V_2O_3 Mott transition visited by TEP under pressure

GDR thermoélectricité:

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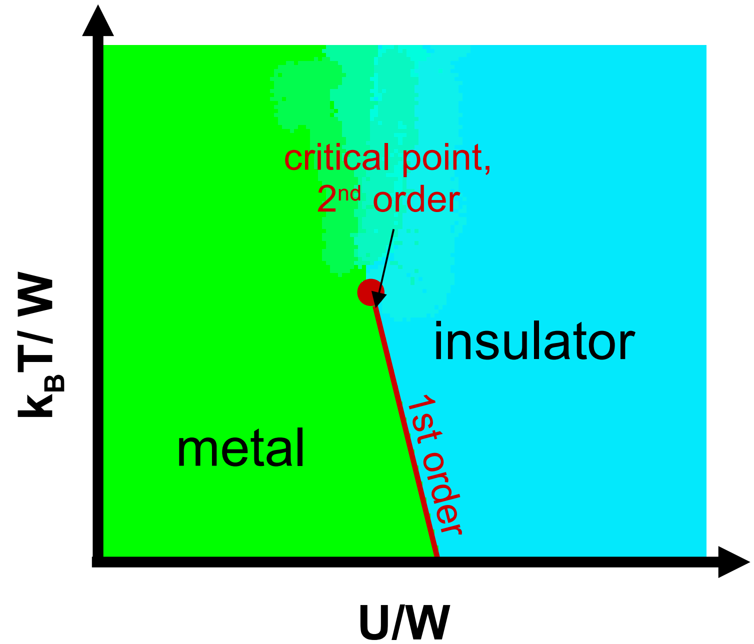
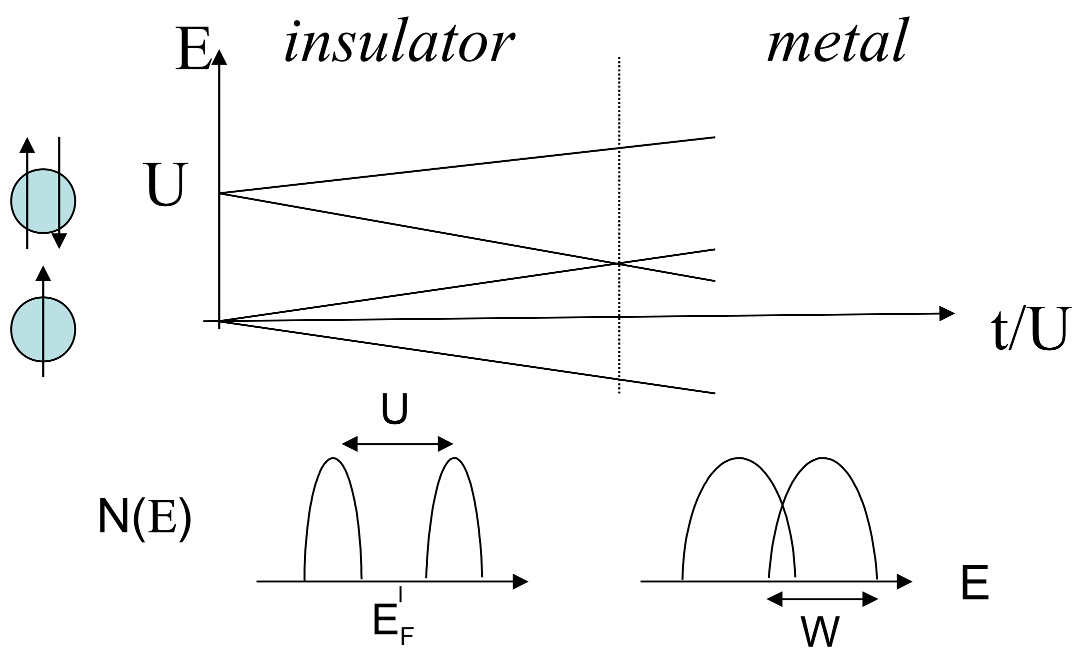
Part of my Ph.D. thesis:
Investigation of the Mott transition
in chromium doped V_2O_3 by means of
ultrasound and thermopower experiments

Nancy, 08.07.2009

The Mott transition: what is a Mott transition?

- First description by N. F. Mott
- Transition between metallic and insulating phase, localisation of charge carriers due to electron-electron interaction
- No symmetry breaking
- First order transition, e.g. induced by external pressure
- Above the critical point continuous crossover



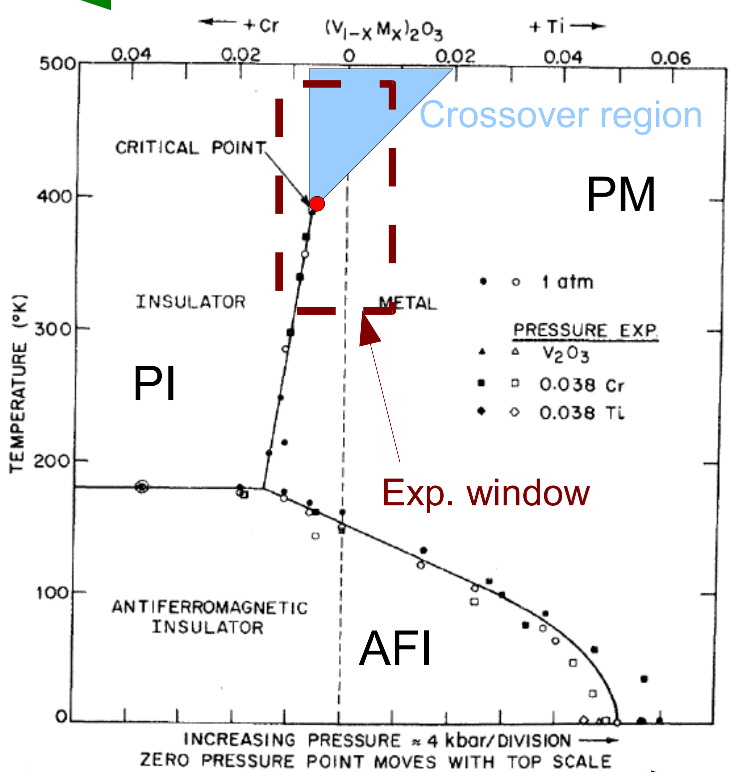


singular quantities:
probability of double site occupation →
-density of states, resistivity etc.

