ANISOTROPY OF CONDUCTIVITY IN RARE-EARTH TRITELLURIDES IN THE STATIC AND SLIDING STATES OF THE CDW

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OUTLINE

- Motivation.
- *R*Te_3 (*R*=Y, La, Ce, Nd, Sm, Gd, Tb, Ho, Dy, Er, Tm) compounds. Properties.
- Conductivity anisotropy in the static and sliding state of the CDW. Experiment.
- Theoretical explanation.
- Conclusion.

Motivation

One fingerprint of the resulting ground states quasi two-dimensional (2D) systems with strong electronic correlations is often the formation of **unidirectional charge or spin modulations (stripes)**.

Investigated in

Cuprates

S.A. Kivelson, et al, Rev. Mod. Phys.,2003

Organic materials

H. Seo, J. Phys. Soc. Jpn, (2000)

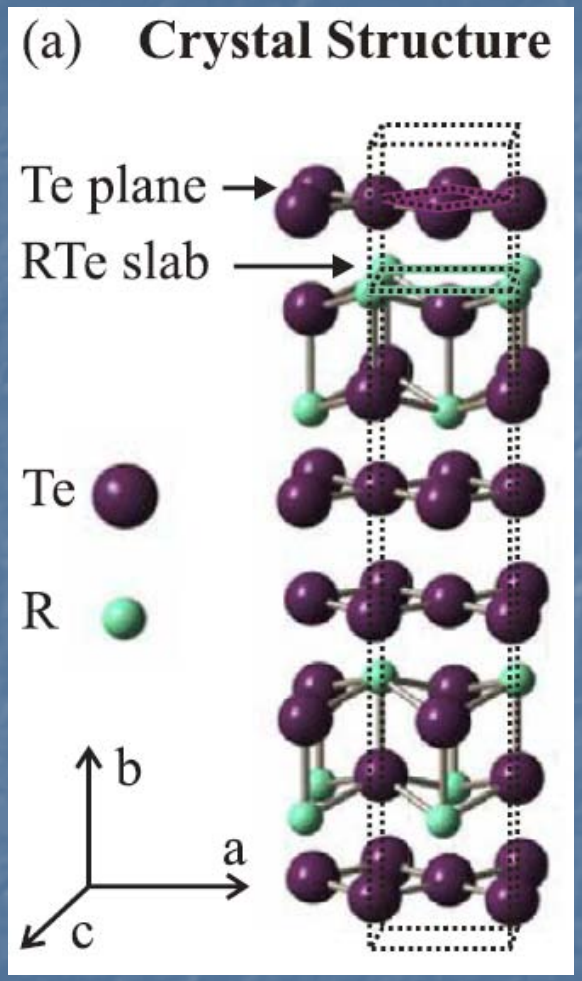
Manganites

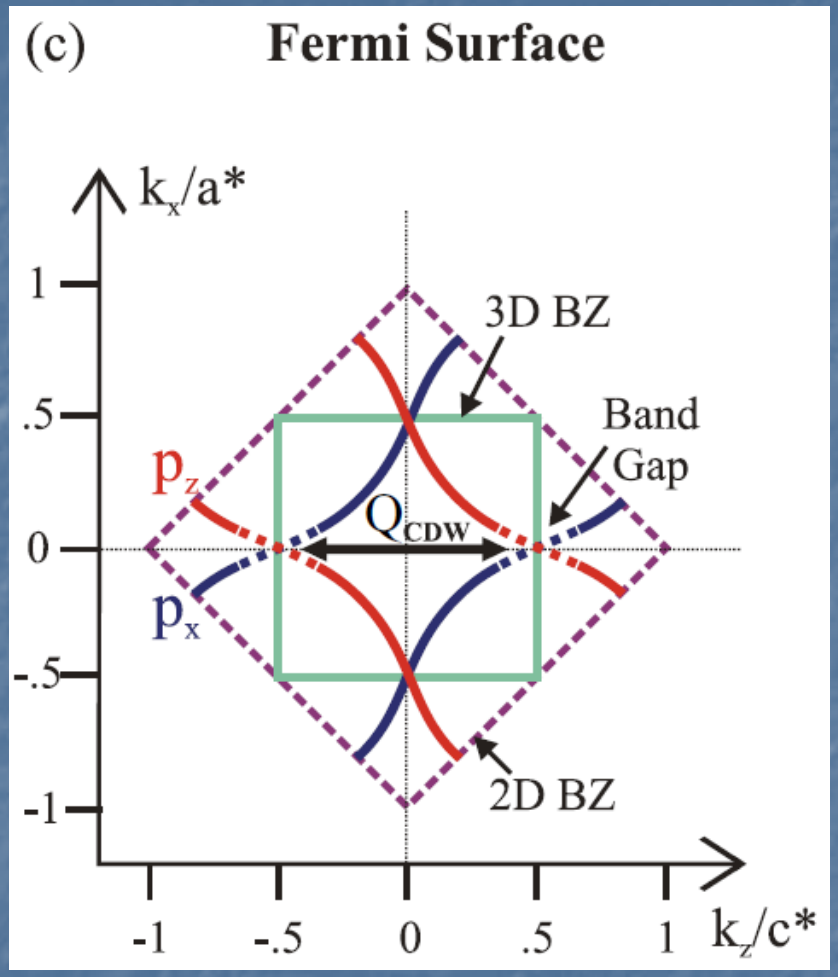
Z. Sun, et al, PNAS, (2011)

Can we find 2D compound with the CDW which can be considered as a model system?

rare-earth tritellurides RTe_3

(*R*=Y, La, Ce, Nd, Sm, Gd, Tb, Ho, Dy, Er, Tm)

