THERMOELECTRIC PROPERTIES OF $Ba_8Au_{5.25}Ge_{40.3}\square_{0.45}$ UNDER HYDROSTATIC PRESSURE

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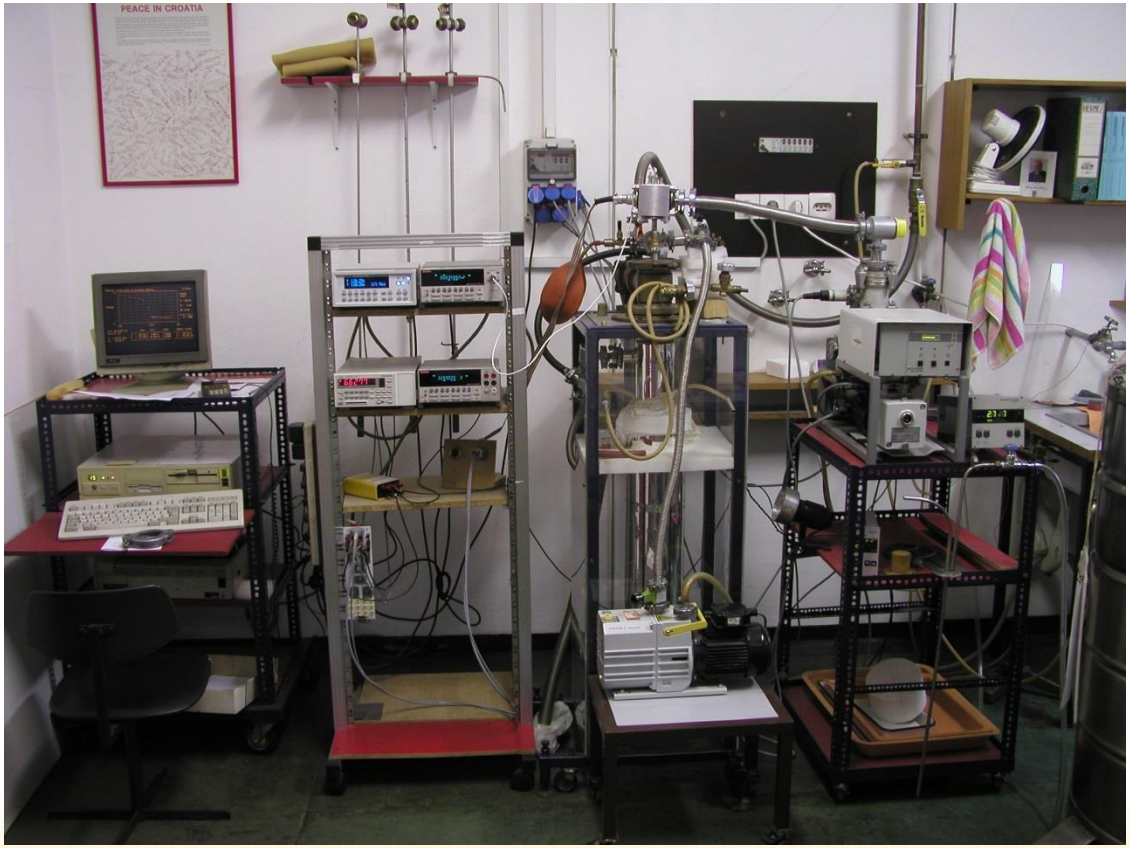
Zagreb

