

# Effect of doping with transition elements on the crystal and magnetic structure of half-Heusler compounds



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# Heusler compounds

Heusler alloys

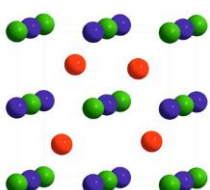
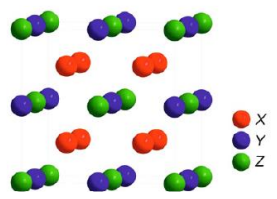
Half-Heusler alloys

Cubic structure



$Ni_2MnSb$ ,  
 $Cu_2MnAl$

$NiMnSb$ ;  
 $CuMnSb$

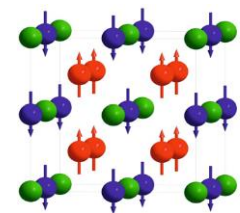


Ni  
Mn  
Sb

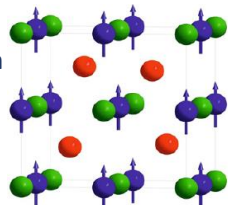
4c  
4b  
4a



Magnetic structure

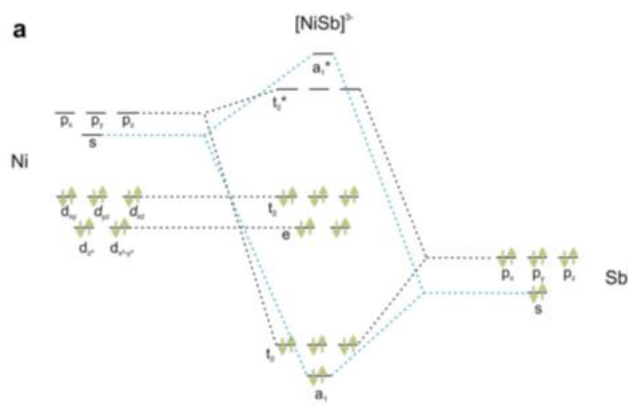


X Ni  
Y Mn  
Z Sb

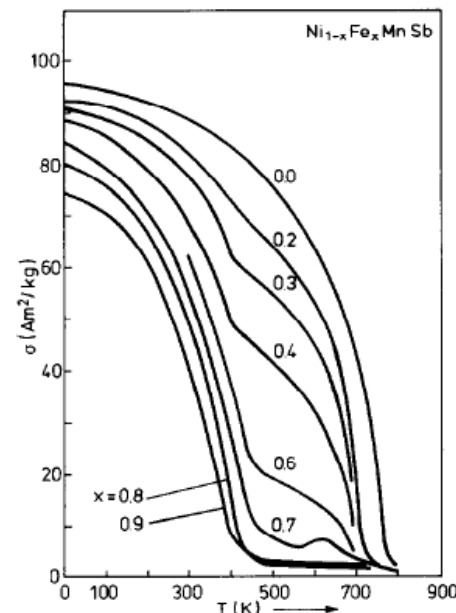
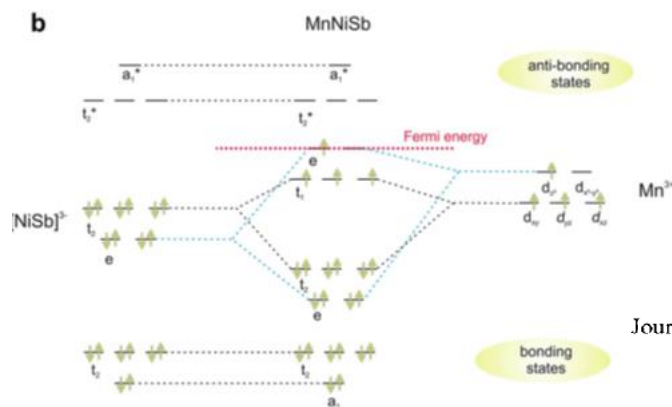


Y  
X  
Z

a

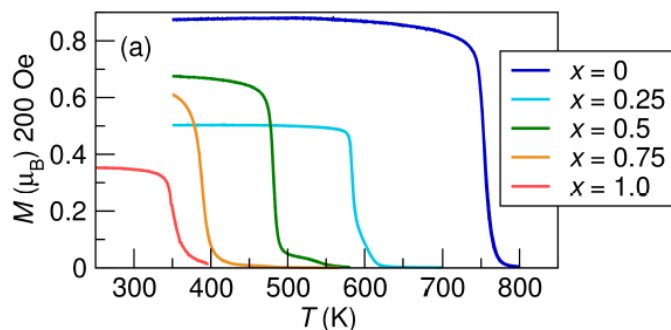


b



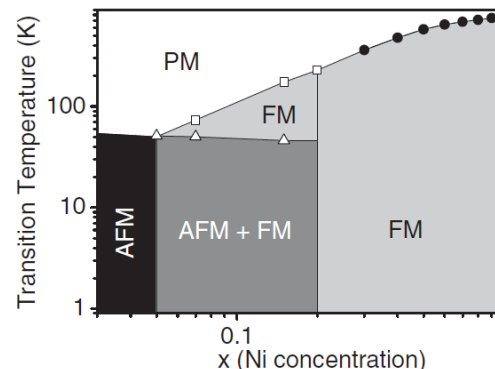
Temperature dependence of the magnetization of various  $Ni_{1-x}Fe_xMnSb$  samples.