The sample system V_2O_3: phase diagram

Phase diagram from resistivity and susceptibility

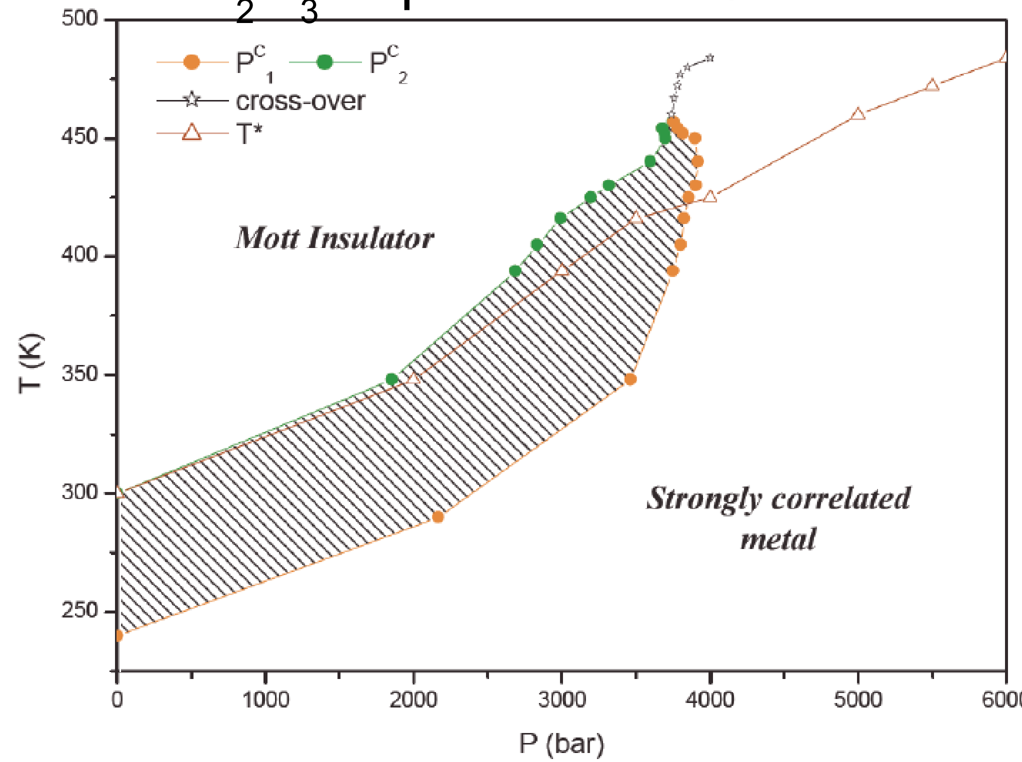
Doping with Cr



Hydrostatic pressure

after McWhan et al. PRL, 1971

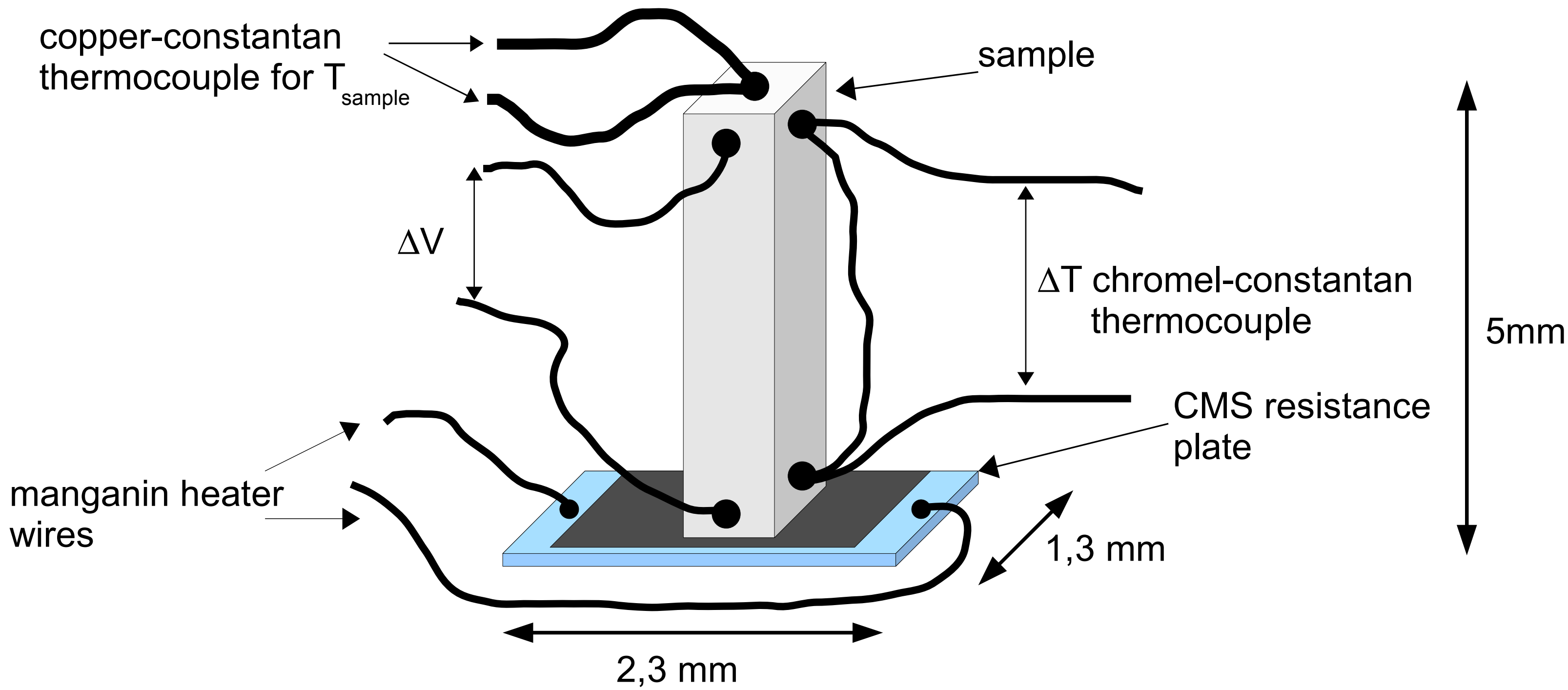
Phase diagram from resistivity for V_2O_3 doped with 1.1% of Cr



