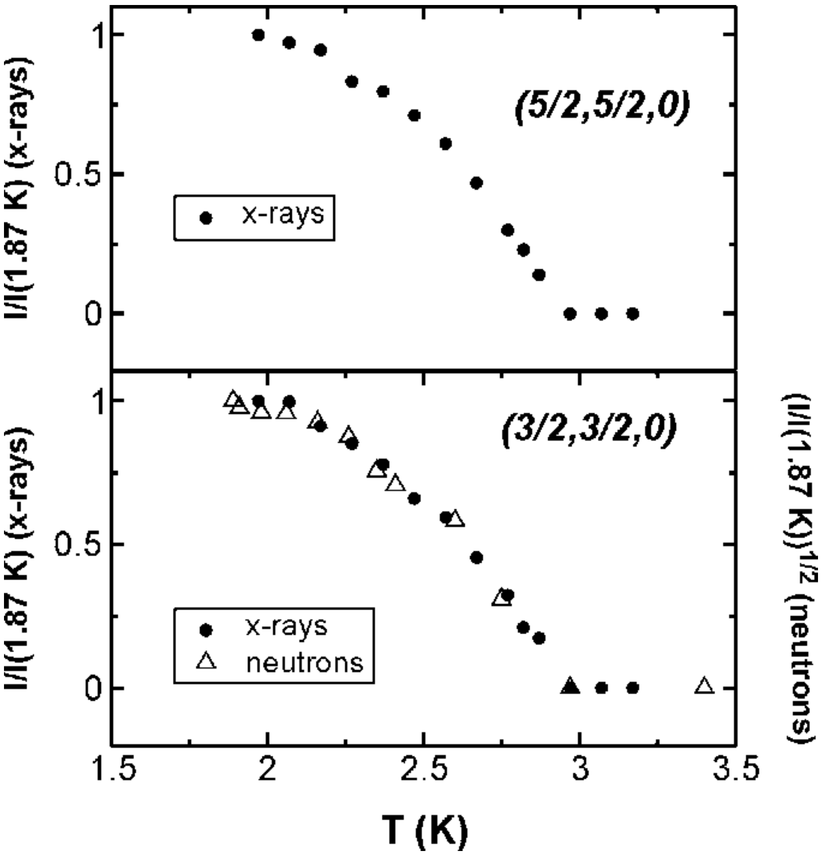
T_{CDW} = 151 K: **q**^{1} = (1/2) **c***   and   **q**^{2} = (1/4±δ) **c***

$T_{lock\text{-}in}$ = 55 K: **q** = (1/4) **c***

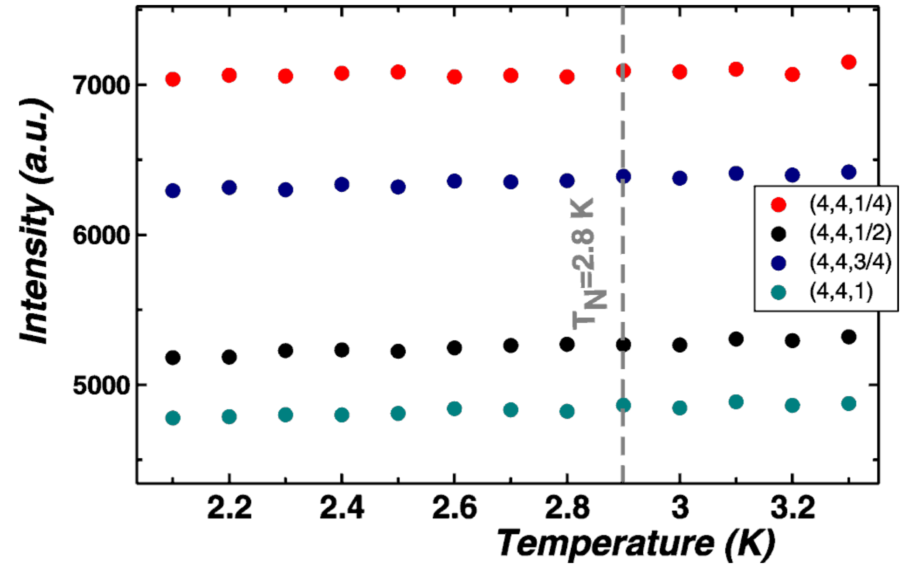
Partial restoration of DOS at the Fermi level

Galli *et al.*, Phys. Rev. Lett. **85**, 158 (2000)