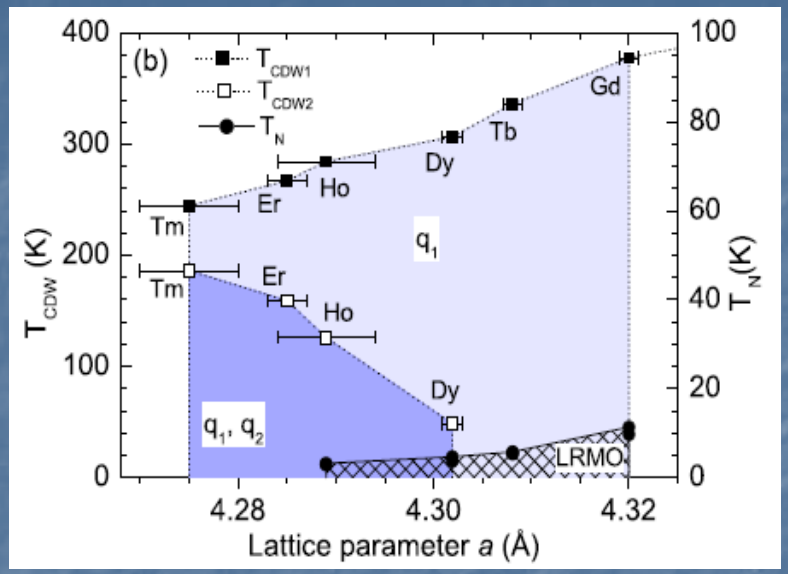




F. Schmitt et al., New Journal of Physics 13, 063022 (2011)

rare-earth tritellurides RTe_3

(R=Y, La, Ce, Nd, Sm, Gd, Tb, Ho, Dy, Er, Tm)



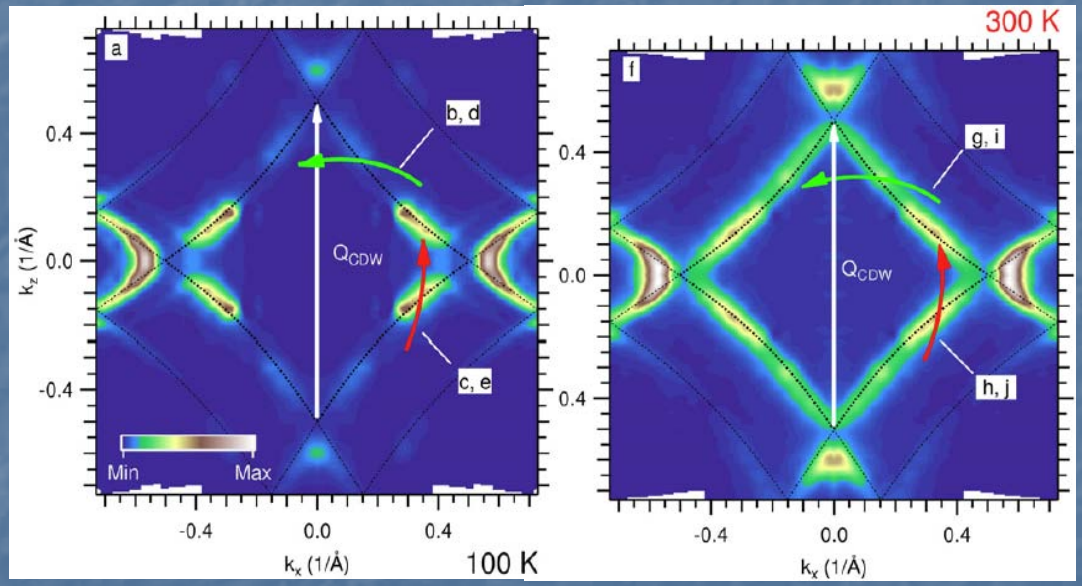
N. Ru, et al, Phys. Rev. B **77**, 035114, 2008

Incommensurate CDW through the whole R series with a wave vector Q_{CDW1}=(0,0,2/7c*).

Peierls transition temperature 240-500K.

For the heavier R (Tb, Dy, Ho, Er, Tm) second CDW at low temperature with the wave vector Q_{CDW2}=(2/7a*,0,0) perpendicular to Q_{CDW1}.

ARPES data on momentum dependence of charge-density-wave (CDW) energy gap in $TbTe_3$



F. Schmitt et al., New Journal of Physics 13, 063022, 2011

rare-earth tritellurides RTe_3

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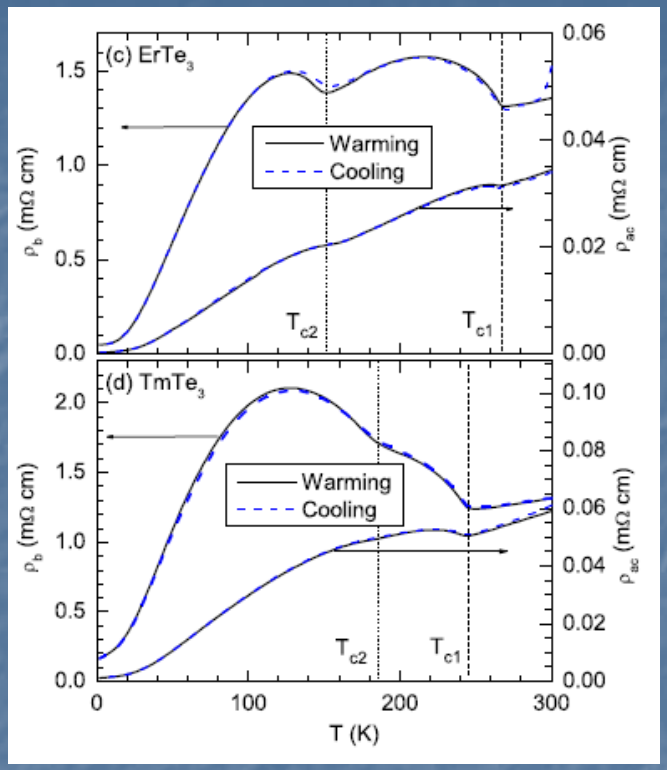