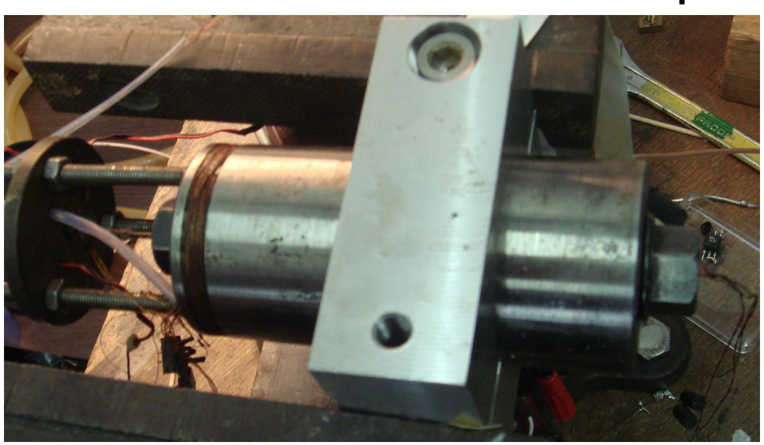
Limelette et al. Science, 2003

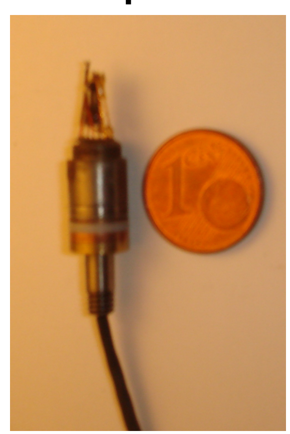
Critical point: (T_c = 457.5 K, p_c = 3738 bar)

Experimental set-up



Set-up in the in pressure cell

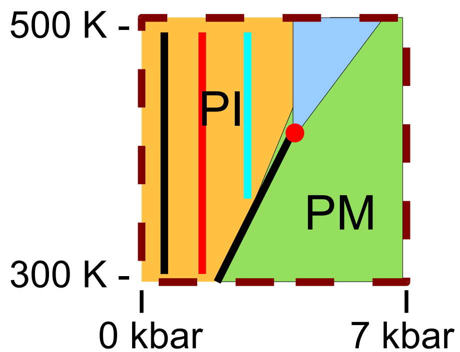


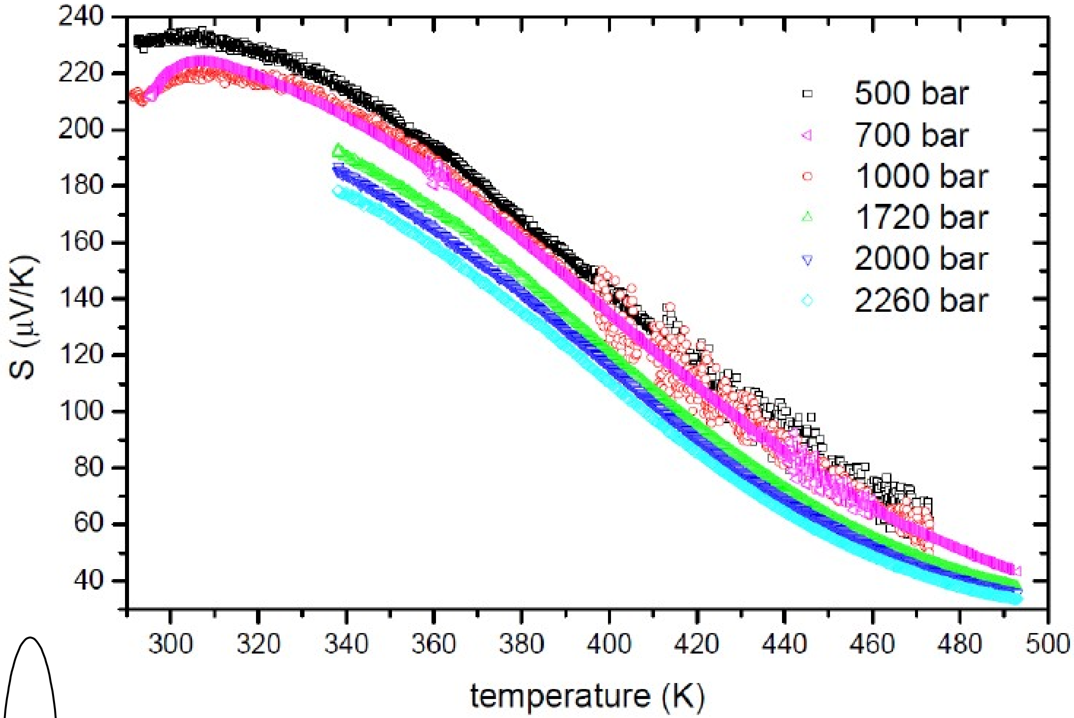


pressure:
$p \leq 7$ kbar

temperature:
$300\ K \leq T \leq 500\ K$

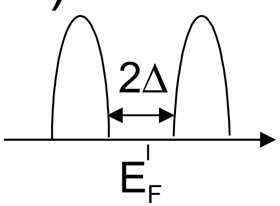
Temperature dependent experiments in the insulating state





Description in terms of a semiconductor (Mott formula):

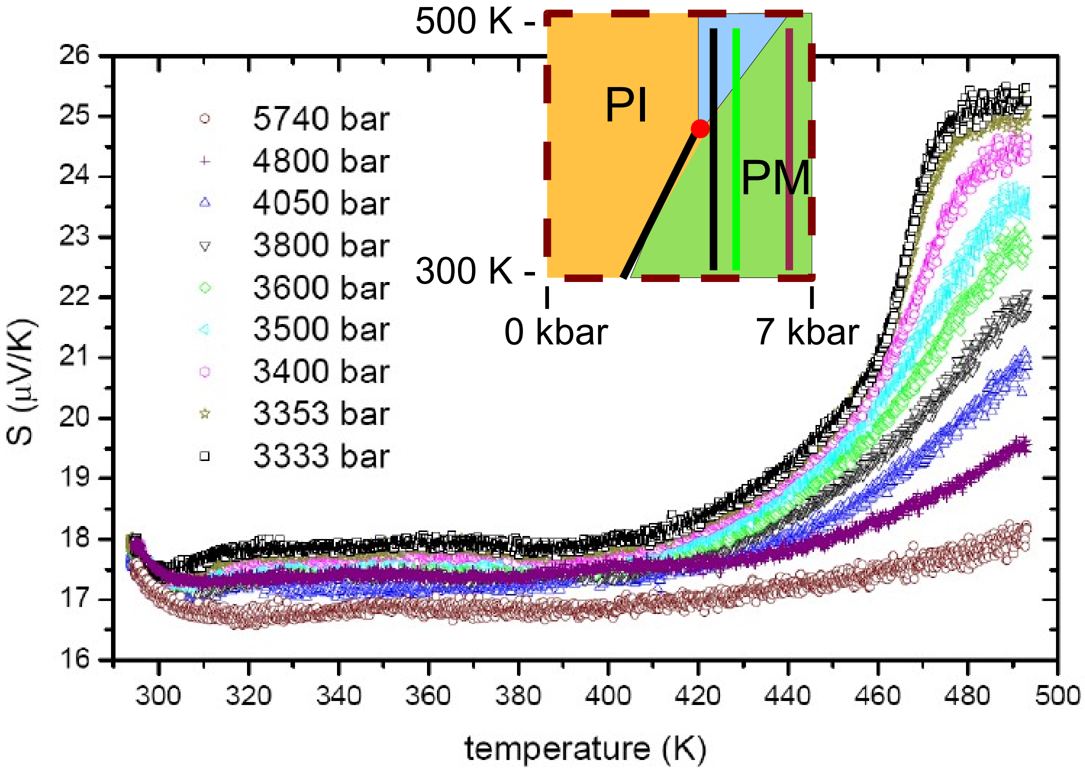
$$S = \frac{k_B}{e} \frac{\Delta}{k_B T} + A$$