Coexistence of CDW and AF magnetic order



Magnetic x-ray and neutron scattering

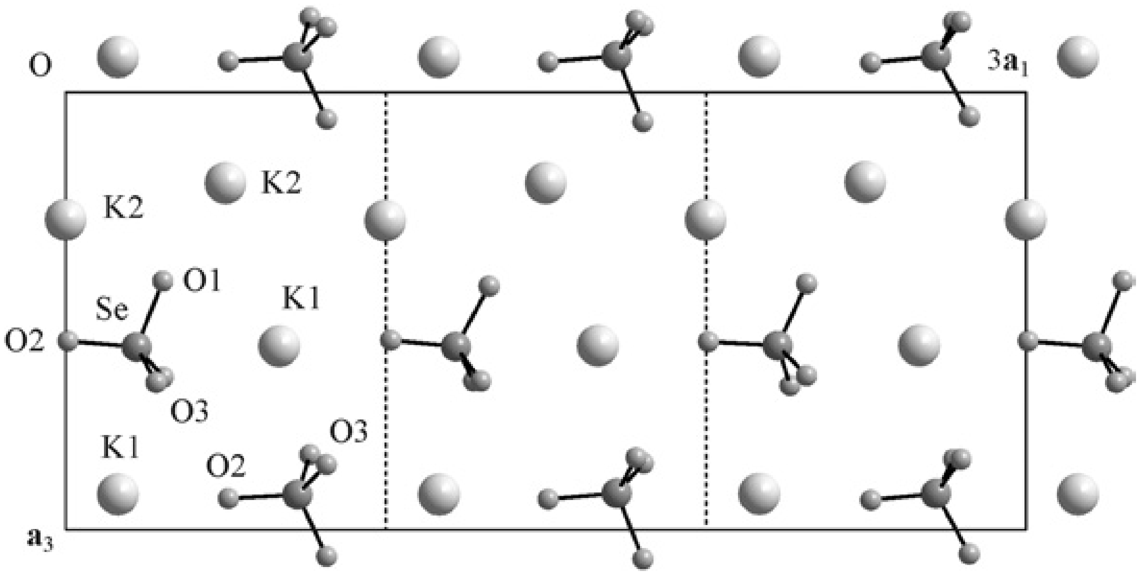


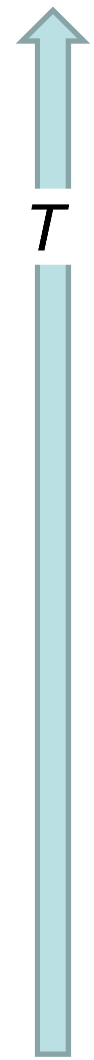
T_N = 2.8 K

fourfold superstructure persists into the state with antiferromagnetic order

Galli *et al.*, J. Phys.: Condens. Matter **14**, 5067 (2002)

