FEATURES OF CDWs IN NbS₃-II REVEALED BY S.G. Zybtsev¹, S.A. Nikonov¹, <u>V.Ya. Pokrovskii¹</u>, V.F. Nasretdinova¹, S.V. Zaitsev-Zotov¹, A. Maizlakh¹, Woei Wu Pai²,

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¹⁰ LT Physics and Superconductivity Department, Lomonosov MSU ¹¹Institute of Physics, Bijenička cesta 46, HR-10000 Zagreb, Croatia ¹²National Research Centre "Kurchatov Institute" The samples were grown from the vapor phase by direct reaction of Nb and S in mole ratio 1:3 with a 10% excess of sulfur. The growth continued for two weeks in a quartz tube at T between 665 and 740 °C in a temperature gradient ~50 °C over the tube length (20 cm)



Microphotos of NbS₃ in TEM



a) NbS₃ I,II,?????.

b) Still more variety, if defects are considered. Stacking faults.

c) CDWs-1,2,3.

3. Shapiro steps (ShSs), what they give?

4. CDW-1: common features of CDWs, utmost

characteristics. ShSs up to 20 GHz. Bessel-type

oscillations. Synchronization of fluctuations near T_{P1} . Phase slippage.

5. CDW-0: high density, but low mobility. *T* dependences of σ_{∞} ??

6. CDW-2: extremely low density and high mobility.

7. Discussion. What the 3 CDWs form from? The nature of CDW-2.



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Structure and superstructure

But...We barely figured out phase II, as a family of new polymorphs were announced



$$a = 4.963 \text{ Å}, b = 2 \times 3.365 \text{ Å}, c = 9.144 \text{ Å}$$

$$\mathbf{a} = \mathbf{9.9} \text{ \AA}$$
, $\mathbf{b} = \mathbf{3.4} \text{ \AA}$, $c = \mathbf{18.3} \text{ \AA}$

- A combination of **4** units of phase I (without dimerization)



FIG. 1. The basic structure of NbS₃-II [$a_0 = 0.96509(8)$ nm, $b_0 = 0.33459(2)$ nm, $c_0 = 1.9850(1)$ nm, and $\beta_0 = 110.695(4)^\circ$]. Large balls represent Nb and the small ones S atoms. There are four symmetry-related pairs of TP columns in the unit cell, three isosceles (Y, O, and P) and one almost equilateral (R). The two inter-column Nb-S bonds of the eight bonds forming the bi-capped trigonal prisms are shown in black. The symmetry elements of the space group $P2_1/m$ are added.

It was only an illusion of systematization

Following Mark Senn we were close to exclaim: "Welcome to the ZOO!" + defects..

Matthew A. Bloodgood,¹ Pingrong Wei,¹ Ece Aytan,² Krassimir N. Bozhilov,³ Alexander A. Balandin,² and Tina T. Salguero^{1,a}



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Nb

^{Nb}Rich Polymorphism of Layered NbS₃

Sergio Conejeros, Bogdan Guster, Pere Alemany, Jean-Paul Pouget, and Enric Canadell*

Nb ISSN 0021-3640, JETP Letters, 2021, Vol. 114, No. 1, pp. 40–44. © Pleiades Publishing, Inc., 2021. (pr Russian Text © The Author(s), 2021, published in Pis'ma v Zhurnal Eksperimental'noi i Teoreticheskoi Fiziki, 2021, Vol. 114, No. 1, pp. 36–40.

CONDENSED MATTER

"NbS₃-VI contains corrugated chains with paired Nb–Nb and uniform chains with unpaired, equidistant Nb centers."



Impact of the chemical vapor transport agent on polymorphism in the quasi-1D NbS₃ system

n

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A recent TEM image in ac plane (\perp to chains)





The basic properties of NbS₃-II Two CDWs at room *T*. RT I-V curves



Zybtsev et al., 2018, http://lt38-conference.ru/



Differential conductivity vs. voltage under RF power up to 18 GHz. (1.6 μ m×0.005 μ m²) Differential conductivity vs. voltage at different strains ϵ . ϵ =0 (the bottom curve), ϵ ~1% (the upper curve). *L*=24 μ m.



What is the profit from the Shapiro steps?

0) CDW velocity, its coherence

1) From j_{CDW}/f (= 18 A/MHz/cm² for NbS₃) one can find *n*: $n = (j_{CDW}/f)/(e\lambda)$

2) From $\sigma(T)$ one can find $\delta\sigma$ and, thus, μ (just above T_P):

$$\mu = \delta \sigma / en = \lambda \, \delta \sigma_{\rm s} / (j_{\rm CDW} / f),$$

or
$$\mu = L\lambda(f / I_{\rm CDW}) \, \delta \sigma.$$

3) Also µ of a CDW !

