Effect of hydrostatic and chemical pressures on spin-reorientation transition, magnetic and magnetocaloric properties of Fe_7Se_8 single crystals

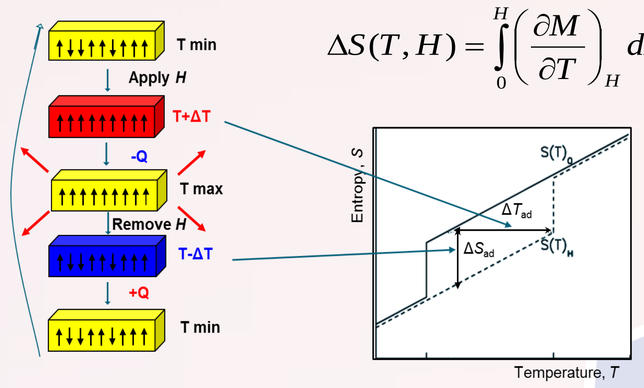
Authors: Y. Konopelnyk[1], I. Radelytskyi[1], P. Iwanowski[1], D. J. Gawryluk[1], M. Berkowski[1], R. Diduszko[2], J. Fink-Finowicki[1], T. Zajarniuk[1], R. Puzniak[1], A. Szewczyk[1] and H. Szymczak[1]

Affiliations: [1]Institute of Physics PAS, Warsaw, Poland, [2]Tele and Radio Research Institute, Warsaw, Poland

Introduction

- The magnetocaloric effect (MCE) is a magneto-thermodynamic phenomenon of the reversible entropy changes in magnetic materials under variation of the applied magnetic field
- Refrigeration systems based on the MCE could significantly decrease energy consumption
- The adiabatic change of magnetic entropy can be calculated from magnetization curves *M(T, H)* using Maxwell's equation:

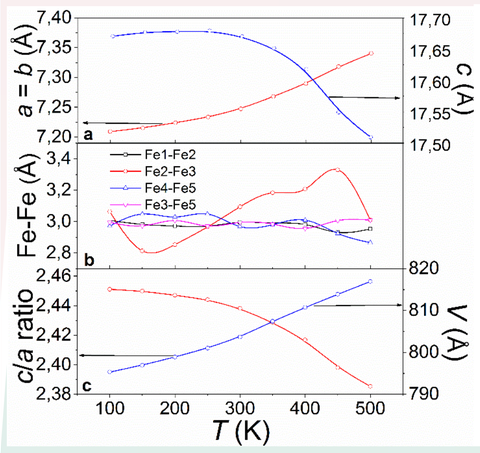
$$\Delta S(T,H) = \int_0^H \left(\frac{\partial M}{\partial T}\right)_H dH$$

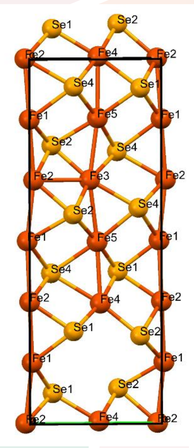


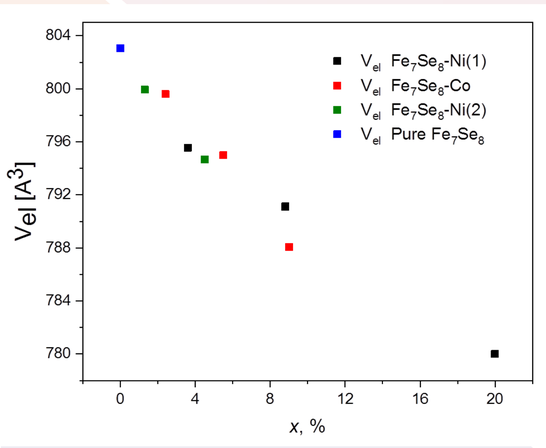
Magnetic refrigeration

- How does hydrostatic and chemical (by doping) pressure can modify the magnetic and magnetocaloric properties of Fe_7Se_8?
- ✓ To answer this question following **concentrations** of dopings were used: Co – 2,5 and 5.5 %, Ni – 1,3; 4,5; 8,5; 11 and 20%.
- ✓ Hydrostatic **pressure**: *P* = 1,25; 3,5; 5; 5,25; 7; 10; 10,25 kbar

