Electric and magnetic properties of $Fe_{7-x}Ni_xSe_8$ single crystals

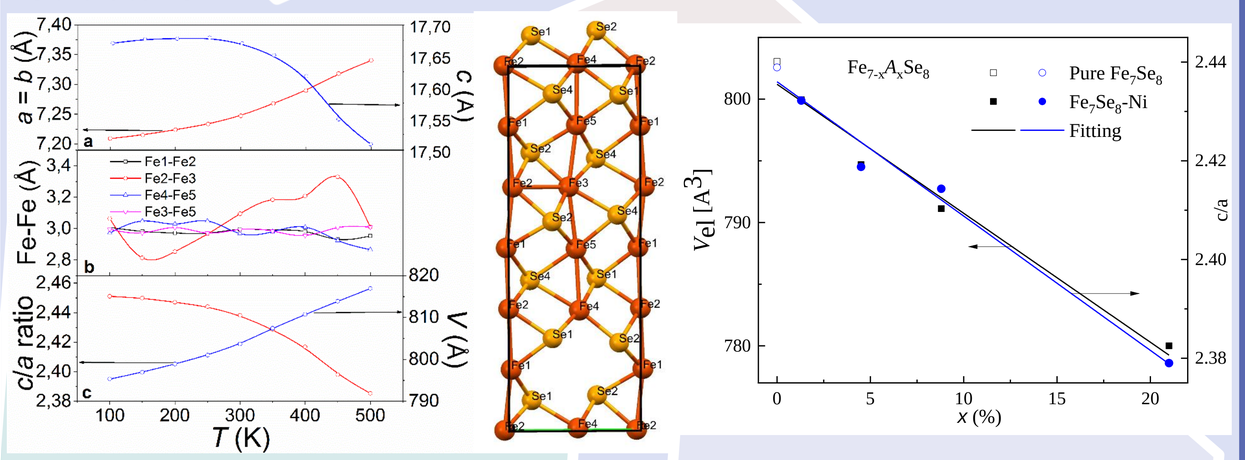
Authors: Y. T. Konopelnyk[1], M. Pękała[2], I. Radelytskyi[1], and P. Iwanowski[1]

Affiliations: [1]Institute of Physics PAS, Warsaw, Poland, [2]Chemistry Department, Warsaw University, Warsaw.

Introduction

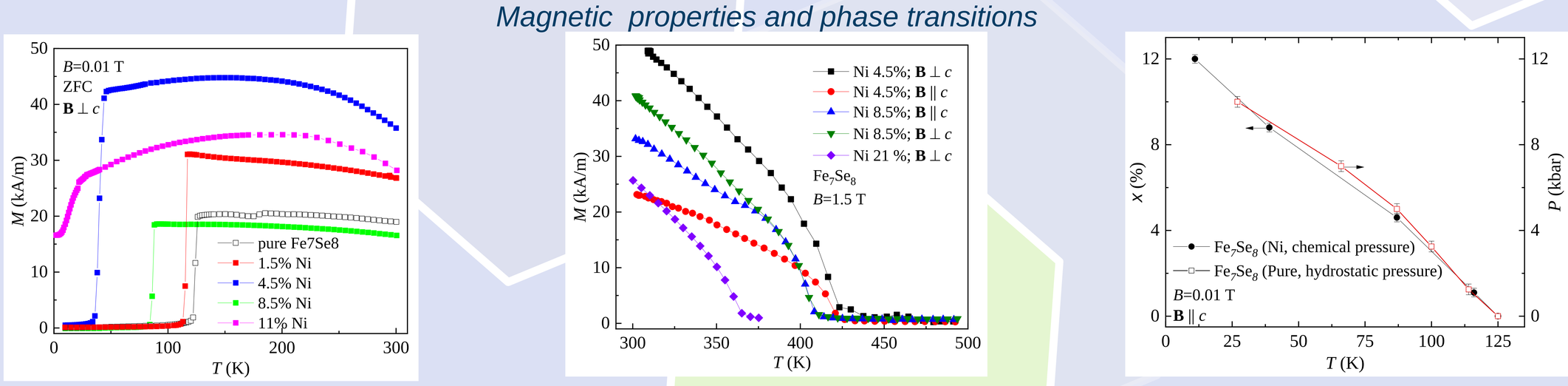
- Generally properties of Fe_7Se_8 depend on interatomic forces, the presence of inhomogeneities, vacancies, and lattice deformations.
- Taking into account previous results describing the crystal structure and magnetic properties of Fe_7Se_8 compounds [1], and because of the lack of relevant data, we investigate the effect of chemical pressure on the magnetic and electric properties of Fe_7Se_8 compounds.
- To answer this question following **concentrations** of dopings were used: Ni – 1.3; 4.5; 8.5; 11 and 21%.
- It was suggested that the explanation of metal-semiconductor transition could be the iron vacancy existence [2].