C-MAC meeting, 14. 10. 2013., Vienna

Laboratory for the physics of transport phenomena

- Thermal conductivity – 1.5 – 300 K

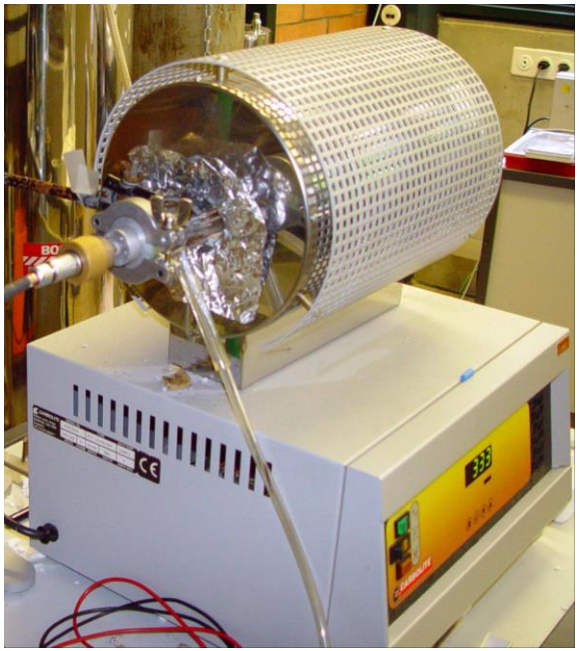


Ana Smontara

Laboratory for the physics of transport phenomena

Ante Bilušić

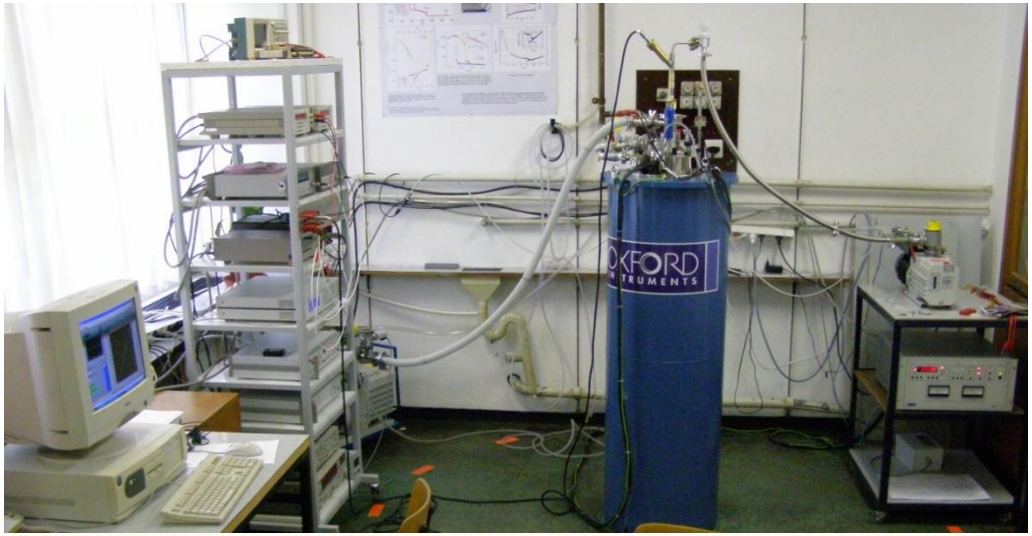
- Thermal conductivity – 1.5 – 300 K
- Electrical resistivity and thermopower (1.5 - 1000K)



Laboratory for the physics of transport phenomena

Kristijan Velebit

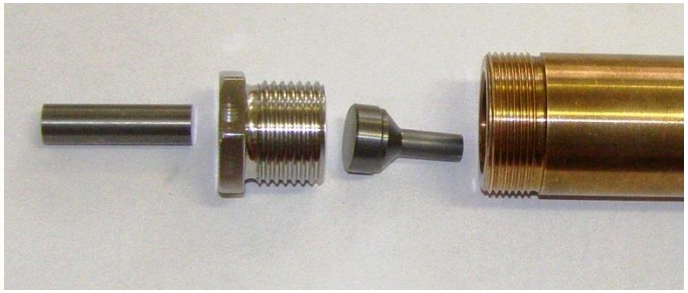
- Thermal conductivity – 1.5 – 300 K
- Electrical resistivity and thermopower (1.5 - 1000K)
- Magnetic field 10 T (thermal conductivity – thermal radiation correction) (*L. Demkó et al., Eur. Phys. J. (2010)*)

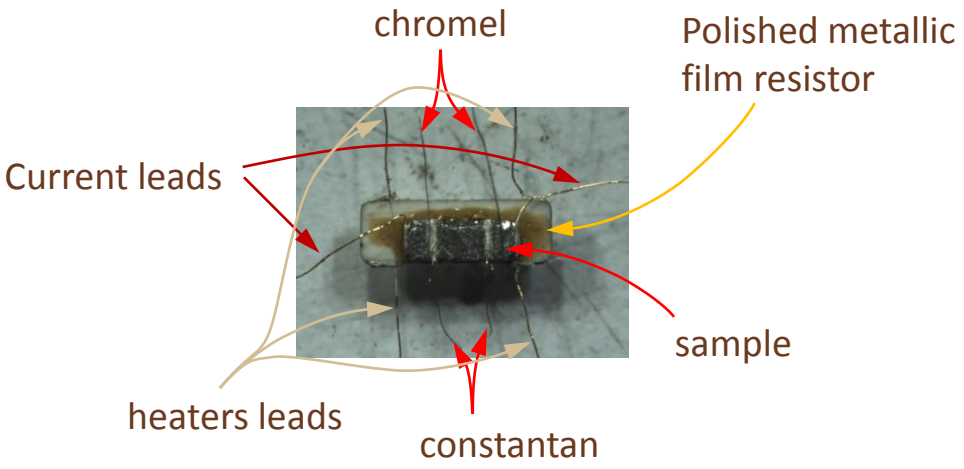


Laboratory for the physics of transport phenomena

Neven Barišić

- Thermal conductivity – 1.5 – 300 K
- Electrical resistivity and thermopower (1.5 - 1000K)
- Magnetic field 10 T (thermal conductivity – thermal radiation correction)
- High pressure
  - 3 GPa – piston-cylinde





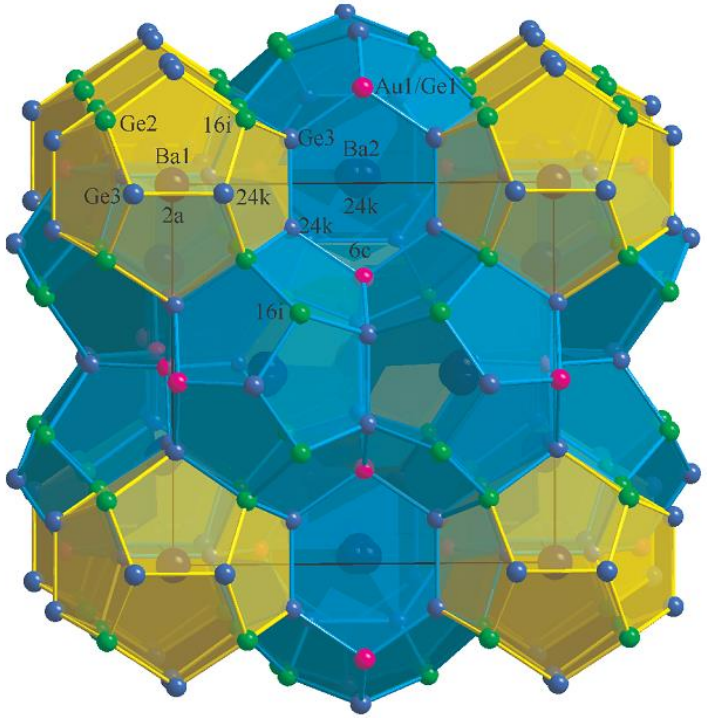
Type I clathrates

- Ba based prospective:
  - $Ba_8Ga_xGe_{46-x}$ ZT - 1.35 for n-type (x=16) *(A. Saramat et al. (2006))*
    1.1 for p-type (x=18) *(H. Anno et al. (2002))*

- $Ba_8Au_xGe_{46-x-y}\square_y$
- $Ba_8Ag_xGe_{46-x-y}\square_y$
- $Ba_8Au_xSi_{46-x}$
- $Ba_8Ag_xSi_{46-x}$

I. Zeiringer, P. Rogl (2011) - study of homo

- some transpo



Yellow - dodecahedra; cyan - tetrakaidecahedra.