Structure

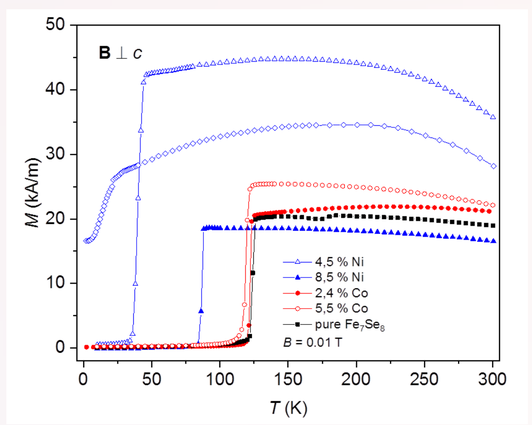


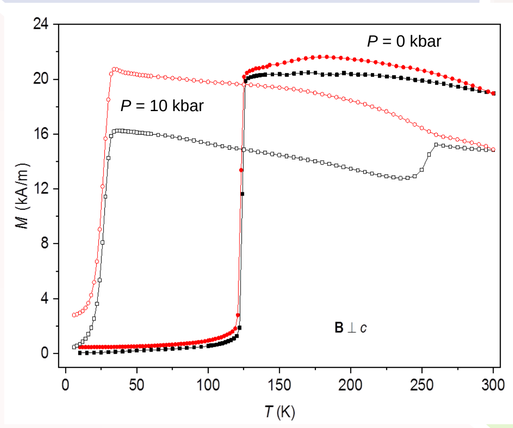


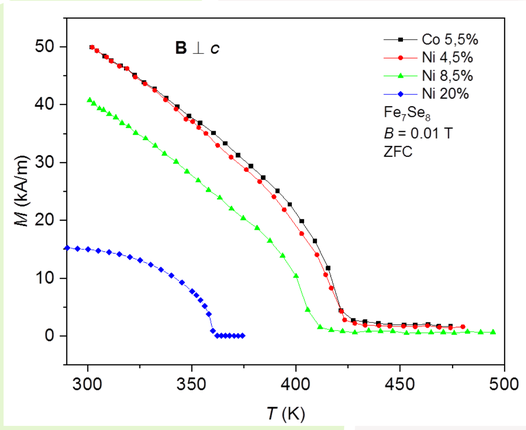


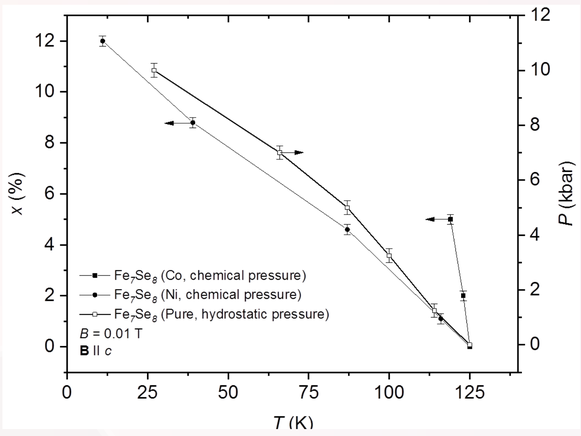
- NiAs-type **hexagonal 3*c*** structure, space group $P3_121$ [2]
- The lattice constant ***a*** increases and ***c*** decreases with the temperature increasing.
- **The volume** of elementary lattice cell V decreases linearly with increasing of Co and Ni concentrations.
- Layers filled with a chalcogen **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

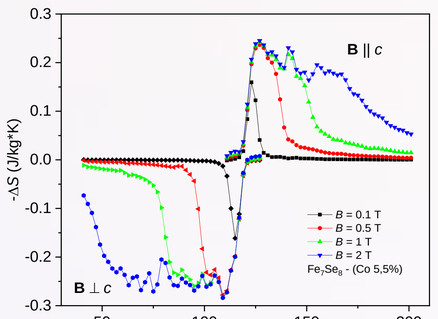


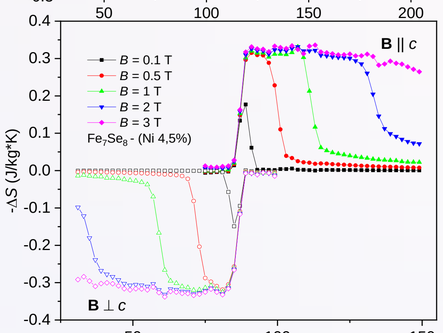






Hydrostatic pressure and chemical dopings provide decreasing of both **first-order** (spin reorientation) and **second order** (Neel temperature) **phase transitions**





Magnetocaloric effect

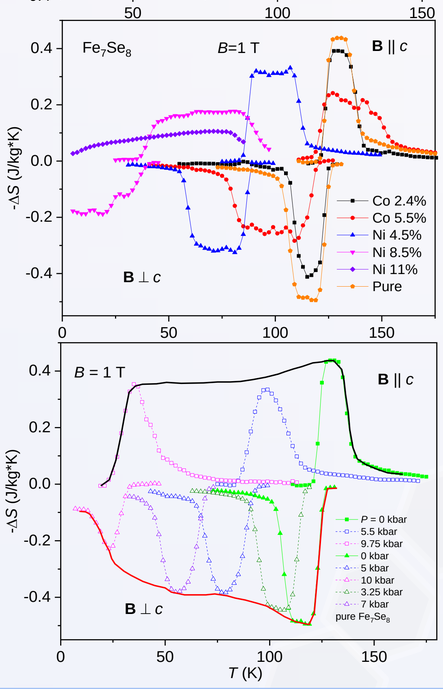
In cobalt substituted (5.5 %) crystals maximum value of ΔS_m **decreases.** Magnetic field provide the expansion of the MCE peak on **14 K** compared to the pure Fe_7Se_8