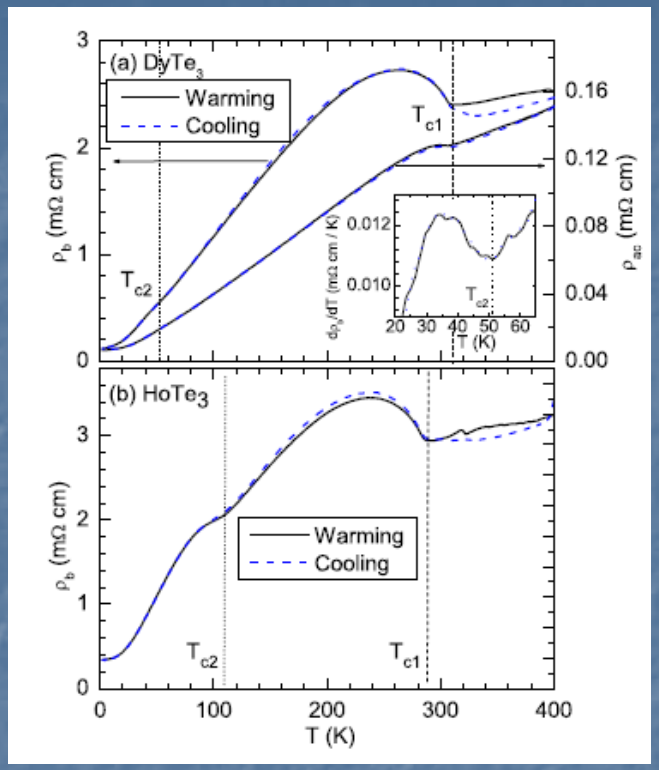

The effect of CDW on the in-plane resistivity is very weak (not more then a few percents) and independent on measurement direction (**?**):

"**In-plane measurements were made for arbitrary current directions in the ac plane, using a standard four point contact geometry.**" (N.Ru, et al, Phys.Rev. B **77**, 035114, 2008).

Does it mean that the system is isotropic not only above Peierls transition, but also below transition???

rare-earth tritellurides RTe_3

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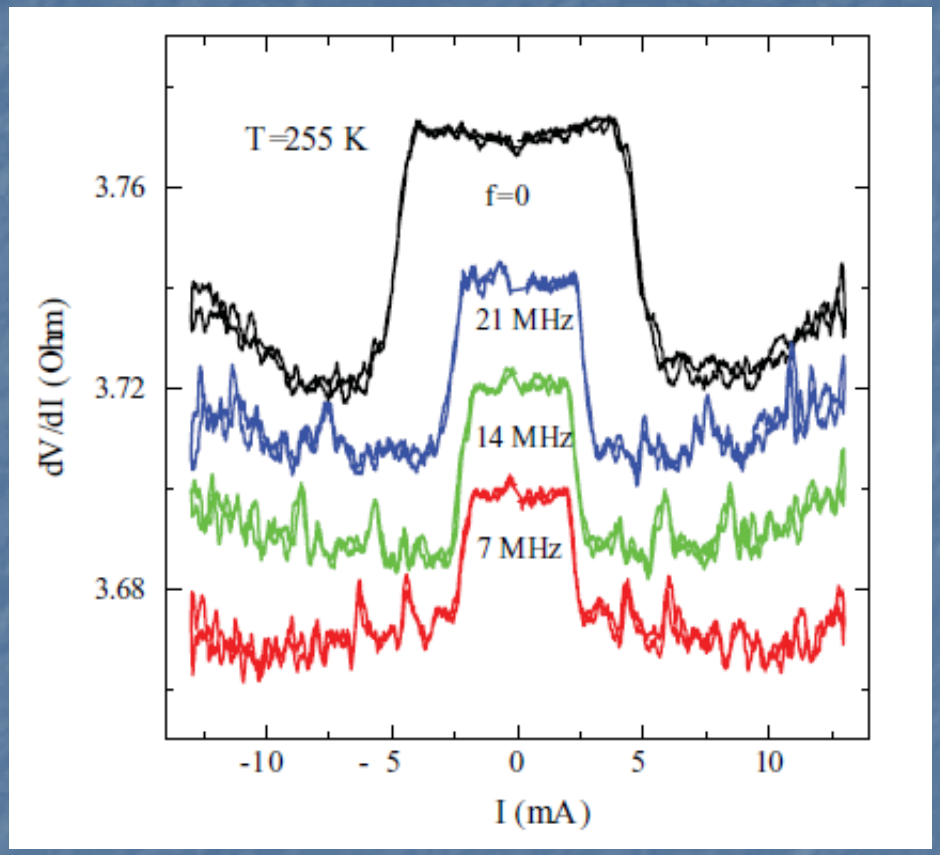
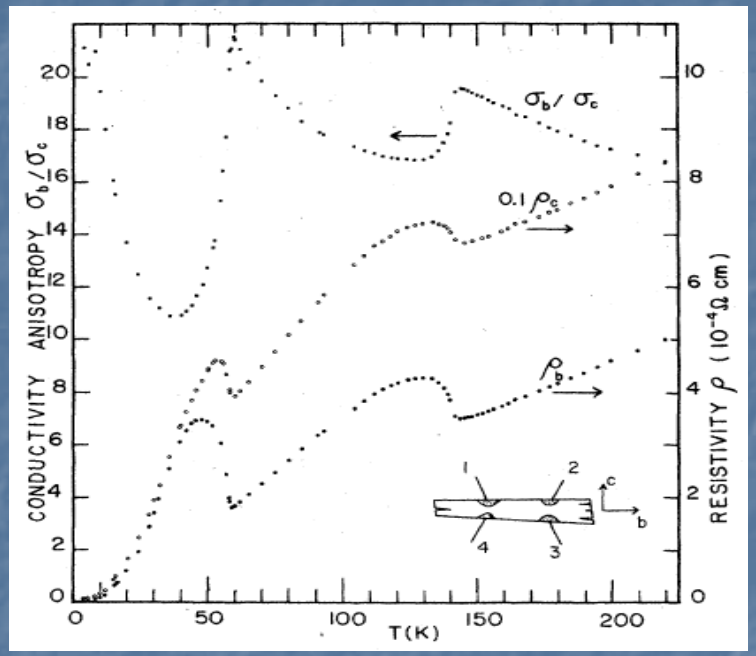