$Ba_8Au_xGe_{46-x-y}\square_y$ ($Pm\bar{3}n$)

- Binary - $Ba_8Ge_{43}\square_3$ – ordering of vacancies in the 6c sites –> $Ia\bar{3}d$
- Au solubility range – $x < 6$
- Lattice parameter increases
- Nonlinear y(x)

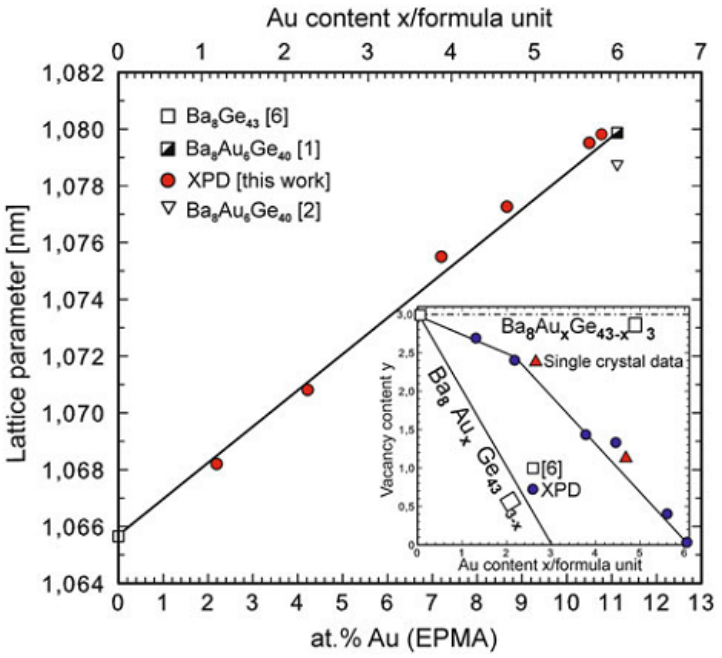


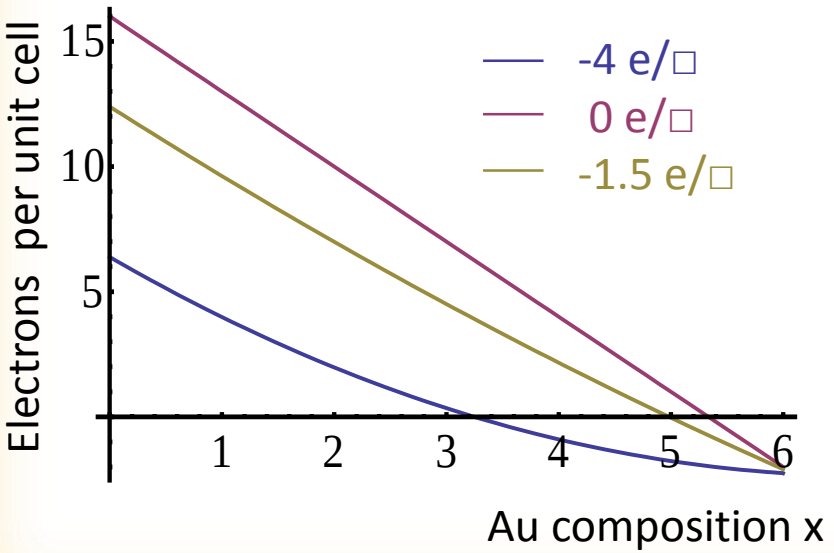
Fig. 1 Lattice parameters vs. Au-content for the clathrate type I solid solution $Ba_8Au_xGe_{46-x-y}\square_y$; the inset shows the filling of vacancies with increasing gold content derived from x-ray Rietveld refinement and single crystal data

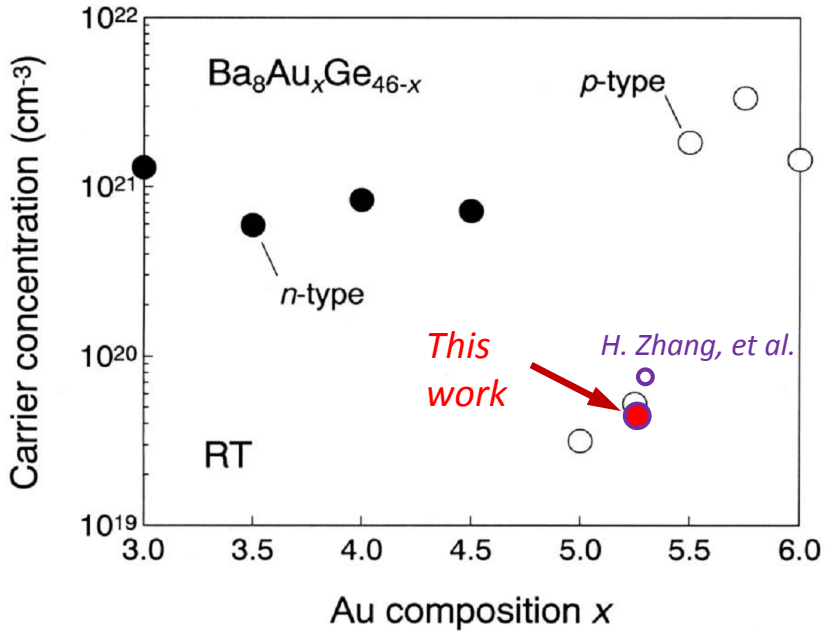
I. Zeiringer et al.(2011)