→ Activation energy: Δ ≈ 200 meV

Photo emission experiment: Δ ≈ 120 meV same order of magnitude
(Mo et al., PRB, 2006)

Temperature dependent experiments in the metallic state



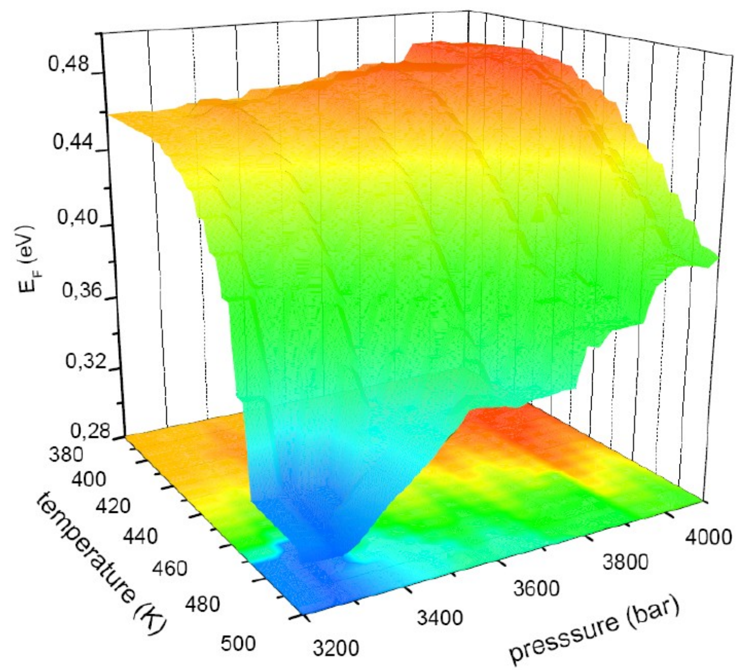
1. Free electron model:

$$S = BT + AT^{-1}$$

Diffusion term:

$$S^d = BT = \frac{\pi^2}{6}\frac{k_B}{e}\frac{T}{T_F}$$

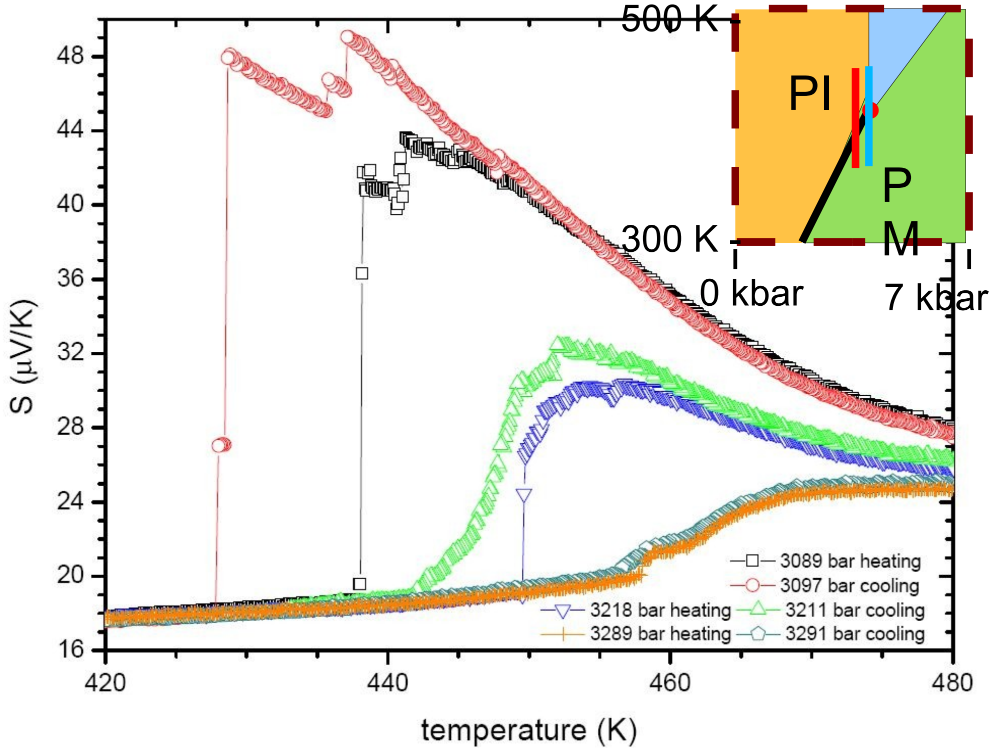
Linear fit of ST vs T^2 plot:
A ≈ const., evolution of E_F:



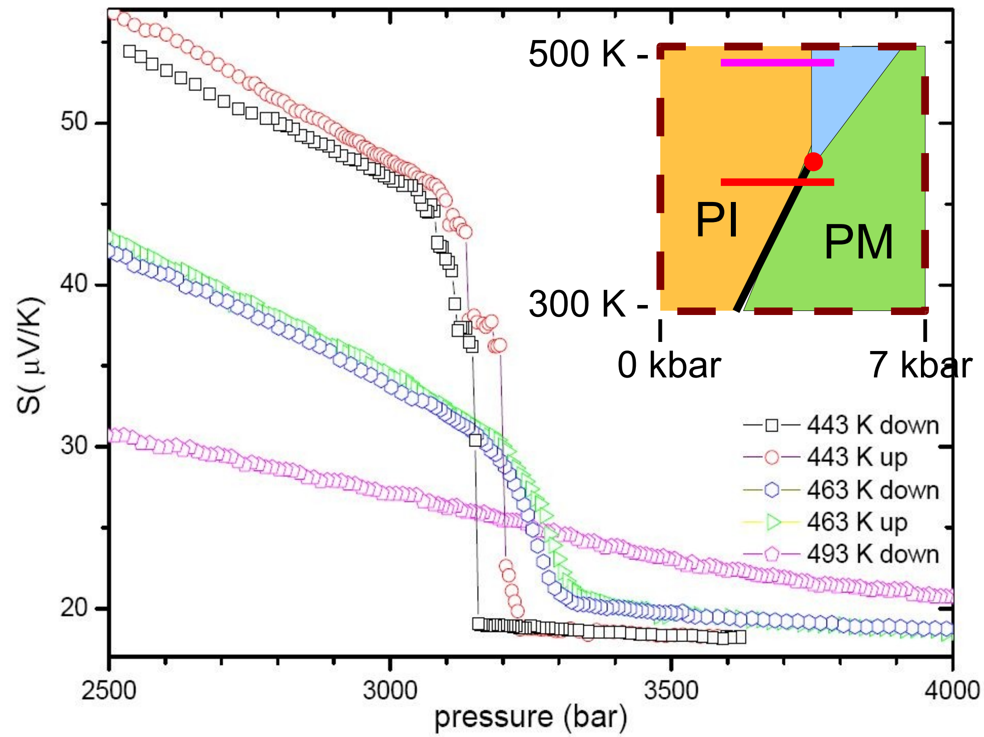
Order of magnitude $E_F \approx 0.5$ eV,
Breakdown of E_F at the transition