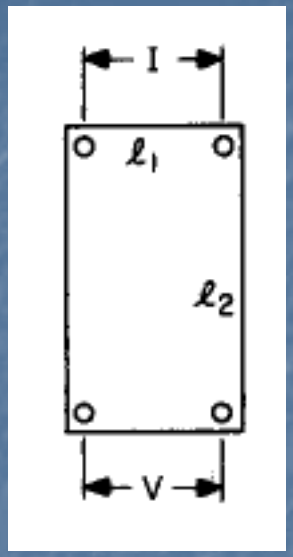
First 2D system where collective CDW motion has been observed: the conductivity of a bridge cut from a thin $DyTe_3$ single crystal increased sharply above a threshold field (E_t ~ V/cm at T=200 K) and under the application of a radio-frequency field Shapiro steps were clearly observed
(Sinchenko, Lejay and Monceau, PRB, 2012).

What is the direction of sliding?

Conductivity anisotropy. Experiment.

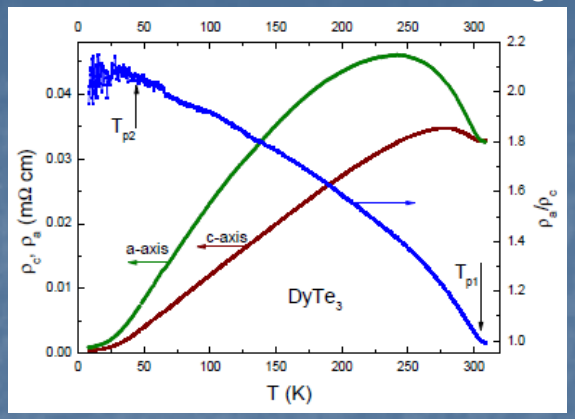
Conductivity anisotropy in $NbSe_3$
(N.P.Ong and J.W.Brill, Phys.Rev.B **18**, 5265,1978)

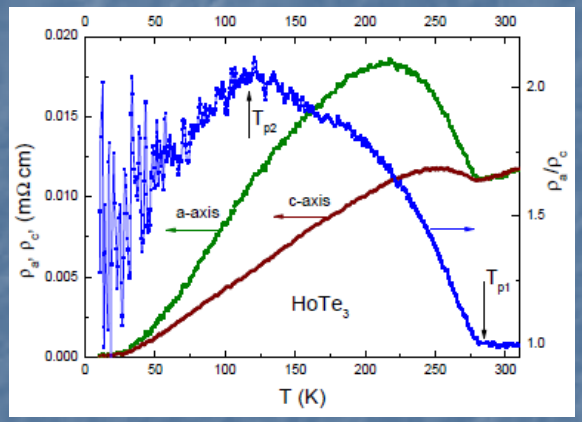




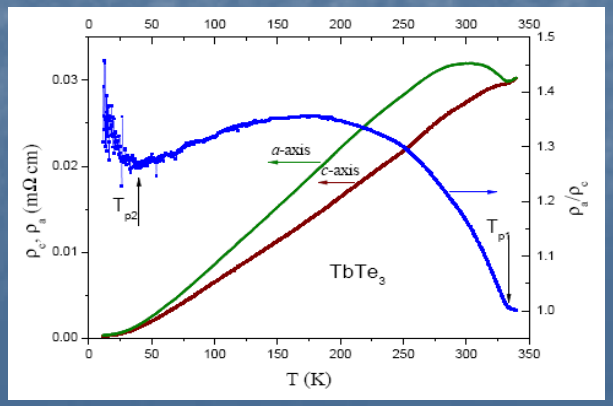
(H.C.Montgomery J.Appl.Phys., 42, 2971,1971)