$Ba_8Au_xGe_{46-x-y}\square_y$ transport porperites

- n to p type crossover at x = 5
- $Ba_8^{2}Au_x^{-3}Ge_{46-x-y}^{?}\square_y$

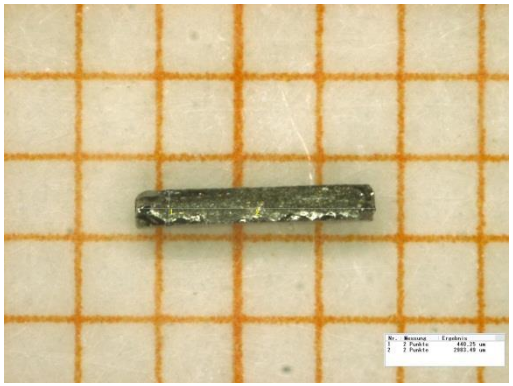
Zintl rule

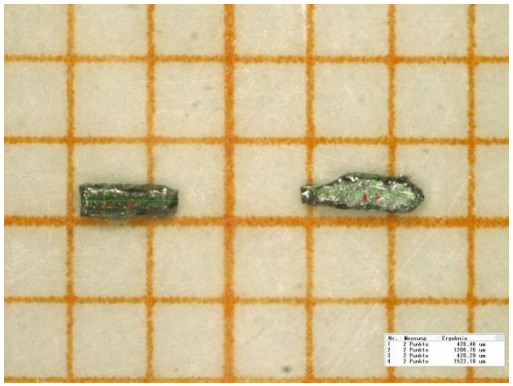


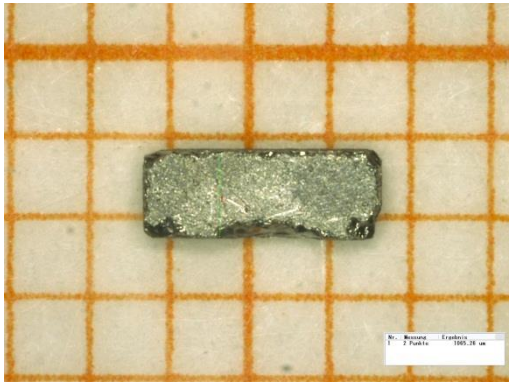


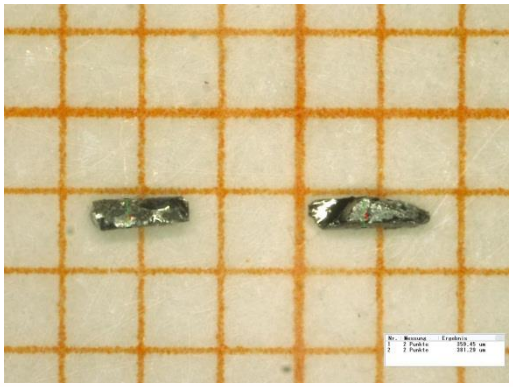
H. Anno et al., (2005)