2. Inflexion points: crossover

Experiments in the transition region



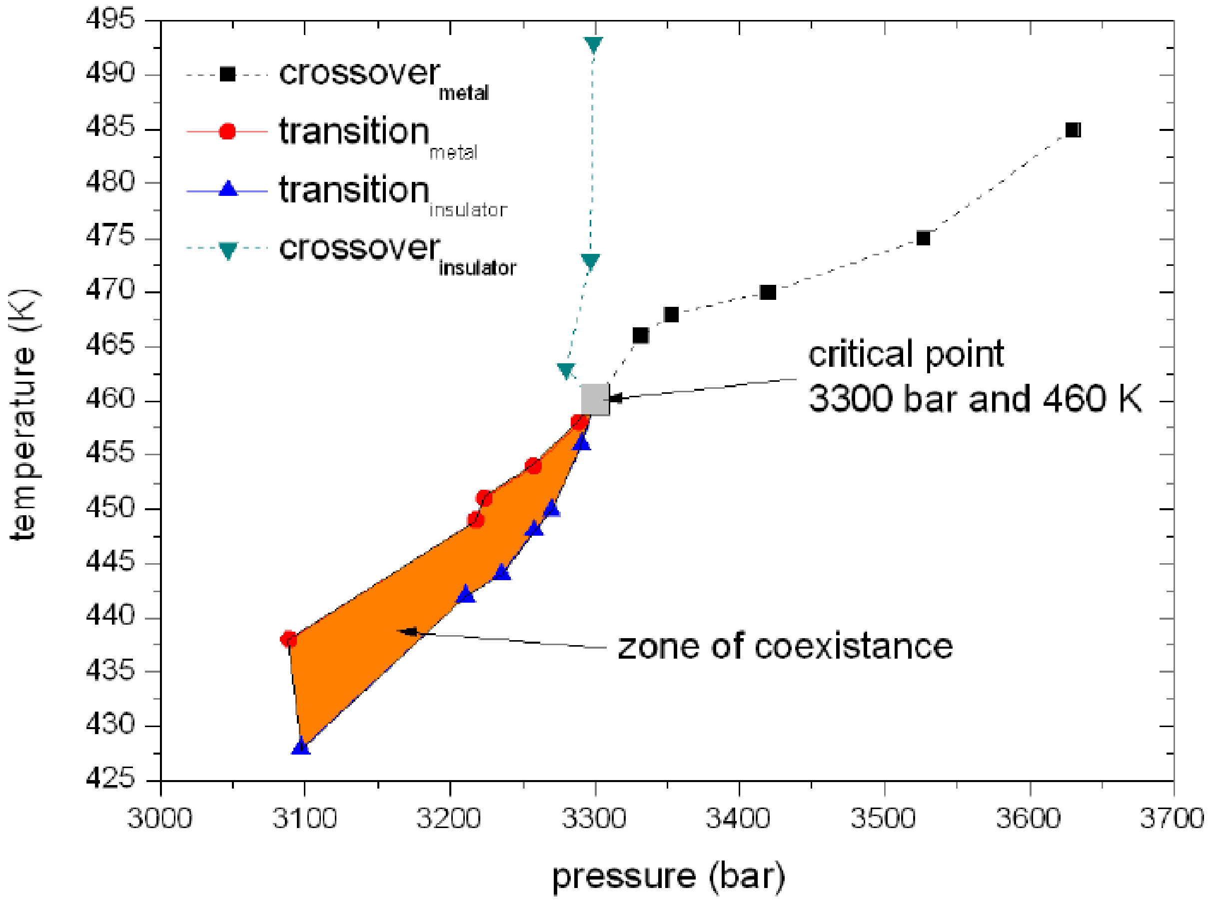
1. Transition temperatures at fixed pressures.
2. Disappearance of discontinuity and hysteresis: T_c = 460 ± 2 K



1. Transition pressures at fixed temperatures
2. Disappearance of hysteresis: p_c = 3300 ± 5 bar
3. Above T_c: second crossover line from inflection points

Phase diagram

- Critical point : (460 ± 2 K, 3300 ± 5 bar)
- several transition temperatures and pressures below critical point
- two crossover lines above the critical point



Comparison: phase diagram of Limelette and ultrasound:

1. T_c within experimental errors identical
2. p_c different due to different doping
3. Qualitatively good agreement

How to interpret thermopower data?

Relaxation time approximation : $S = \frac{K_1}{eTK_0}$

where $K_n = -\frac{1}{3}\int 2\tau_k v_k v_k \left(-\frac{\partial f_0}{\partial \epsilon}\right)|_{\epsilon=\mu} (\epsilon(k) - \mu)^n \, d^3k$

Definition electrical conductivity with transport coefficients: $\sigma = e^2 K_0$

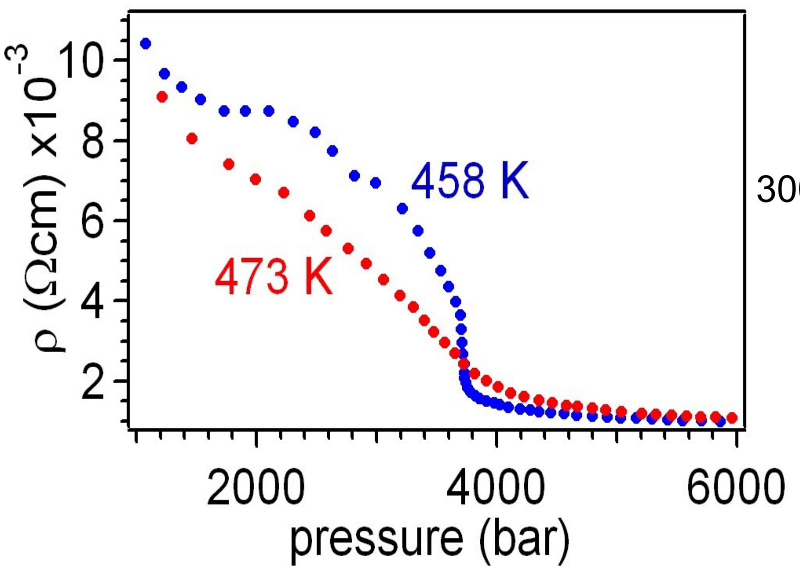
$\longrightarrow \rho \propto K_0^{-1}$

Relation of our data for *S* to resistivity gives information about transport coefficient K_1: $K_1 \propto \frac{ST}{R}$

