Different types of correlations in $Fe_{7-x}A_xSe_8$ single crystals (A=Ni, Co)

Authors: Y. Konopelnyk, H. Szymaczak
Affiliations: Institute of Physics PAS, Warsaw, Poland

Introduction

➤ Generally properties of Fe_7Se_8 crystals 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 [1,3], and because of the lack of relevant data, we investigate the effect of hydrostatic and chemical pressures on the magnetic 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%, Co - 2.5; 4.9; 9%. And the values of hydrostatic pressure up to the P = 10.25 kbar.

➤ The analysis of **correlations** between the properties of studied matter is a very useful phenomenological research method. The correlated effects observed for various groups of materials are particularly important because there exist different mechanisms determining the correlations, even in one fixed group of materials.

Structure
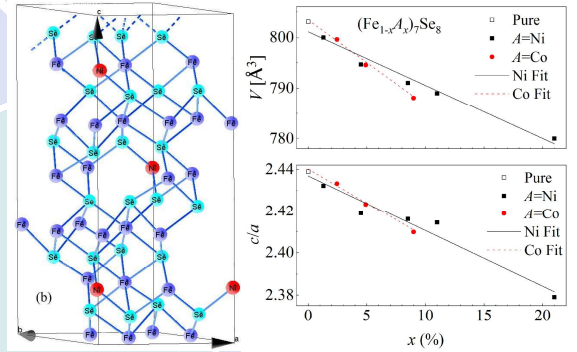
➤ NiAs-type **hexagonal 3c** structure, space group $P3_121$ [1]
➤ Layers filled with a chalcogen **alternate** with metal layers with vacancies
➤ The first-order phase transition (spin reorientation) temperature is determined to be $T_{SRT}\approx125$ K
➤ Ferrimagnetic metal with $T_N \approx 450$ K (second-order phase transition)
➤ The easy direction along the c-axis exists below the T_{SRT} and the easy c-plane above this temperature.
➤ The substitution of Fe with Ni or Co induces a systematic decrease in the lattice constant a and c and unit-cell volume, which are dependent on the average ionic radius of the transition metal.

Correlation between hydrostatic and chemical pressures
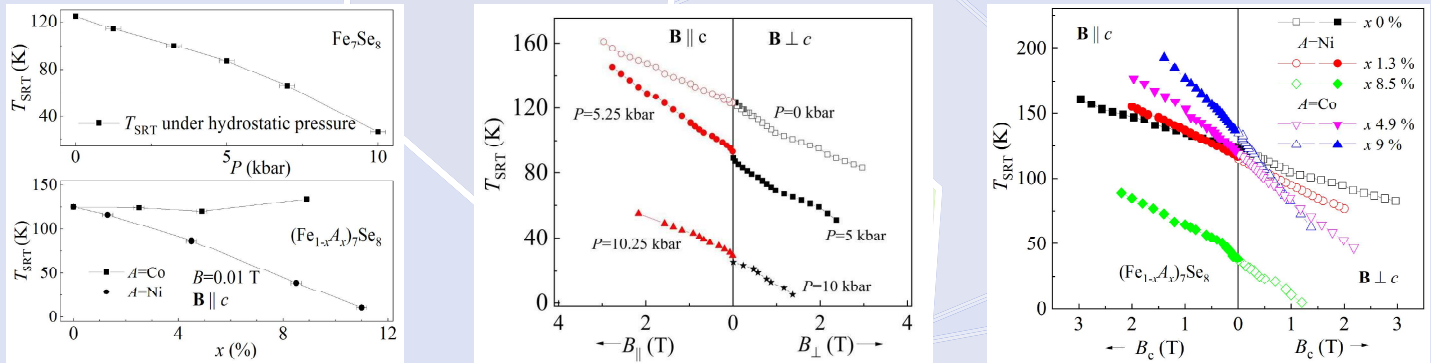
The "chemical pressure" affects the T_{SRT} **(first-order transition)** similarly to the action of the magnetic field and hydrostatic pressure