$Ba_8Au_{5.25}Ge_{40.3}\square_{0.45}$ samples



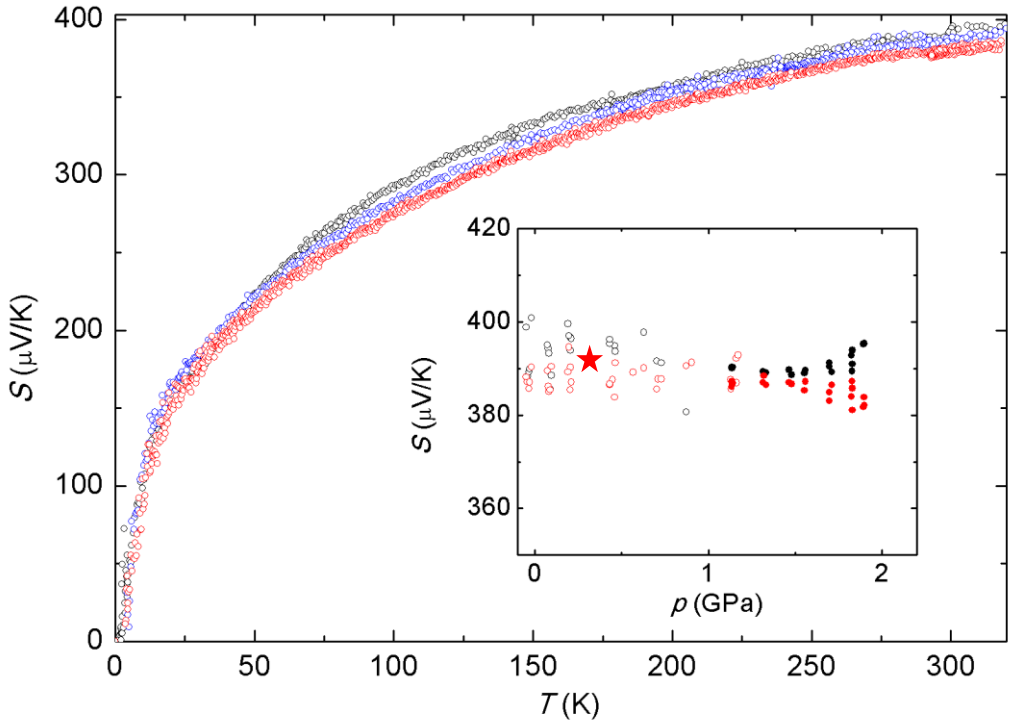






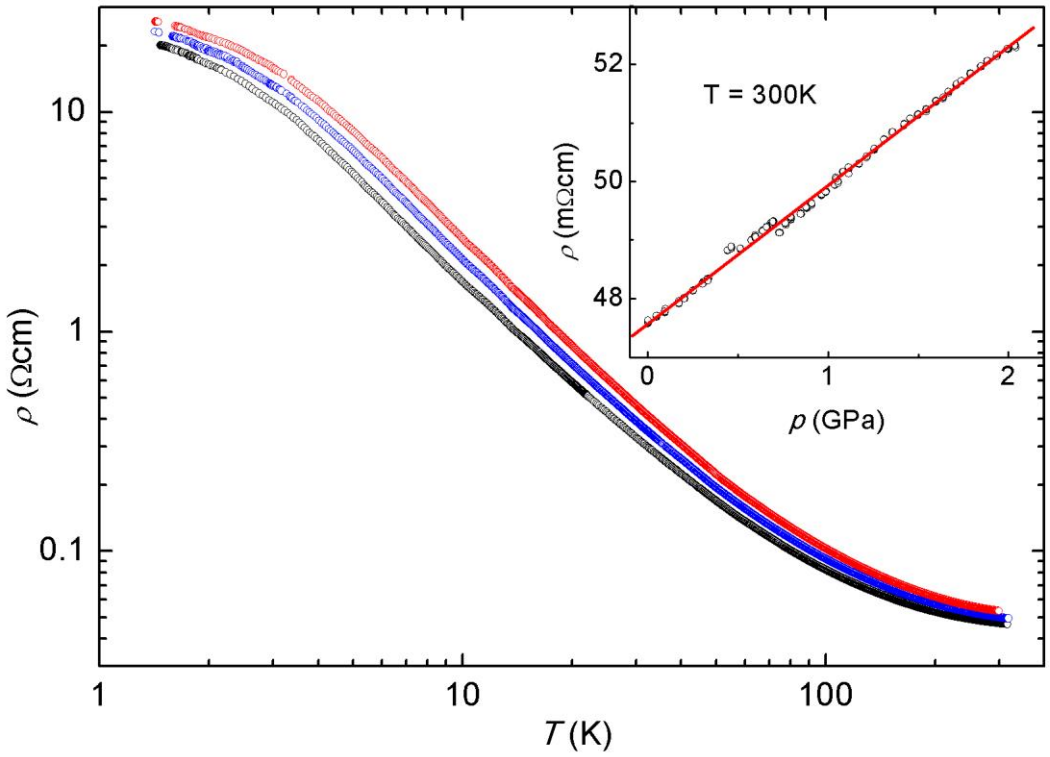
$Ba_8Au_{5.25}Ge_{40.3}\square_{0.45}$ under pressure