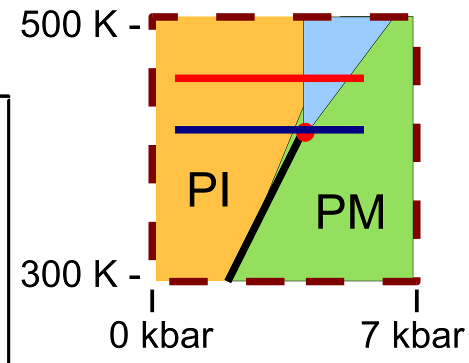
K_1 sensitive to particle hole symmetry, perfect symmetry: $K_1 = 0$

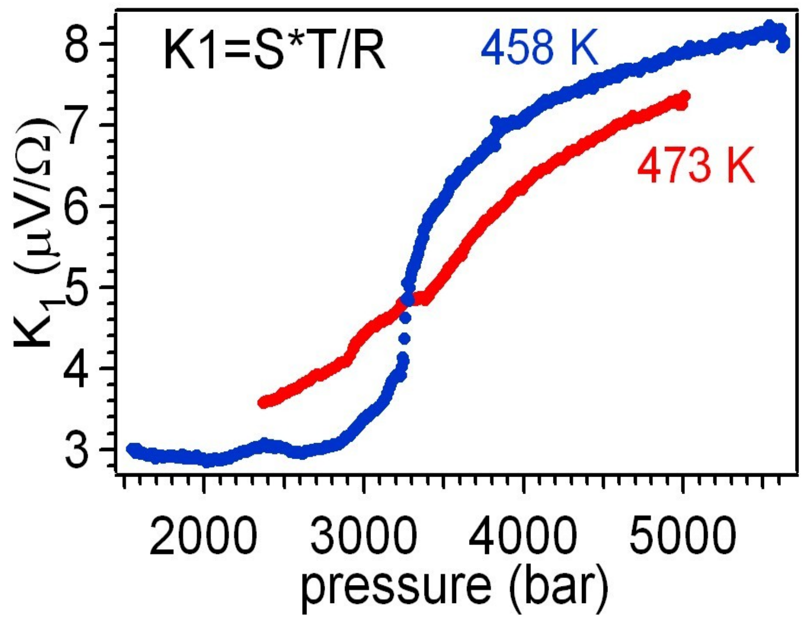
Estimation of K_1 yields information about the quasi-particle peak that is responsible for the conduction

Comparison to data from resistivity measurements



Resistivity data: P. Limelette PhD thesis, 2003





Qualitative explanation: increasing pressure approaches metallic phase → quasi-particle peak becomes well defined → asymmetries less averaged out → increase of K_1

Interpretation: change in K_1 smaller than the one of the conductivity

→ evolution of the particle hole symmetry plays no crucial role in the transition

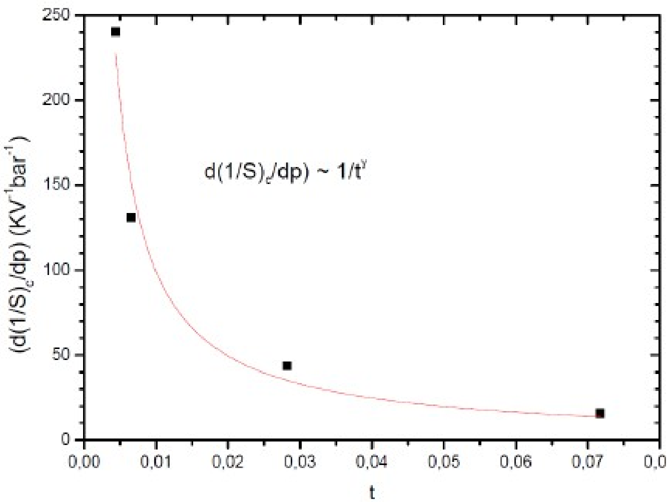
Scaling with the scaling laws of resistivity

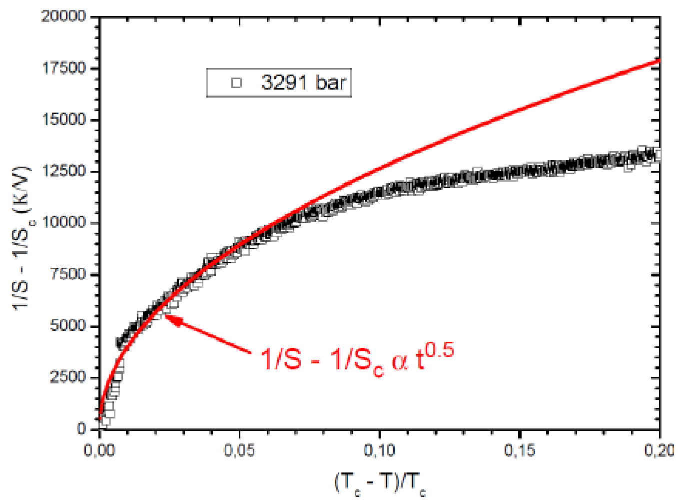
$$\frac{1}{S} \propto \frac{\sigma T}{K_1}$$

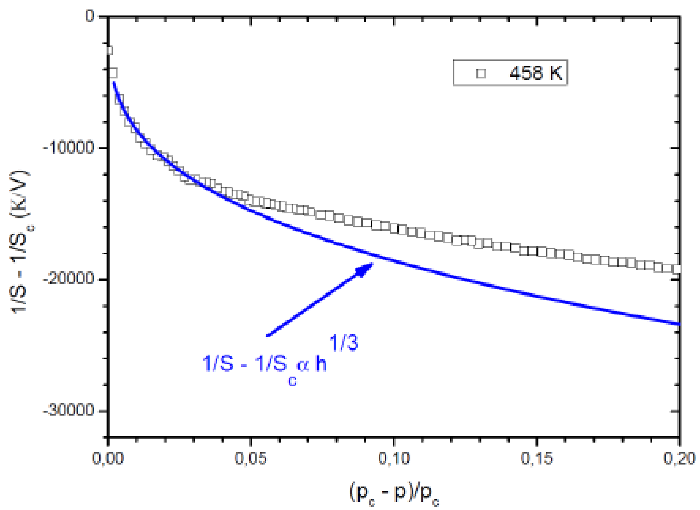
Vicinity of transition: T ≈ constant, change in conductivity dominates → $\frac{1}{S} \propto \sigma$