Incommensurability by competing interactions





P*nma*

Pnma(σ 0 0)0s0

$\sigma = 2/3 + \delta$

$Pn2_1a$

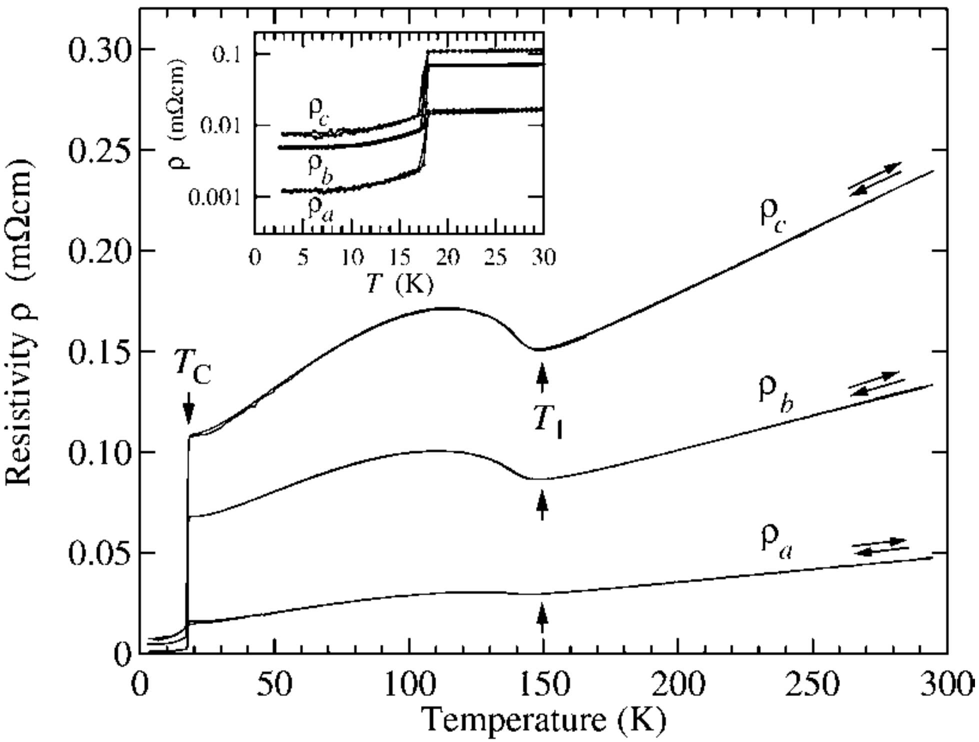
3**a-**supercell

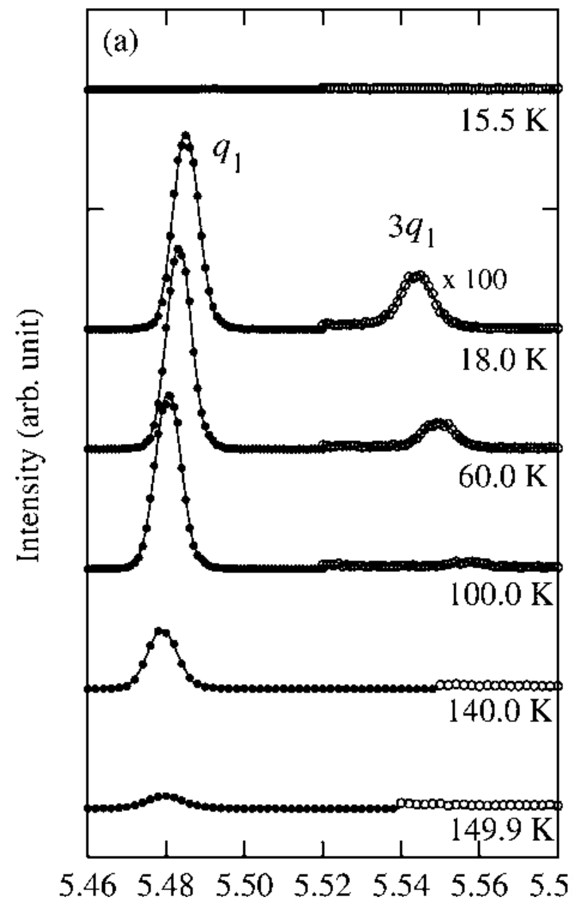
A_2BX_4 ferroelectrics (K_2SeO_4):