- Thermopower
  - logarithmic temperature behavior
  - „No" pressure dependence

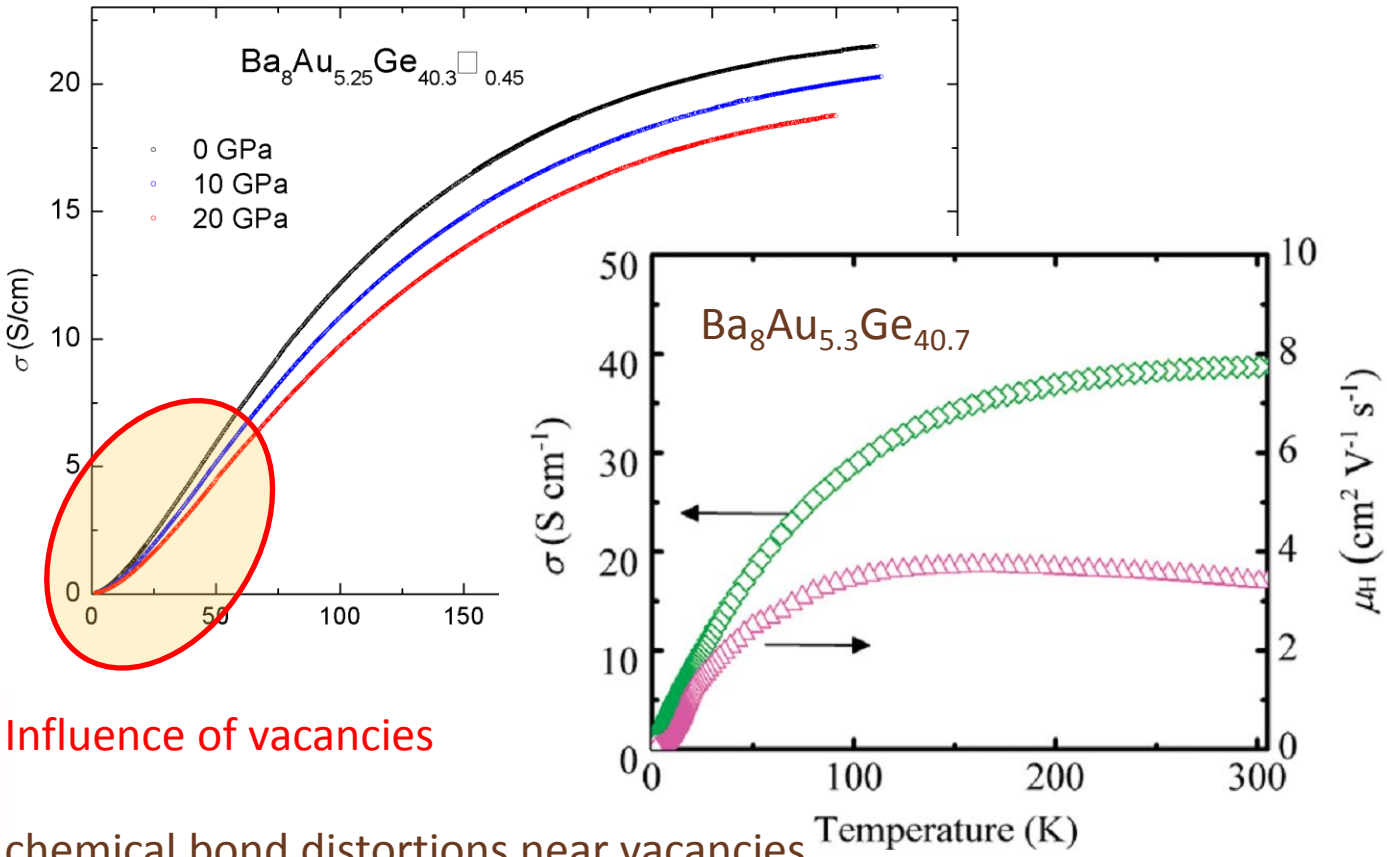


$Ba_8Au_{5.25}Ge_{40.3}\square_{0.45}$ under pressure

- Electrical resistivity



$Ba_8Au_{5.25}Ge_{40.3}\square_{0.45}$ under pressure

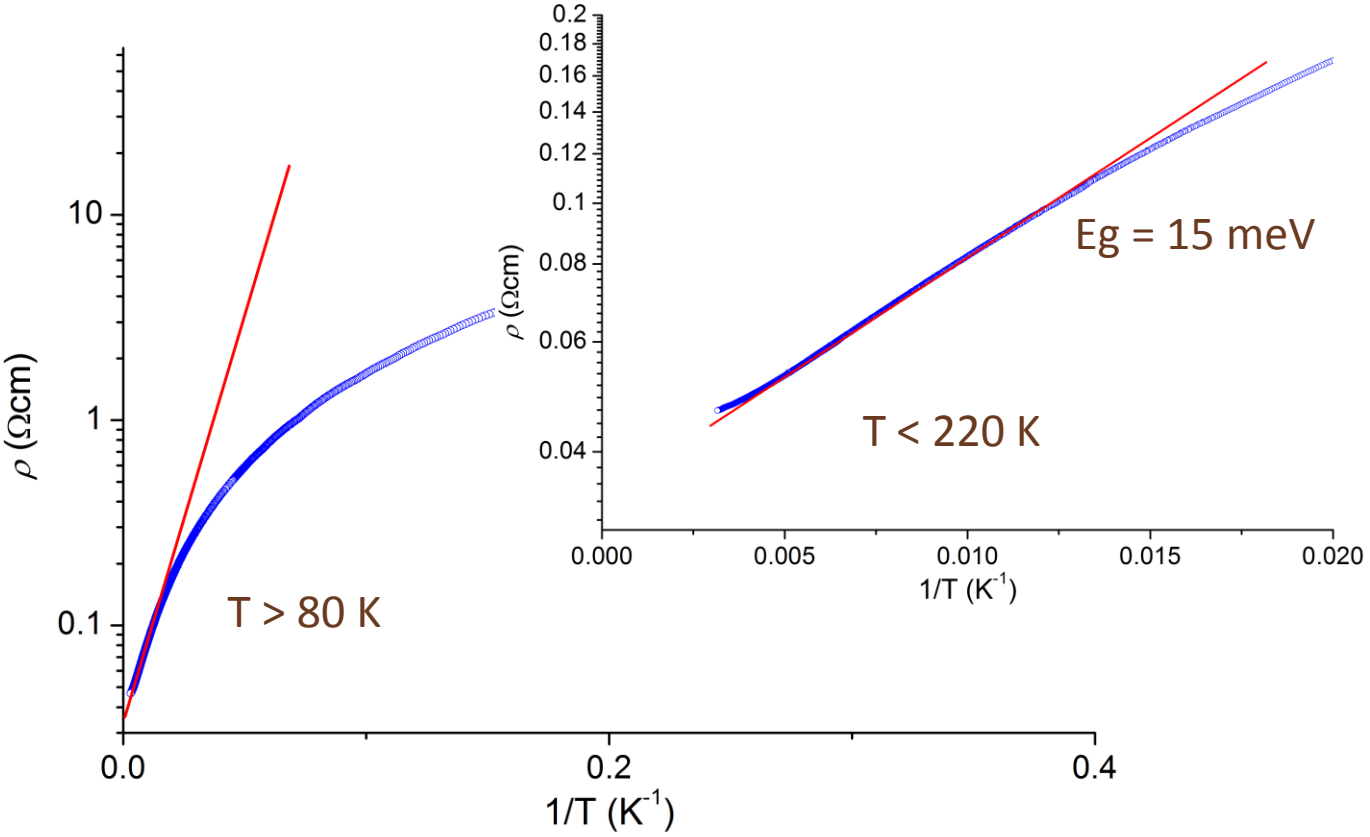


Influence of vacancies

chemical bond distortions near vacancies.