Comparison with power laws from σ (Limelette et al. Science 03):

$$\left(\frac{dm}{dp}\right)_{p=p_c}(T) \propto \frac{1}{t^\gamma} \qquad \sigma - \sigma_c = t^\beta \qquad \sigma - \sigma_c = h^{1/\delta}$$





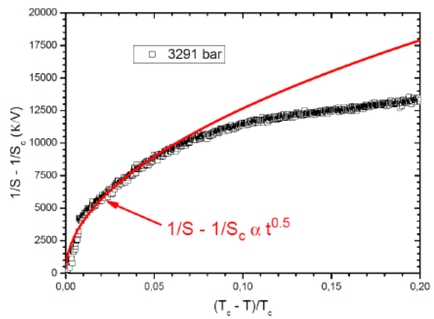


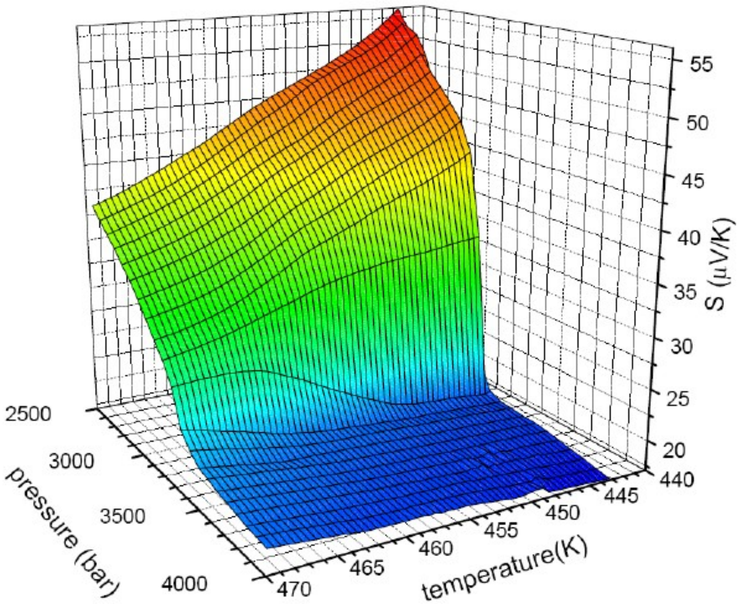
Near the transition good agreement with the mean field exponents γ=1, β=0.5, and δ=3

- assumptions are correct
- critical behaviour of S is governed by σ

Conclusion and outlook

- Conclusion
  - Thermopower experiment: adapted for high temperatures and variable pressure cell
  - Observation of the MIT by TEP
  - Scaling with mean field exponents





- Further work
  - More realistic band structure calculations needed for theoretical understanding of the data (LDA+DMFT) of the thermopower experiment

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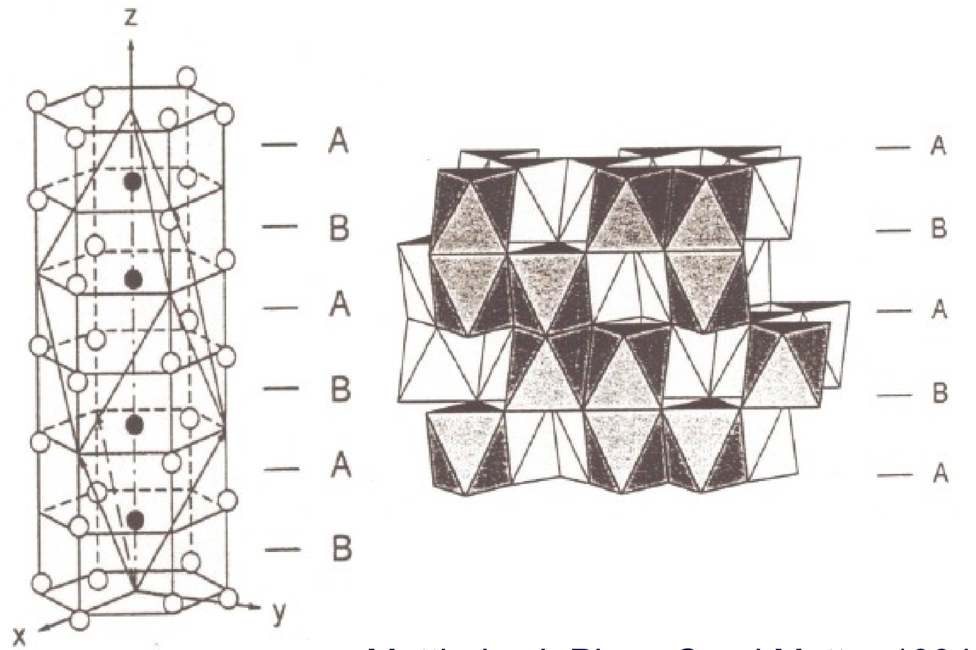
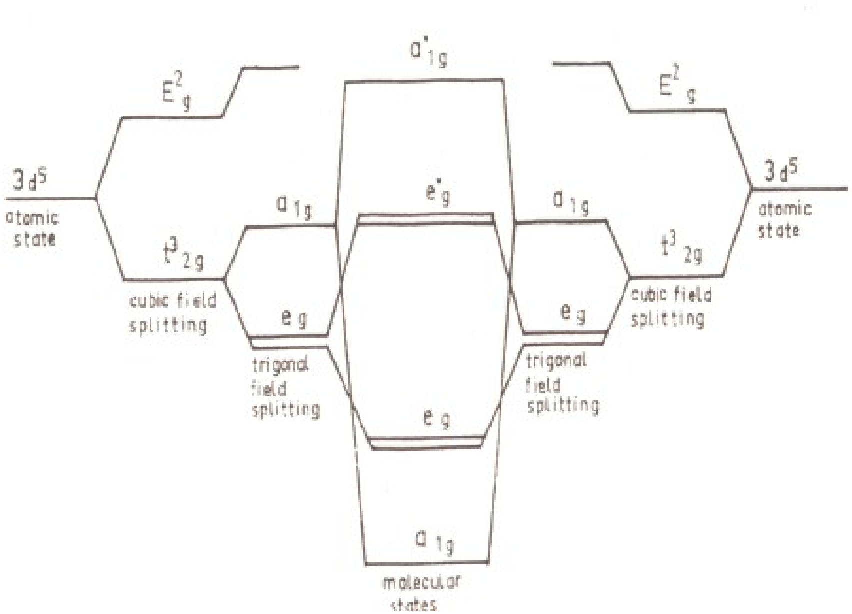
Thank you for your attention!