local interactions vs optimized packing

N. Yamada *et al.*, J. Phys. Soc. Jpn. **53**, 2565-2574 (1984).

Strongly coupled CDW in $SmNiC_2$



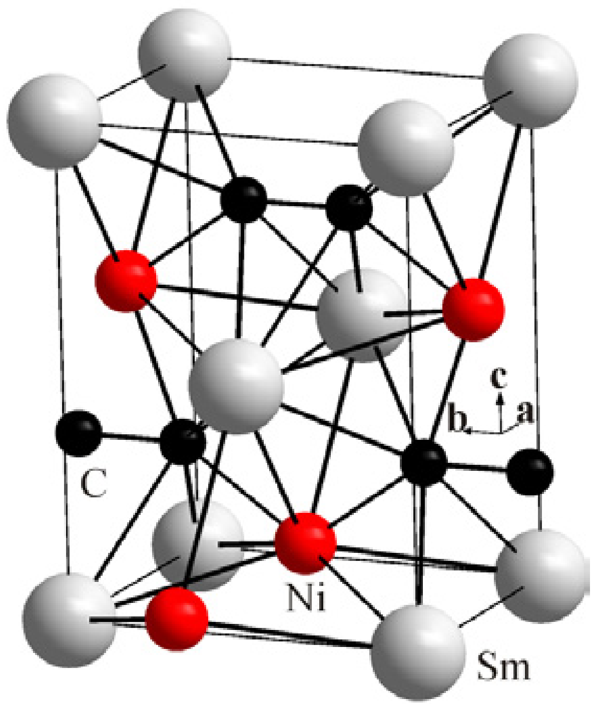


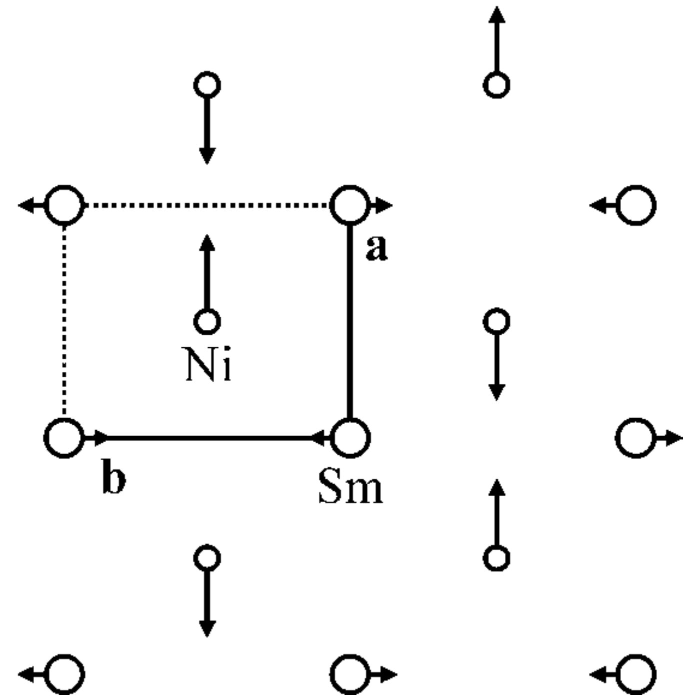
R(**a**) : R(**c**) = 1 : 5 T_c = 148 K

R(**a**) : R(**b**) = 1 : 2.8   **q** = (1/2, 0.516, 0)

S. Shimomura *et al.*, Phys. Rev. Lett. **102**, 076404 (2009)

Incommensurability of the CDW by frustrated interlayer coupling in $SmNiC_2$





SSG 38.1.16.13 Amm2(1/2 β 0)000

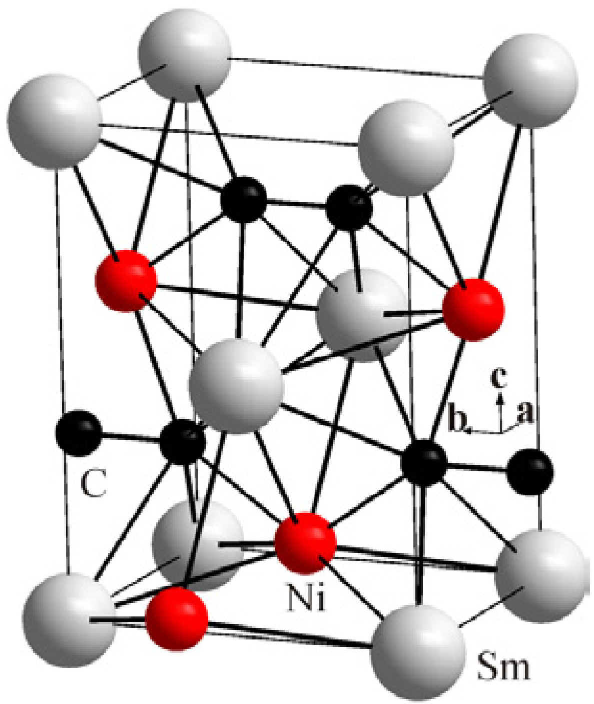
a = 3.70, *b* = 4.53, *c* = 6.10 Å

q = (1/2, 0.516, 0)

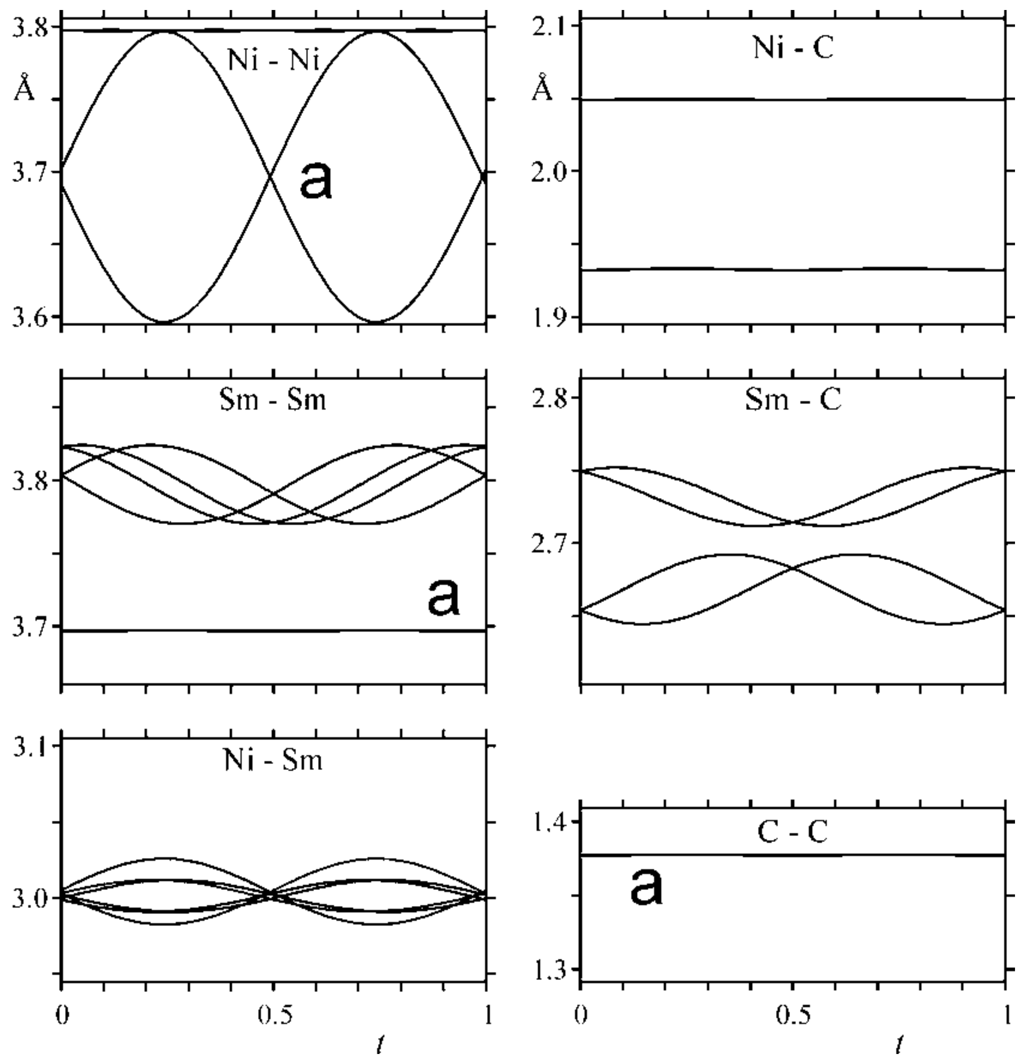
Atomic displacements (x 25)