For orthorhombic TaS₃ with $\delta \sigma_s \approx 2.5 \cdot 10^3 (\Omega \text{cm})^{-1}$, $j_{\text{CDW}}/f = 38 \text{ A/cm}^2/\text{MHz}$ and $\lambda = 13 \text{ Å}$, $\mu = 8.5 \text{ cm}^2/\text{Vs}$, in agreement with Hall mobility at 300 K.

380

For K_{0.3}MoO₃ for the 21 µm-length sample $I_{CDW}/f=1.6 \times 10^{-12}$ A/Hz and $\delta\sigma=3.4 \times 10^{-3} \Omega^{-1}$. With $\lambda=30$ Å we get µ=1.31 cm²/Vs. For T=158 K the Hall mobility 1.18 cm²/Vs can be found.

ShSs of CDW-1 – common features of CDWs. Oscillations of ShS's magnitudes.



ShSs of CDW-1 – common features of CDWs. ShS's at $T \rightarrow T_{\rm P}$.



 $I_{\rm CDW}/fk \, {\rm vs} \, f_{\rm f}$, at selected temperatures. k is the harmonic. O-f=50 MHz, $\triangle - f = 80 \text{ MHz}, \Box$ *f*=400 MHz, ◊ − *f*=800 MHz. The broken lines approximate the dependencies as A+B $\arctan(f/f_0)$.

Temperature dependence of f_0 determined from the arc tan approximation (closed circles) and visually. The slope corresponds to W=11000 K.

We synchronized CDW fluctuations and found their characteristic time vs. T!

2.82





The closed signs correspond to measurements under f = 50 MHz, the open signs – without irradiation. 297K: CDW-1 is sliding. 381K: CDW-0 is sliding. 17 µm × 0.013 µm².



 $\sigma_{\rm d}$ vs $I_{\rm CDW}$ under RF 400 MHz (a) 297K: CDW-1 is sliding. (18 A/MHz/cm²) and (b) 122 K: CDW-2 is sliding. 170 μ m x 0.2 μ m²

Densities and mobilities of CDW-0,1,2.



A still stronger assumption: $\sigma_{\infty}(T)$ follows $\sigma_{qp}(T)$?? And $\mu_{CDW}(T)$ follows $\mu_{qp}(T)$?? On the origin of CDW-0,1: what is condensing therein?



On the origin of CDW-2: stacking faults?



An STM image in the *bc* plain. T=160 K, **above** T_{P2} .

CDW-0 and CDW-1 are seen. The stacking fault is without



/ith resolved surface S columns ins, as well as strongly (S) and esponding IFFT, obtained with modulation along and between = 140 K.

Check for update

ı NbS2-II



CDW

The same at *T*=140 K, **below** *1* superstructure with 2*b* (or 2.2*b*

ARTICLE

COMMUNICATIONS

https://doi.org/10.1038/s41467-021-26105-1 OPEN

Robust charge-density wave strengthened by electron correlations in monolayer 1T-TaSe₂ and 1T-NbSe₂

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The conclusions.

1. NbS_3 crystallizes in a number of polytypes, and phase II is reproducible with certain reservations.

2. NbS_3 -II shows 3 CDWs, which can slide.

3. CDW-1 reveals common features of sliding CDWs:

-ShSs up to 20 GHz.

-The oscillations of ShS magnitudes are periodic in CDW travel in t=1/(2f).

-ShSs are observed up to T_{P1} . Time of fluctuations can be found.

4. ShSs allow estimation of charge density of a CDW. Knowing $\delta\sigma$ at T_P one can estimate the mobilities of a CDW and *its* quasiparticles.

5. For all the 3 CDWs
$$\sigma(E \to \infty) \approx \sigma_{qp}$$
.
6. For CDW 2,1,0: $n_2:n_1:n_0 \sim (1/3-1/1000): 1 : 2,$
 $\mu_2:\mu_1:\mu_0 = 3 : 0.6: 0.05 \text{ (in cm}^2/\text{Vs)}.$

7. CDW-2 is seen on the low-Ohmic, S deficient, samples. It is likely, that CDW-2 are 2D formations on the stacking faults.

8. CDW-0 seems to form from hopping holes. Also hopping?

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+ "hidden" questions:

- high-*E* limit of CDW conductions

- distribution of CDW between chains



The most recent effects observed NbS₃-II without T_{P1} ?!





Examples of the correlation between σ_{CDW} ($E \rightarrow \infty$) and σ_{qp} . TaS₃ – 0 and m







Fig. 3. Differential conductivity vs. voltage at different *T* for a low-ohmic (a) and a high-ohmic (b) samples.