Crystal structure of V2O3

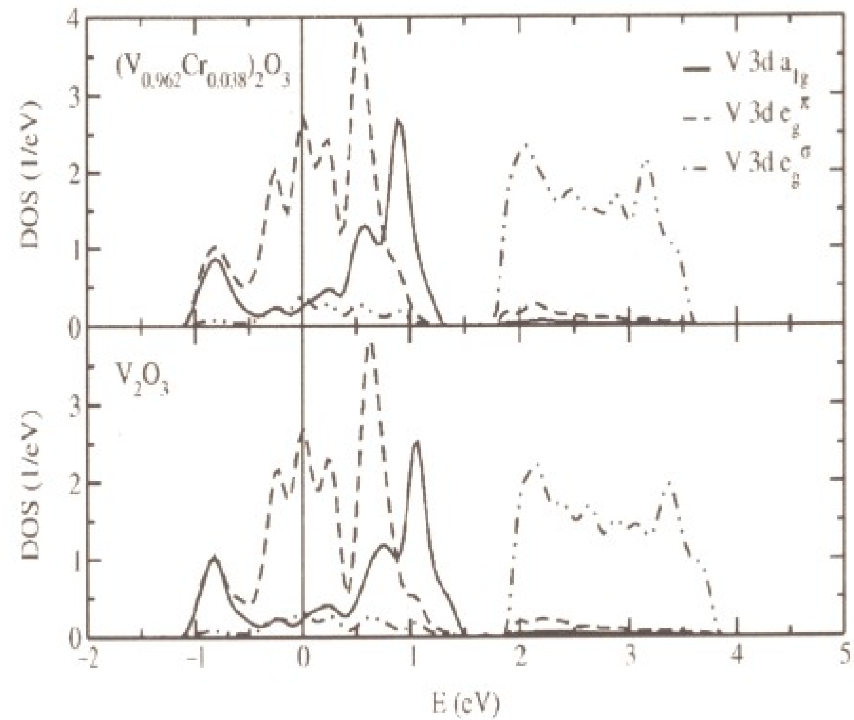


Mattheis, J. Phys: Cond Matter 1994

Band structure

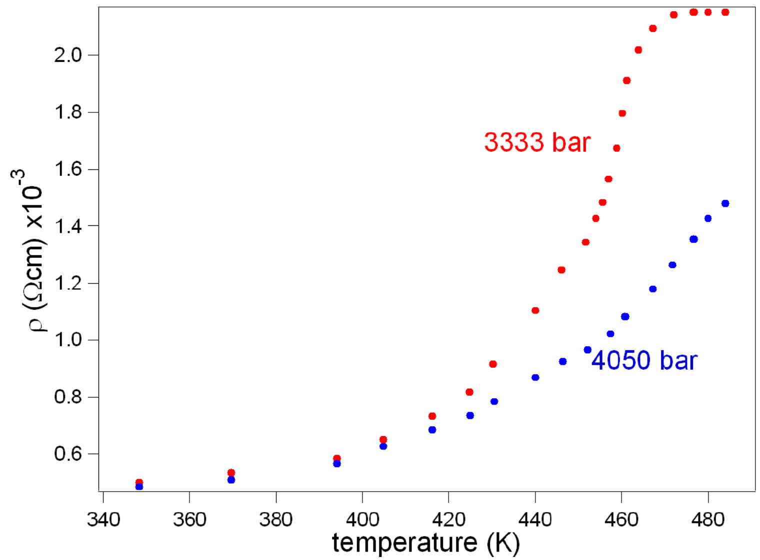


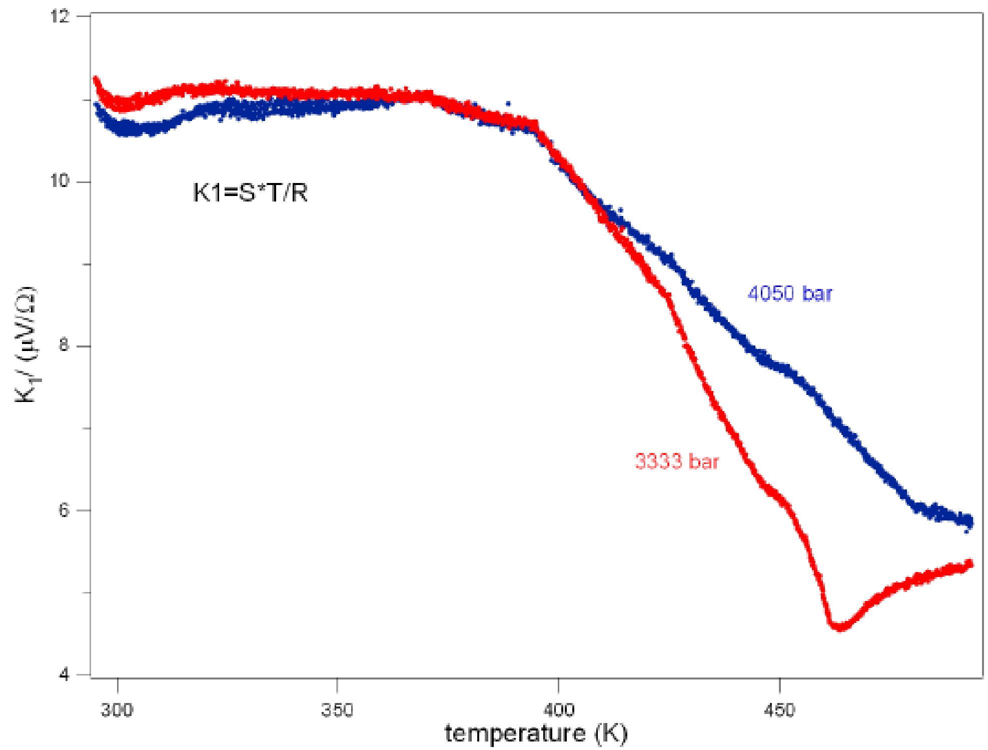
Castellani et al., PRB 1978



Held et al., PRL 2001

Comparison to resistivity in dT experiments





- Metallic phase: quasi-particle peak is well defined, stays unchanged until 390 K
- Approaching the insulating or the crossover region: quasiparticle peak starts to broaden, asymmetries are more and more averaged out → K_1 becomes smaller

$ZT \approx 3\text{-}4 \times 10^{-3}$ (at 400 K and 5000 bar, in the metallic phase)