Structure

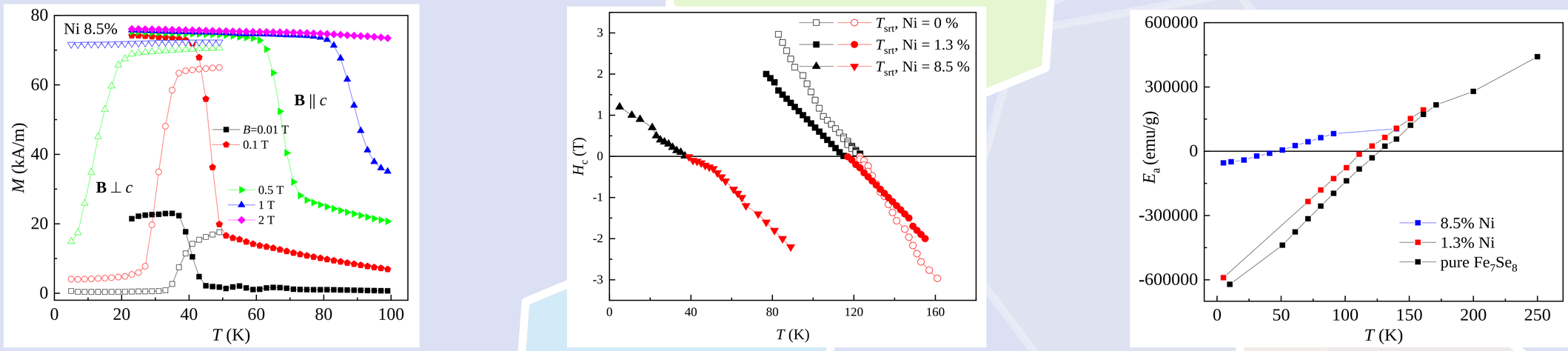


- NiAs-type **hexagonal 3*c*** structure, space group $P3_121$ [1]
- The lattice constant ***a*** increases and ***c*** decreases with the temperature increasing.
- The substitution of Fe with Ni induces a systematic change in the unit-cell volume, which is dependent on the average ionic radius of the transition metal.
- Layers filled with a chalcogen **alternate** with metal layers with vacancies
- The first-order phase transition (spin reorientation) temperature is $T_{SRT} \approx 125$ K
- Ferrimagnetic metal with $T_N \approx 450$ K (second-order phase transition)
- The easy direction along the *c*-axis exists below the T_{SRT} and the easy *c*-plane above this temperature.

Magnetic properties and phase transitions

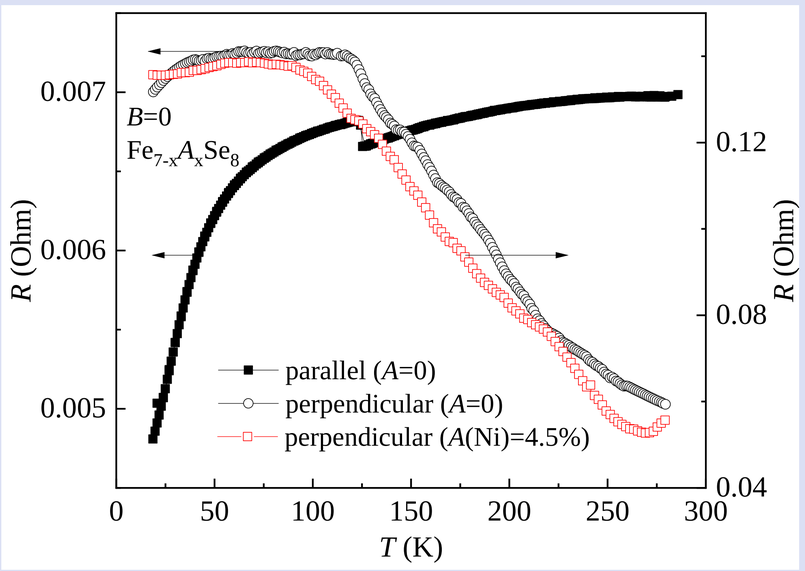


The “chemical pressure” affects both the T_N (**second order transition**) and the T_{SRT} **(first-order transition)** similarly to the action of the magnetic field and hydrostatic pressure