Conductivity anisotropy in RTe_3



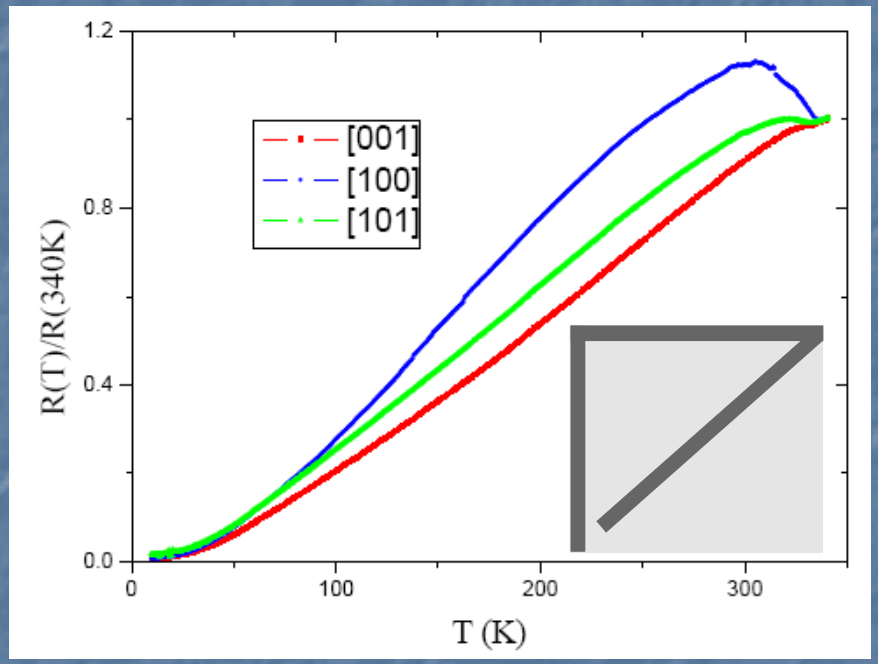


The transition into the CDW state in rare-earth tritellurides leads to a stronger increase of resistance in the direction perpendicular to the CDW *Q*-vector than in the direction parallel to the CDW *Q*-vector. Such behavior is inverse to that observed in quasi-one dimensional compounds with a CDW where the anisotropy is considerable in the normal state and strongly decreases below the Peierls transition

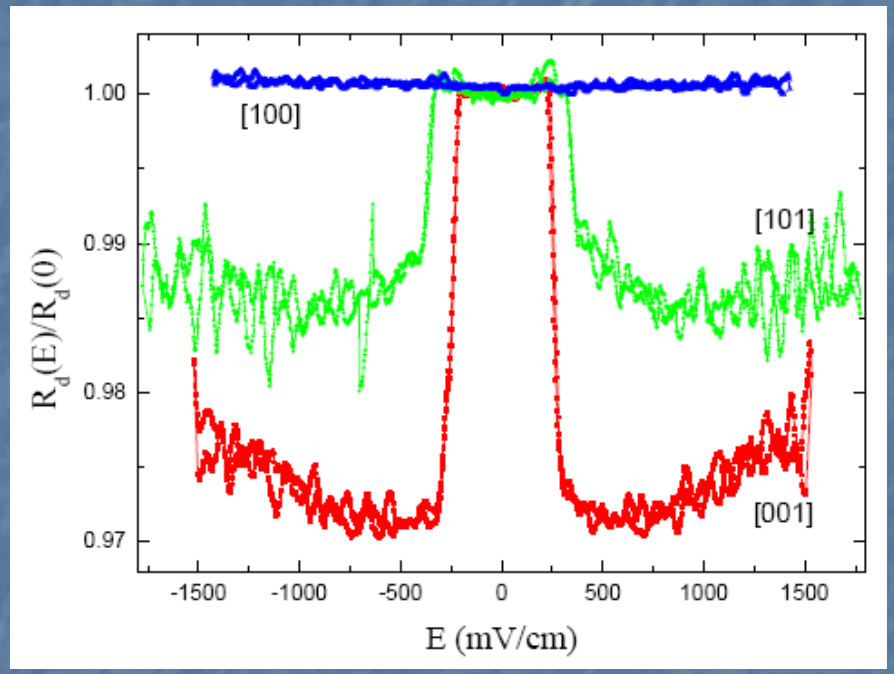


Conductivity anisotropy. Experiment.

R(T) for $TbTe_3$ bridges cut in [001]; [100] and [101] directions



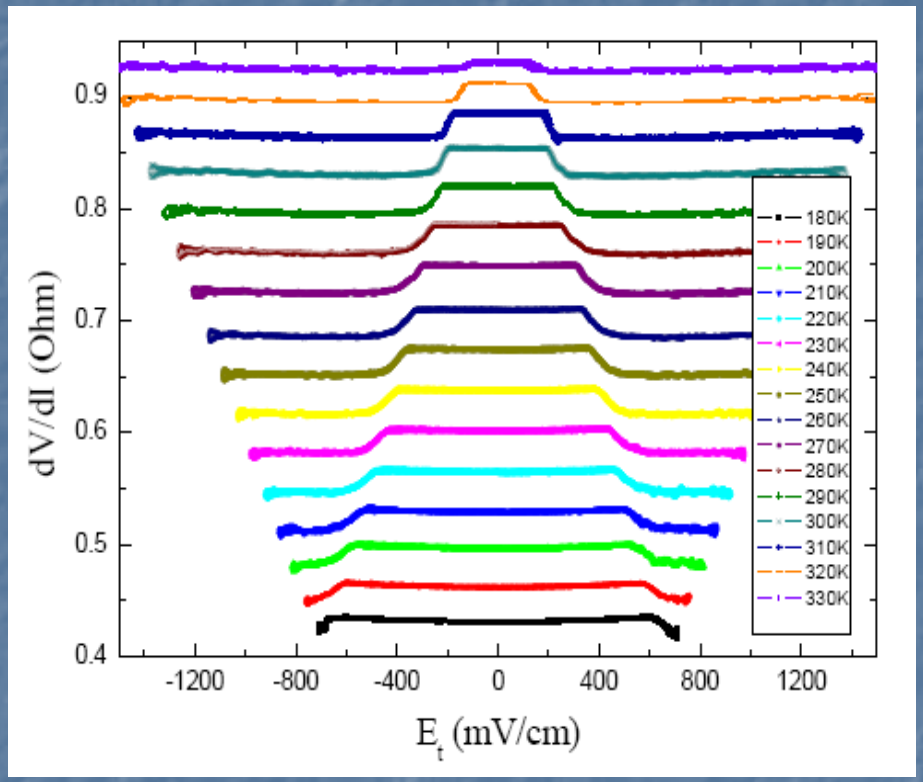
Differential IVs of $TbTe_3$ bridges cut in [001]; [100] and [101] directions