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

Correlation between magnetocaloric properties and magnetostriction
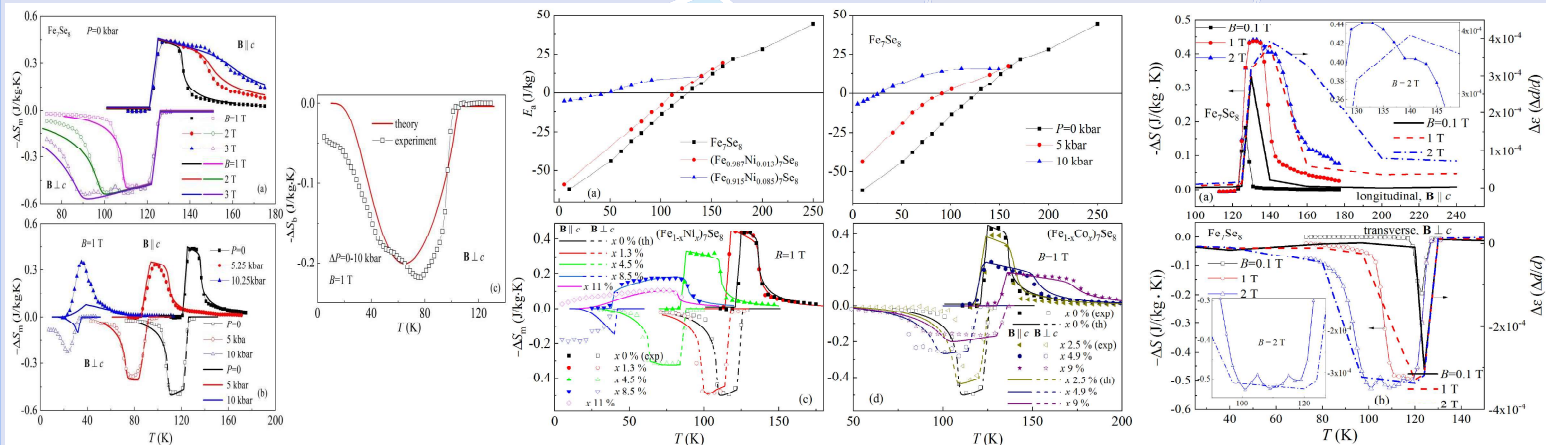
Entropy change, ΔS_m, in Fe_7Se_8, subjected to a combined variation of the magnetic field and hydrostatic pressure, attains large values in a wide range of temperatures.
The application of hydrostatic pressure induces a strong **barocaloric effect** - BCE

Existence of the strong **correlation** between hydrostatic and chemical pressures.
T_{SRT} is slightly shifted towards **higher temperatures** with Co substitution for iron, while for Ni substitution T_{SRT} **decreases** considerably.

Giant negative **magnetostriction** ("-") below T_{SRT}, and positive ("+") above T_{SRT} was observed.
The temperature and magnetic field dependences of the magnetostriction $\Delta\varepsilon$ **correlate** well with the MCE in different fields by a simple relation $\Delta S_m \sim \Delta\varepsilon$.

Conclusions

● The temperature of phase transition T_{SRT} monotonously **decreases with increasing** Ni concentration and applied hydrostatic pressure.

● The **normal and inverse magnetocaloric effects** were observed in the pure and nickel-/cobalt-doped Fe_7Se_8 single crystals in the external magnetic field.

● A **correlation between hydrostatic and chemical pressures** can be established from the measurements of phase transition temperature.

● There is strong correlation between **magnetostriction and magnetocaloric effect.** The mechanism determining both in the case of Fe_7Se_8 has the **same origin** (related to magnetocrystalline anisotropy) and can be used as an indirect method to estimate the change in magnetic entropy.

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).
3. Y. Konopelnyk et al, *J. Magn. Magn. Mater.* **543**, 168626 (2022).