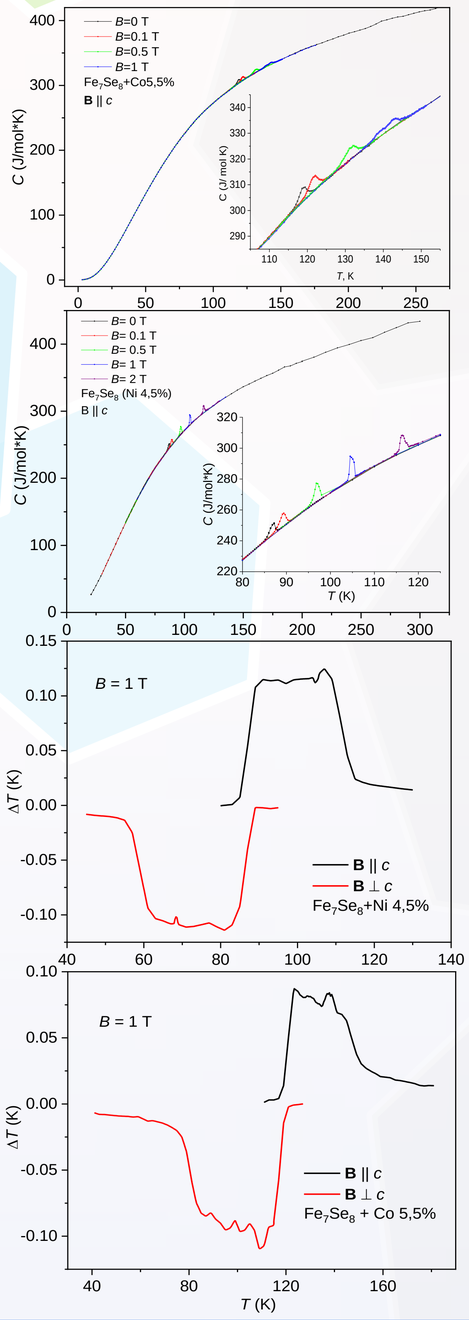
Substitution by nickel (4.5 %) provide a **decrease** of ΔS_m. MCE peak is almost **2 times** wider compare to the pure Fe_7Se_8

The **normal** MCE is smaller than the **inverse** magnetocaloric effect. In the case of Cobalt substitution, the ΔS_m peak is slightly shifted to the lower temperatures but in the case of Nickel substitution ΔS_m peak shifts **dramatically** to the lower temperatures.

Very wide working temperature range of about 100 K in the magnetic field *B* = 1 T.

Applying of hydrostatic pressure leads to the **decreasing** of MCE value and temperature of spin reorientation transition similar to the effect of chemical pressure.

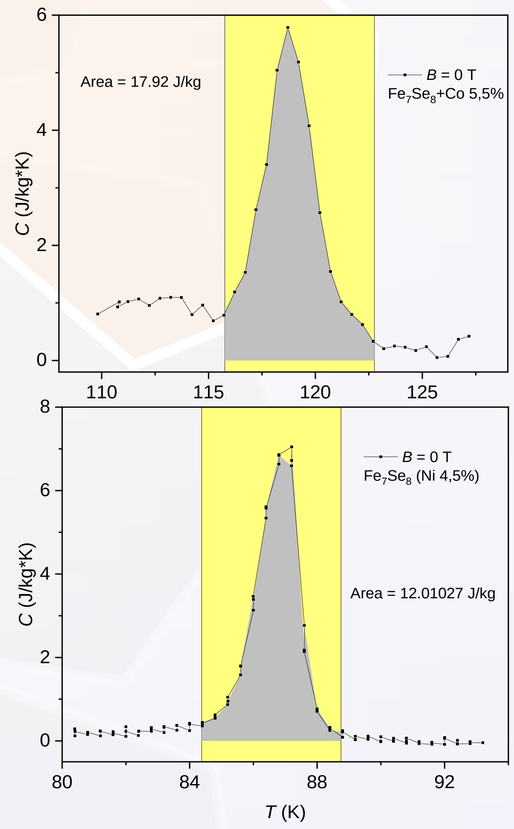




Heat capacity

Heat capacity maximum is **shifted** under influence of the magnetic field.

Values of the heat capacity and the anomaly peak, related to the **hidden heat** of first-order phase transition decrease in substituted crystals



The **adiabatic temperature** change induced by the external magnetic field, can be calculated using heat capacity:

$$\Delta T = -\frac{T\Delta S}{C}$$

Conclusions

- The temperature of phase transition T_{SRT} monotonously decreases with increasing of hydrostatic pressure and/or Ni/Co concentration.
- The normal and inverse magnetocaloric effect can be observed in pure Fe_7Se_8 under hydrostatic pressure and cobalt/nickel substituted Fe_7Se_8 single crystals in an external magnetic field

References

1. T. Kamimura J. Phys. Soc. Japan 43 (1997) 1593
2. I. Radelytskyi et al, Journal of Applied Physics 124, 143902 (2018

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