Wölfel, Liang Li, Shimomura, Onodera & van Smaalen, Phys. Rev. B **82**, 054120 (2010)

Interatomic distances in the CDW phase of $SmNiC_2$

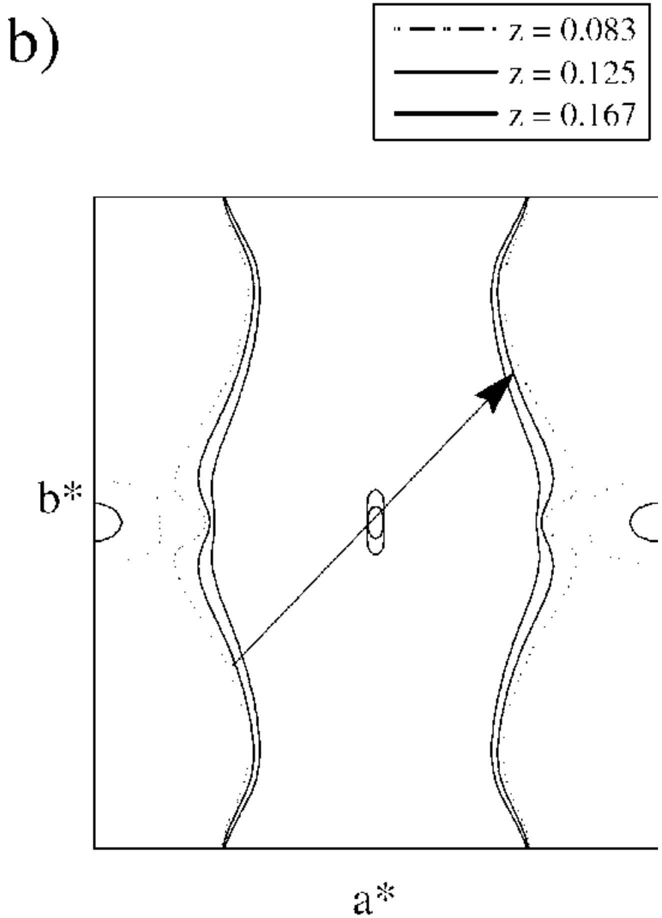


q = (1/2, 0.516, 0)