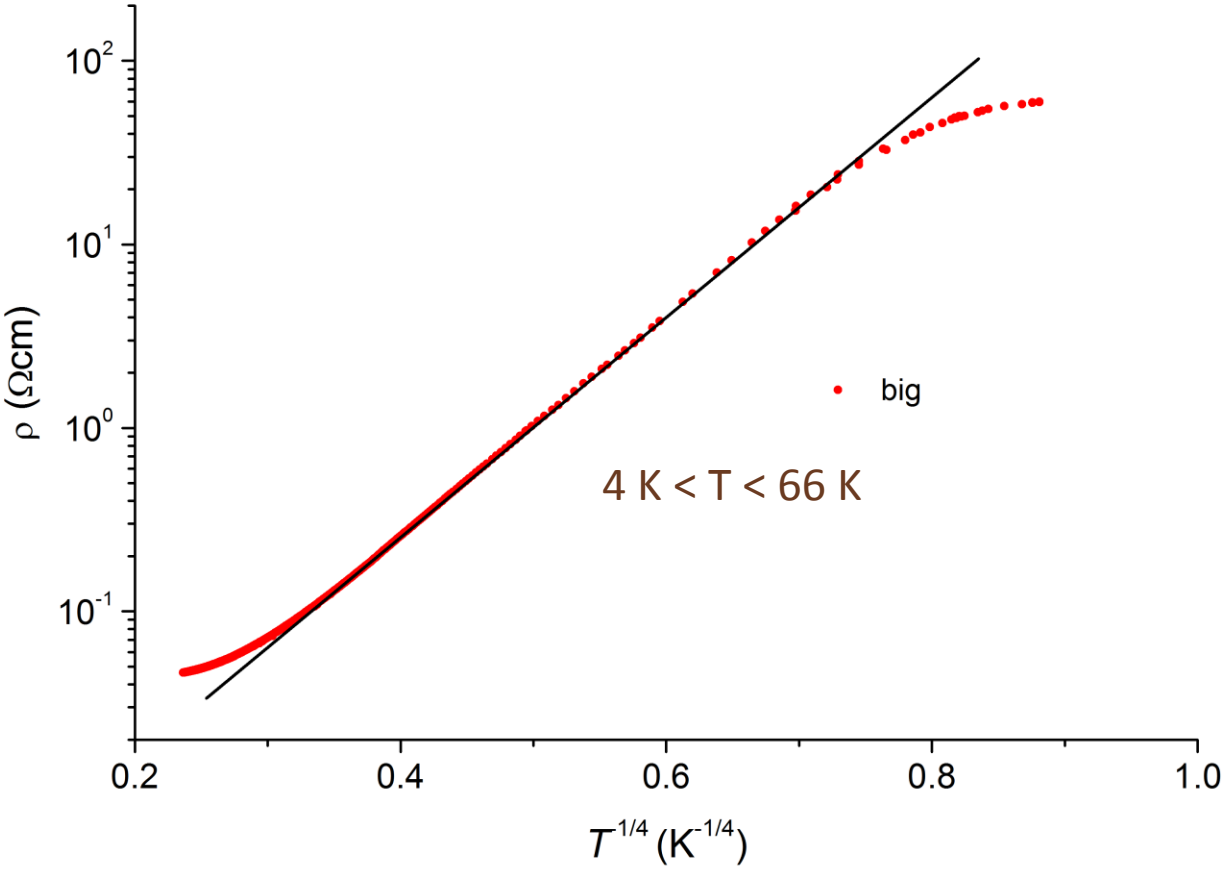
H. Zhang, et al., Inorg. Chem. ***50****, 1250 (2011).*

Semiconducting?