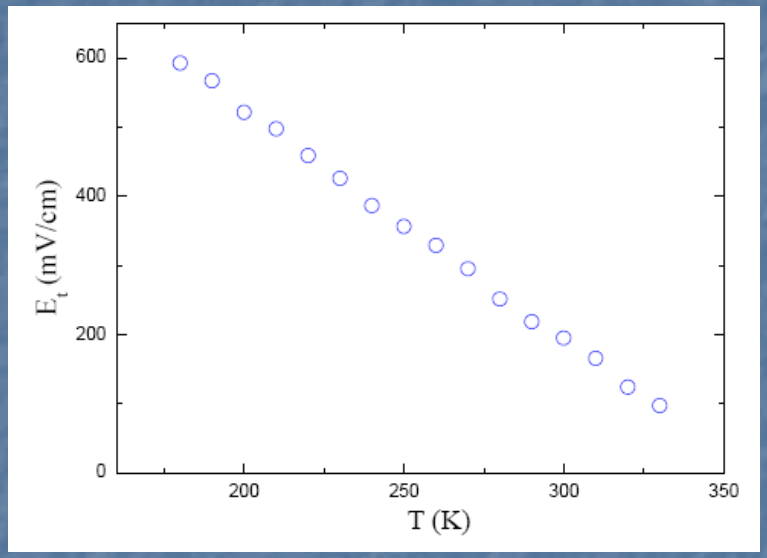


For [001] direction the threshold behavior, typical for the transition to the sliding CDW state, is clearly seen: the IVs are Ohmic for electric field less than some threshold electric field E_t, and for field in excess of this value the differential resistance decreases sharply. For bridges oriented in [100] direction such a sliding behavior is absent completely.

Conductivity anisotropy. Experiment.

temperature dependence of the threshold electric field





$$E(T) = E(0)(1 - \frac{T}{T_0})$$

- relative change of the differential resistance from static to sliding state is very small ⟹ the contribution of the CDW to the electron transport in these quasi-2D CDWs is very low.
- E_t is a linear function of T in the whole range of temperature

Explanation

Effect of momentum asymmetry of CDW gap.

Electron dispersion without CDW determined from band-structure calculations:

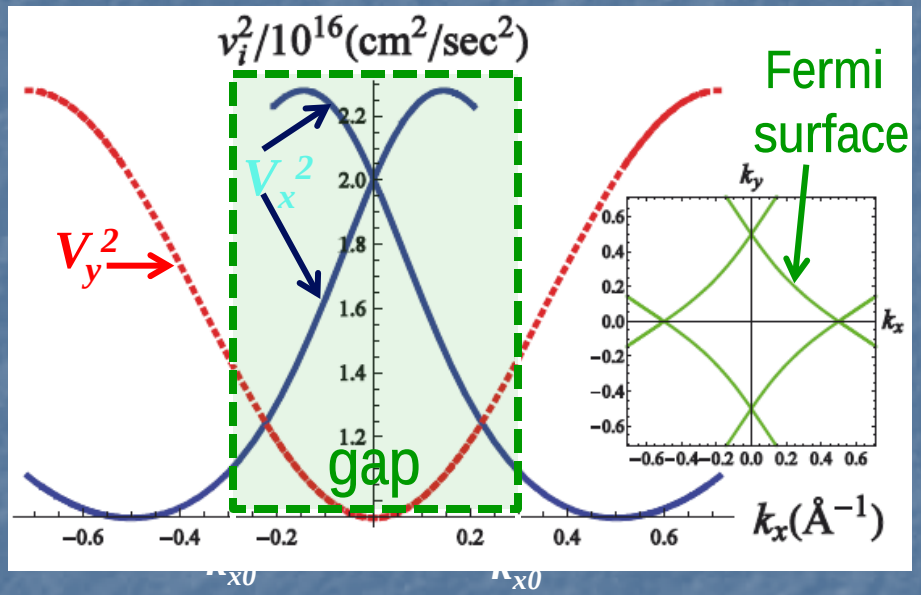
$$\varepsilon_1(k_x,k_y) = -2t_{\parallel}\cos[(k_x+k_y)a/2] - 2t_{\perp}\cos[(k_x-k_y)a/2] - E_F,$$
$$\varepsilon_2(k_x,k_y) = -2t_{\parallel}\cos[(k_x-k_y)a/2] - 2t_{\perp}\cos[(k_x+k_y)a/2] - E_F,$$

=>

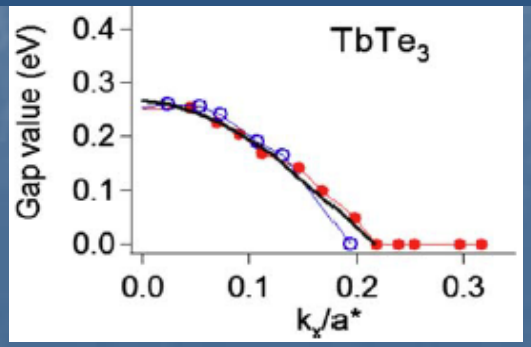
where $t_{\parallel} \approx 2$ eV, $t_{\perp} \approx 0.37$ eV

$E_F \approx 1.48$ eV and $a \approx 4.4\mathring{A}$ for $TbTe_3$

The momentum dependence of electron velocity without CDW:



momentum asymmetry of CDW gap:

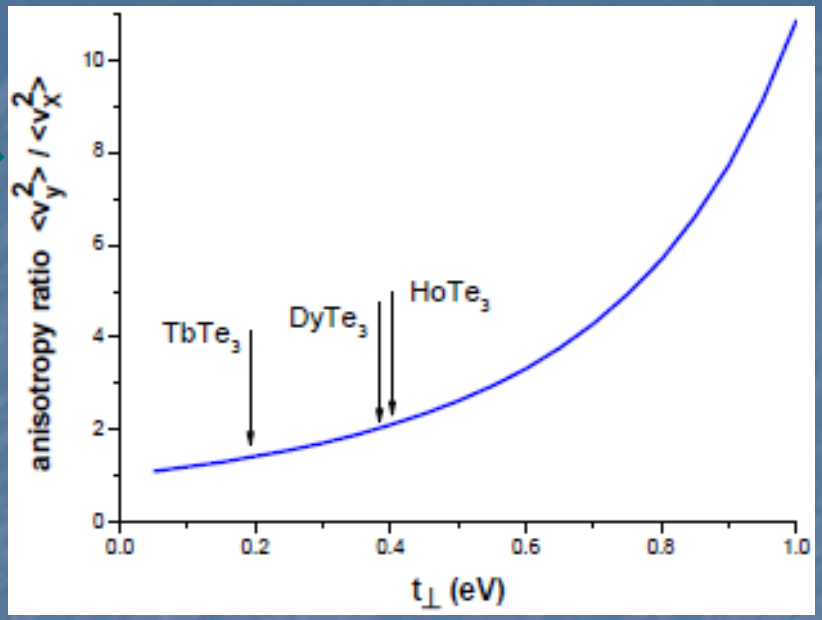


Electron conductivity: $\sigma_i(T) = 2e^2\tau \sum_{\boldsymbol{k}} v_i^2(\boldsymbol{k})\left(-n_F'[\varepsilon(\boldsymbol{k})]\right)$

! CDW energy gap removes the electron states from FS parts with larger component V_x^2, thus breaking the x-y isotropy of conductivity.

Explanation

The anisotropy ratio depends strongly on $t_\perp / t_\parallel$ in the electron dispersion without CDW. This can help to extract $t_\perp$ from experiment.



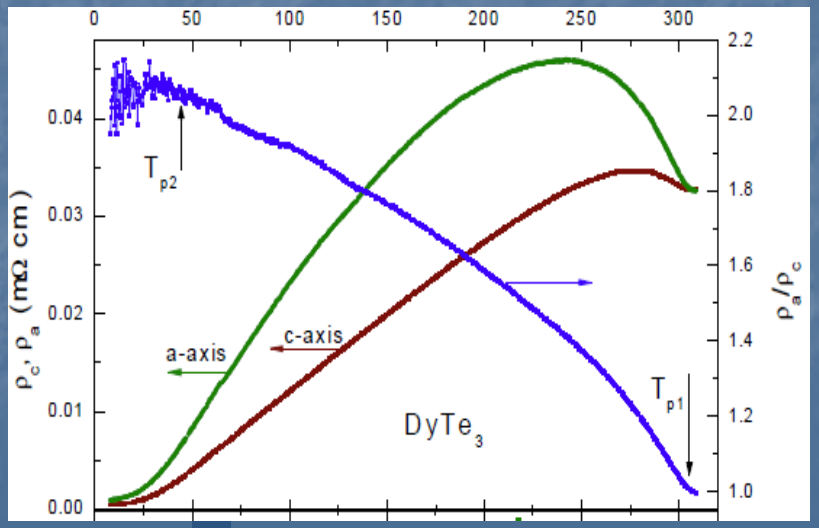
For RTe_3 where R=Tb,Dy,Ho,

with $t_\parallel \approx 2 \text{ eV}, \; t_\perp \approx 0.37 \text{ eV}$

and the calculated maximum anisotropy ratio (at T=0)

$$\frac{\sigma_{yy}}{\sigma_{xx}} \approx \frac{\int_{|k_x| \geq k_{x0}} dk_x \sqrt{1 + \left|\frac{dk_y}{dk_x}\right|^2_{FS}} v_y^2}{\int_{|k_x| \geq k_{x0}} dk_x \sqrt{1 + \left|\frac{dk_y}{dk_x}\right|^2_{FS}} v_x^2} \approx 1.96.$$

agrees with experiment, where this ratio ≈ 2



Explanation

Calculation of the temperature dependence of resistivity (from Boltzmann transport equation)

Electronic conductivity in the τ-approximation:

$$\sigma_i(T) = 2e^2\tau \sum_{\boldsymbol{k}} v_i^2(\boldsymbol{k})\left(-n_F'\left[\varepsilon(\boldsymbol{k})\right]\right)$$

CDW energy gap:

$$\Delta(T,\boldsymbol{k}) \approx \Delta_0(T)\,\Delta(\boldsymbol{k}) \approx \Delta_0(T)\left(1 - k_x^2/k_{x0}^2\right)$$

$$\Delta_0(T) \approx \Delta_0\left(1 - T^2/T_c^2\right)^{\alpha},\ \alpha \geq 1/2.$$

For $TbTe_3$ $\Delta_0 \approx 0.27\text{eV}$ $k_{x0} \approx 0.29\mathring{A}^{-1}$

Electron dispersion in the CDW state $E(\boldsymbol{k}) = \sqrt{\varepsilon^2(\boldsymbol{k}) + \Delta^2(T,\boldsymbol{k})}.$

Electron velocity:

$$v_{i\Delta}(\boldsymbol{k}) = \frac{\partial E(\boldsymbol{k})}{\partial k_i} \approx \frac{\varepsilon(\boldsymbol{k})\ \partial\varepsilon(\boldsymbol{k})/\partial k_i}{\sqrt{\varepsilon^2(\boldsymbol{k}) + \Delta^2(T,\boldsymbol{k})}} = v_i(\boldsymbol{k})\frac{\varepsilon(\boldsymbol{k})}{E(\boldsymbol{k})}.$$