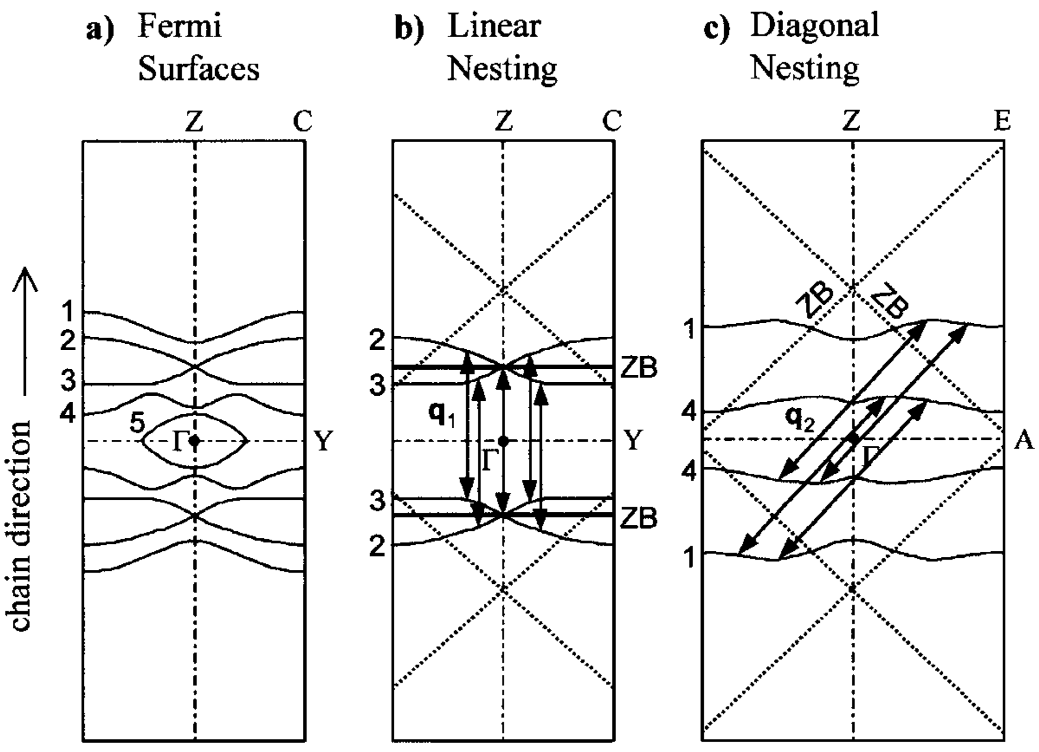


Wölfel, Liang Li, Shimomura, Onodera & van Smaalen, Phys. Rev. B **82**, 054120 (2010)