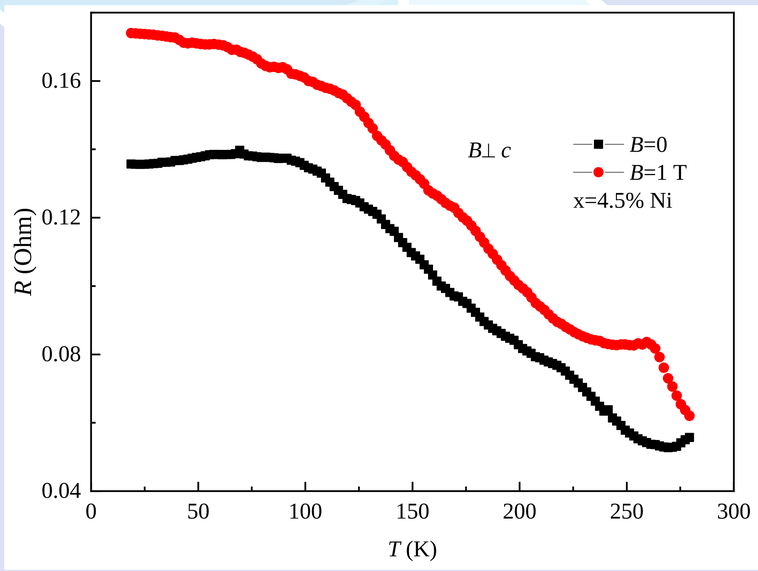


Increasing of Ni concentration changes phase transition order from **first to second**, leads to **magnetization decreasing** and changes of **magnetocrystalline anisotropy**

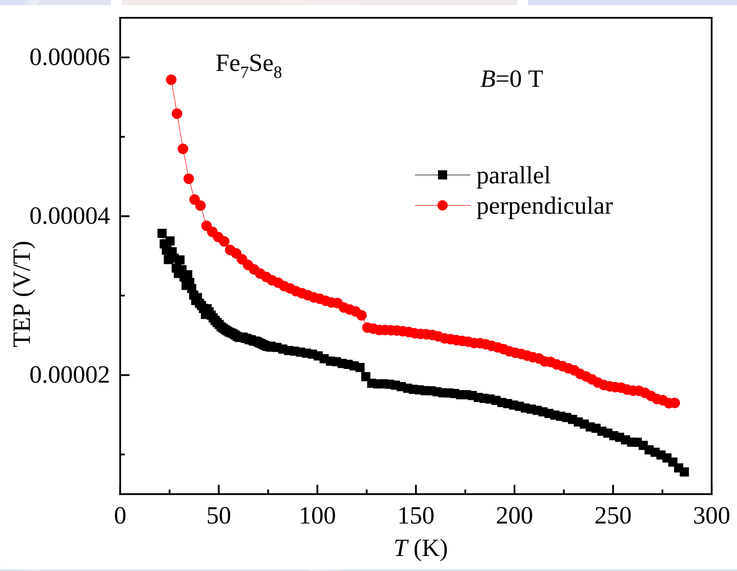
Electric properties



Existence of metal-semiconductor transition at the same temperature as T_{SRT}. Substitution Fe by Ni (4.5 %) provide a **decrease** of T_{SRT} and temperature of metal-semiconductor transition



The appearance of remarkable positive magnetoresistance is observed



The jump in TEP curve is about 125 K at the same temperature and as the spin-reorientation transition in pure Fe_7Se_8

Conclusions

- The temperature of phase transition T_{SRT} monotonously decreases with increasing Ni concentration.
- The metal-semiconductor transition transition and positive magnetoresistence can be observed in pure and nickel substituted Fe_7Se_8 single crystals.
- A correlation between hydrostatic and chemical pressure can be established from the measurements of phase transition temperature.

References

1. I. Radelytskyi et al, Journal of Applied Physics 124, 143902 (2018
2. G. Li, B. Zhang, T. Baluyan, J. Rao, J. Wu, A. A. Novakova, P. Rudolf, G. R. Blake, R. A. de Groot, and T. T. M. Palstra, *Inorg. Chem.* ***55***, 12912 (2016).

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