Conductivity components

$$\sigma_i(T) = \frac{e^2\rho_F\tau}{d}\int_{-\pi/a}^{\pi/a}\frac{a\,dk_x}{2\pi}\sqrt{1+\left(\frac{dk_y}{dk_x}\right)^2}\,v_i^2(k_x) \times \int\frac{d\varepsilon}{v_F}\frac{-n_F'\left[\sqrt{\varepsilon^2+\Delta^2(T,k_x)}\right]\varepsilon^2}{\varepsilon^2+\Delta^2(T,k_x)},$$

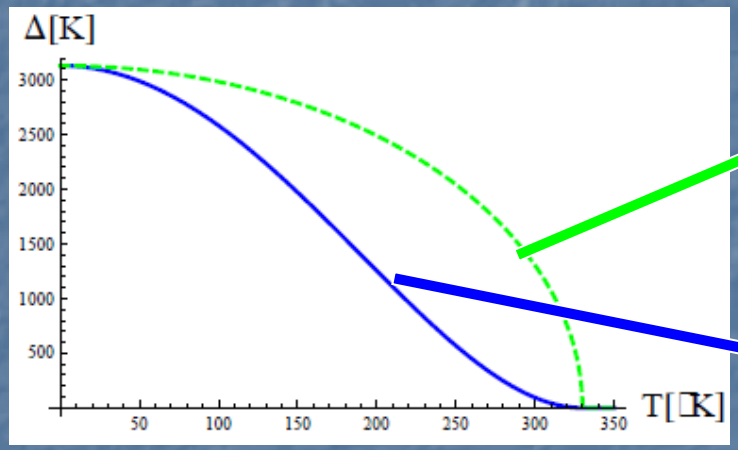
where $\varepsilon(\boldsymbol{k})$ **is the electron dispersion without CDW**

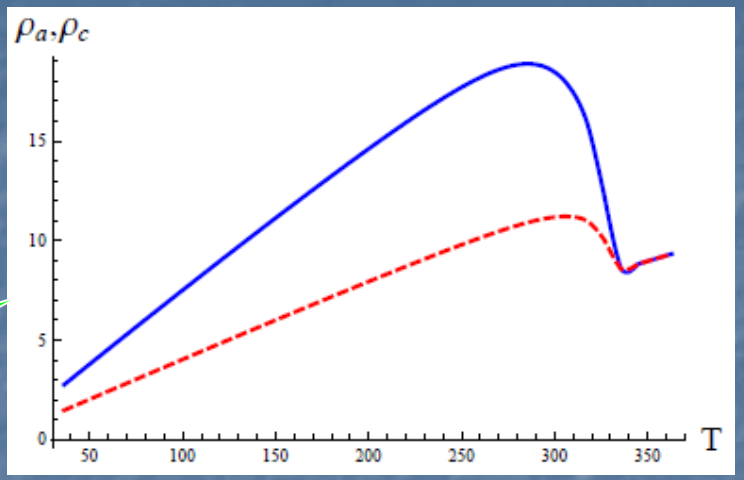
Explanation

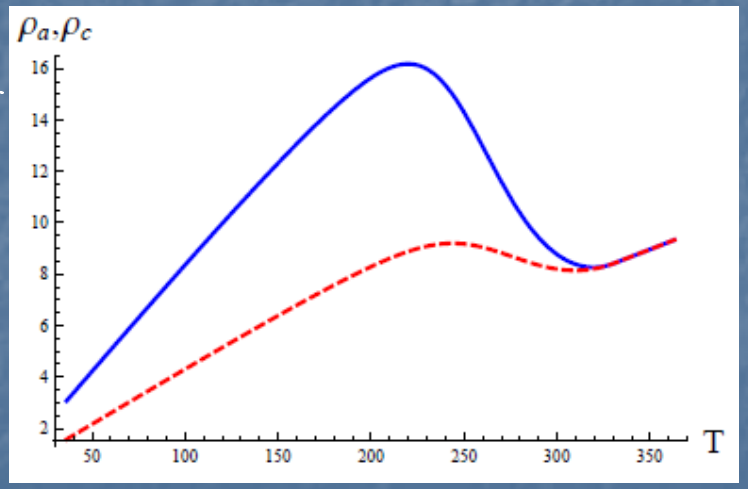
temperature dependence of CDW gap is given by

$$\Delta_0(T) \approx \Delta_0\left(1 - T^2/T_c^2\right)^{\alpha}, \ \alpha \geq 1/2.$$

α=1/2 (solid blue line)
α=2 (dashed green)







Temperature dependence of various conductivity components is sensitive to the T-dependence of CDW gap Δ(T), determined by fluctuations. This allows to compare various theoretical predictions of Δ(T) with experiment.
It best agrees well with experiment for $\alpha \approx 1.5$
.

Conclusion

The quasi-isotropic conductivity in the normal state of untwinned RTe_3 compounds is broken by the CDW gap appearing below T_{CDW}

The sliding of CDW in rare-earth trirellurides is only observed when the current is applied along the direction of the Q-vector, namely c-axis. That is the clear manifestation of the unidirectional CDW in these two-dimensional systems.

We explain conductivity anisotropy by the momentum-dependent CDW gap. It removes the electron states from FS parts with larger component V_a^2, thus breaking the a-c isotropy of conductivity.

The performed calculations of conductivity in the τ-approximation with electron dispersion modified by the momentum-dependent CDW gap (determined from ARPES) agrees well with experimental data on conductivity in various RTe_3 compounds.

This allows to specify the electron dispersion parameter $t_\perp$ and the temperature dependence of CDW gap close to T_{CDW}

Similar calculation allows to obtain information about the momentum dependence of the CDW/SDW energy gap even if ARPES data are not available