Fermi surface of $SmNiC_2$



$NbSe_3$

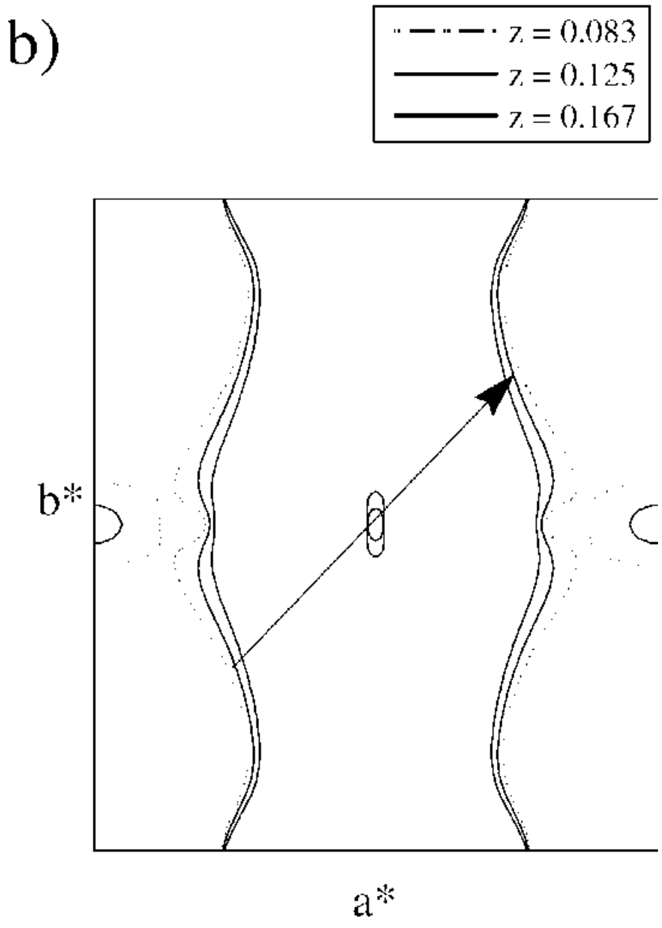


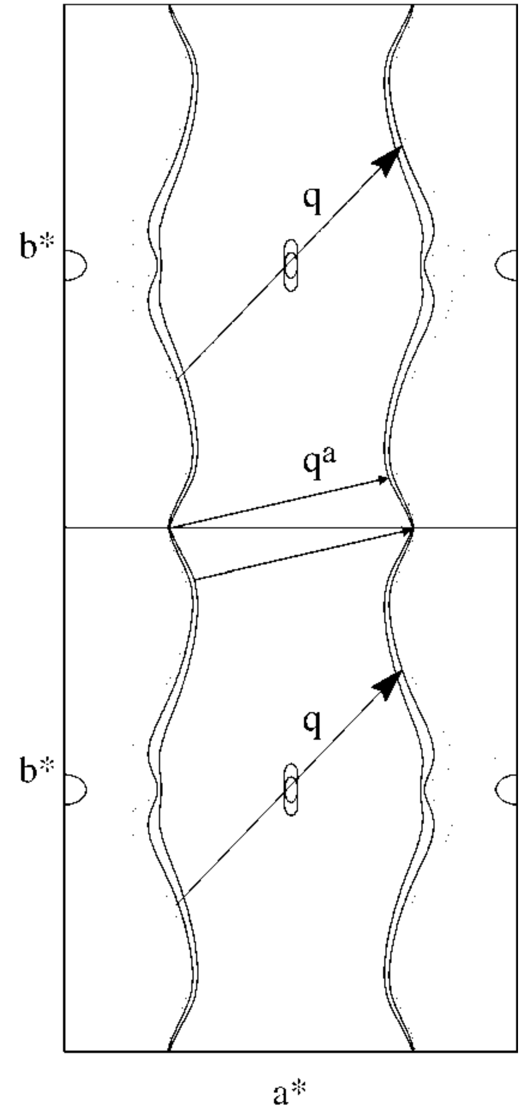
A. Wölfel *et al.*, Phys. Rev. B **82**, 054120 (2010)

J. Laverock *et al.,* Phys. Rev. B **80**, 125111 (2009)

J. Schafer *et al.,* Phys. Rev. Lett. **87**, 196403 (2001)

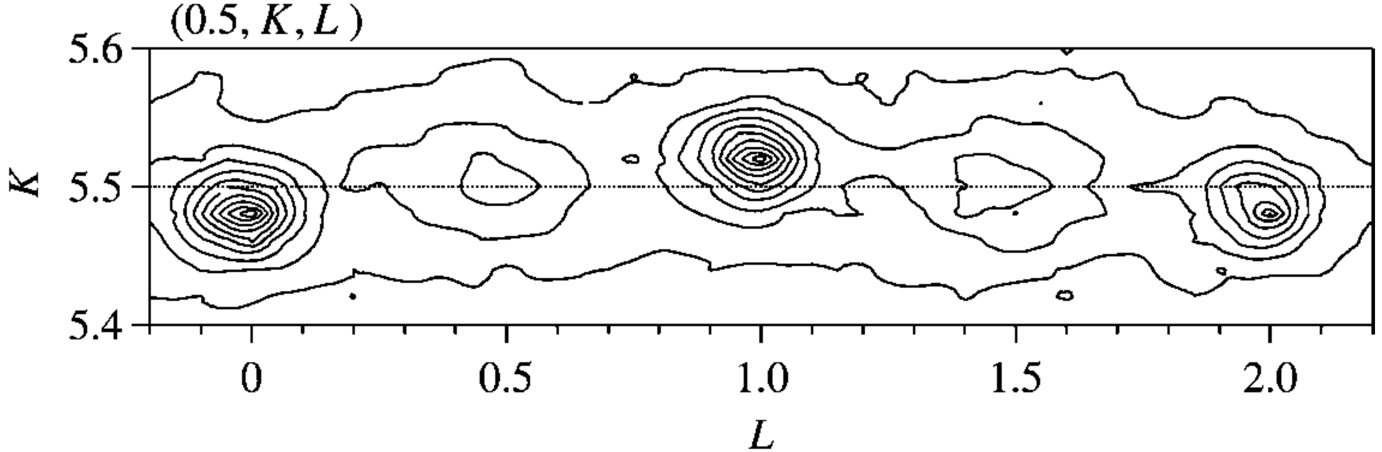
Extended zone Fermi surface of $SmNiC_2$