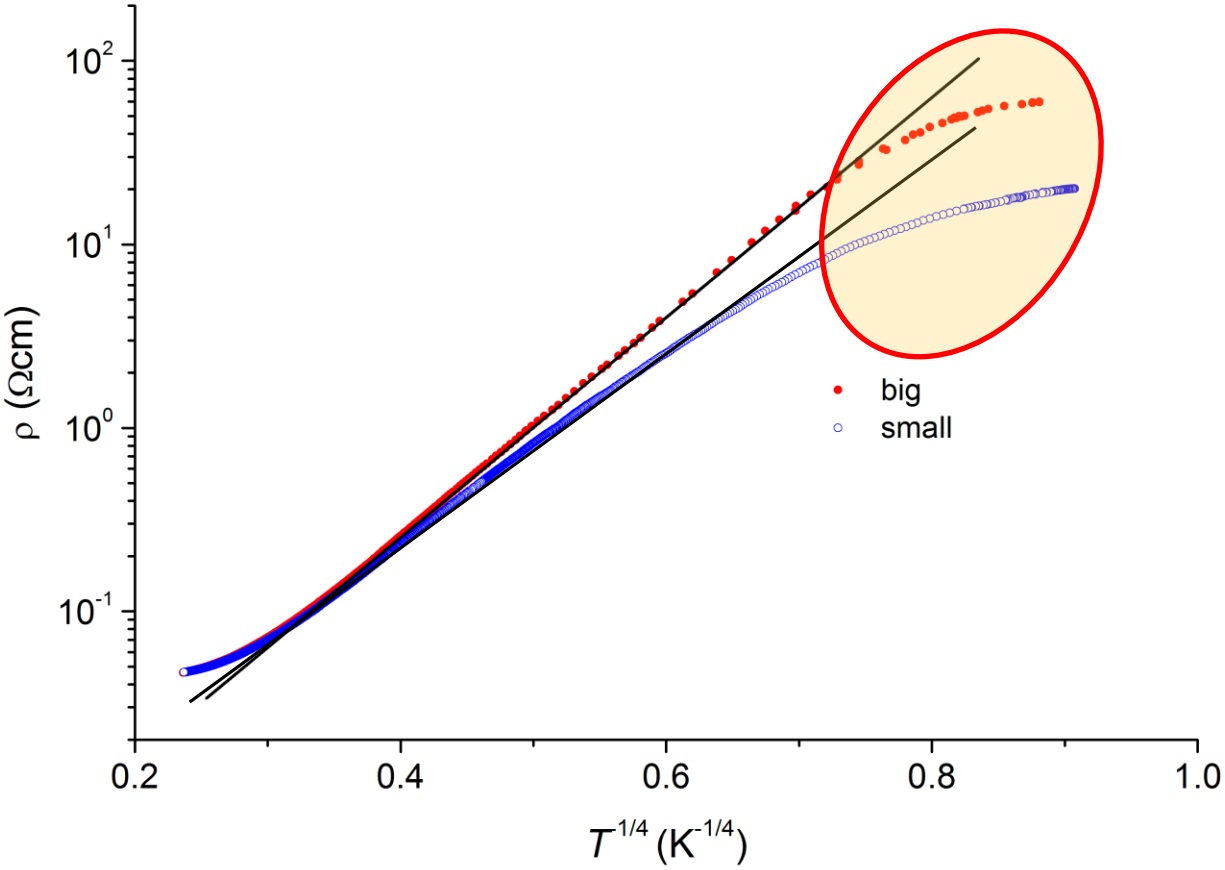


Eg = 300 meV, *(H. Zhang et al. (2011)).*

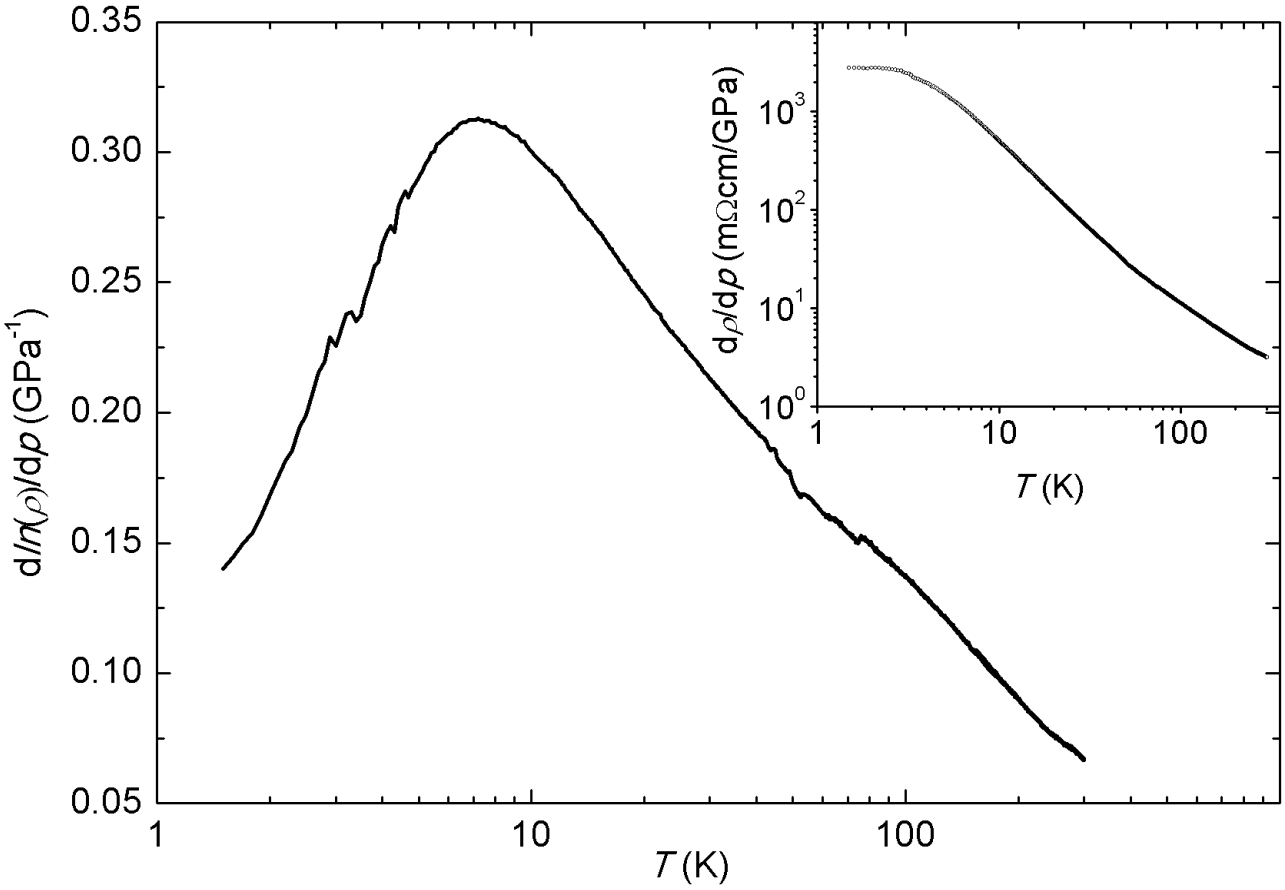
Hopping?



Hopping?



Influence of pressure



Summary

- Vacancy concentration –
  - preparation technique dependent
  - Influences transport properties at low temperatures
- Pressure -> broadens the gap
- Thermopower
  - logarithmic behavior
  - „Pressure independent”
- Investigate vicinity of x = 5 to determine gap dynamics and influence of vacancies

Thank you for your attention