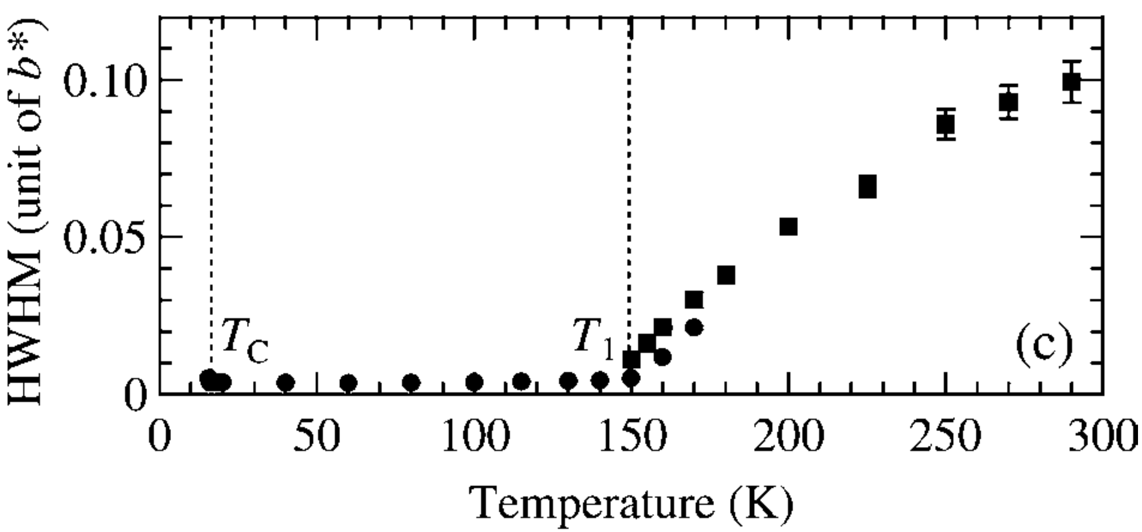




J. Laverock *et al.*, Phys. Rev. B **80**, 125111 (2009)

Diffuse X-ray scattering for $T > T_c$ of $SmNiC_2$



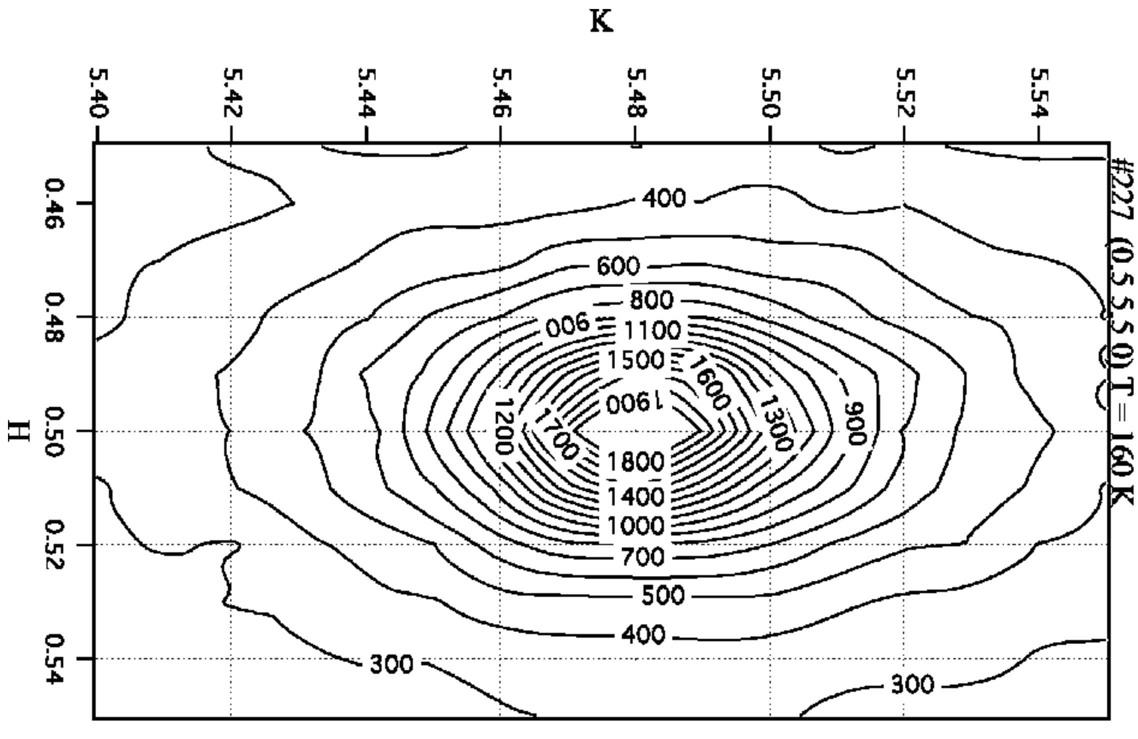


$T > T_c = 148$ K

Increasing temperature gives increasing FWHM and decreasing correlation length

S. Shimomura *et al.*, Phys. Rev. Lett. **102**, 076404 (2009)

H, K-Plane of diffuse X-ray scattering of $SmNiC_2$



$T > T_c = 148$ K

T = 160 K

Correlation length from FWHM

116.3 Å along **a**

94.3 Å along **b**

X-ray data by S. Shimomura *et al.*

Summary

CDW involves conduction band and atomic modulations

Sliding of incommensurate CDW (phason degree of freedom)

Commensurate CDW in $SmNiC_2$ along **a**

- Lowest electrical resistance along **a**
- Magnitude and direction of largest modulation amplitude
- Warped planar Fermi surface perpendicular to **a**
- Correlation length of CDW fluctuations above T_c

CDW in $SmNiC_2$ is rendered incommensurate by frustration of interchain interactions