Journal of Magnetism and Magnetic Materials 61 (1986) 330-336



$Ni_{1+x}MnSb$  ( $x = 0, 0.25, 0.5, 0.75, 1$ )

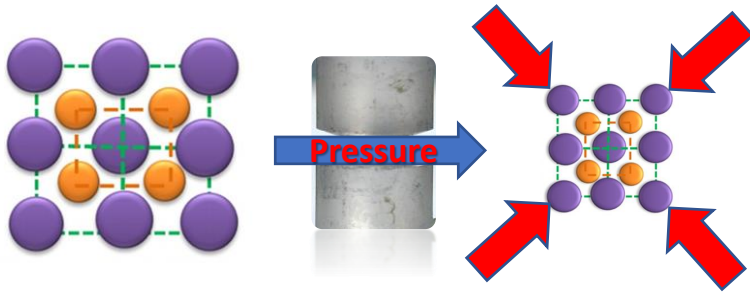
PHYSICAL REVIEW MATERIALS 1, 075003 (2017)



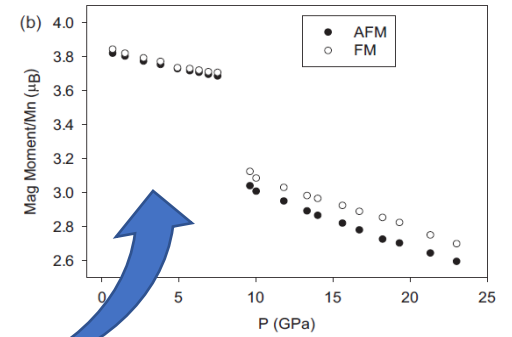
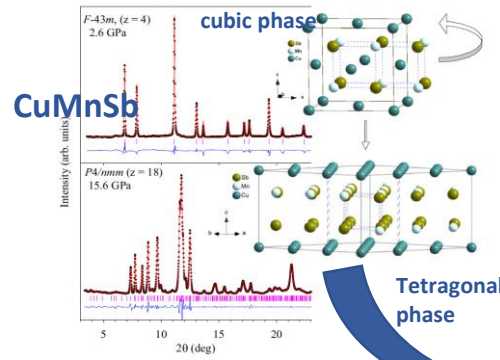
Magnetic phase diagram of the  $Cu_{1-x}Ni_xMnSb$  Heusler alloys series from  $x = 0.03$  to 1.

PHYSICAL REVIEW B 84, 094435 (2011)

# Half-Heusler alloys under pressure



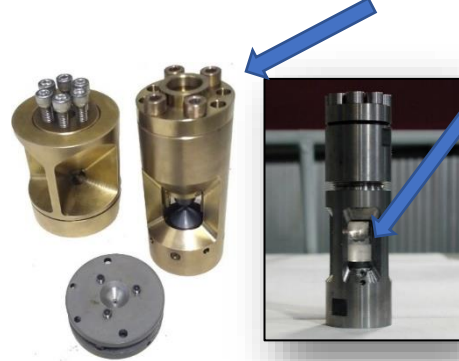
Pressure is direct method to change interatomic distances and valence angles.



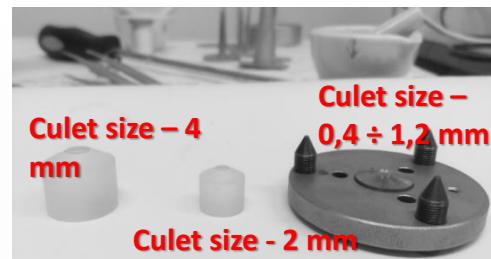
PHYSICAL REVIEW B 98, 054431 (2018)

## High pressure technique at Frank Laboratory of Neutron Physics (FLNP JINR, Dubna, Russia)

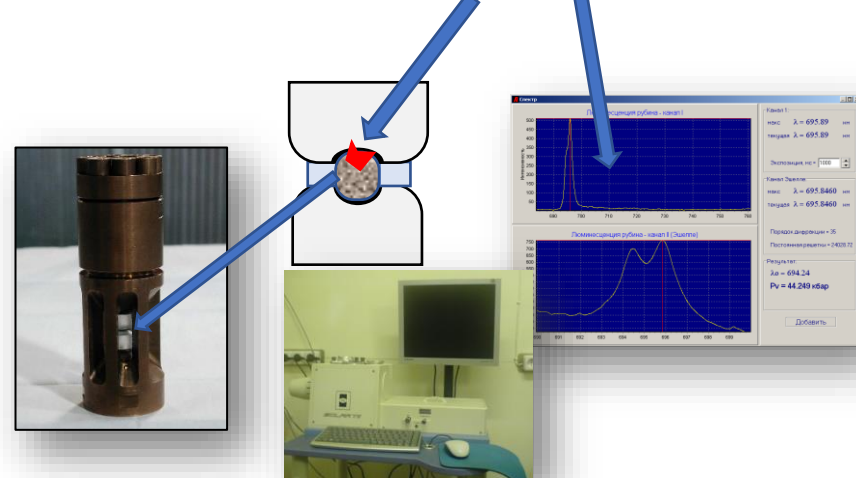
The high pressure cells with diamond and sapphire anvils



Deferent tapes of anvils



The pressure is measured by the ruby luminescence shift.



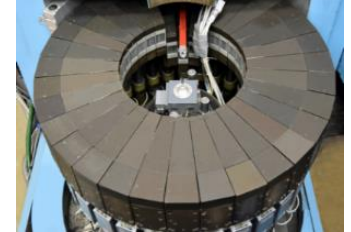
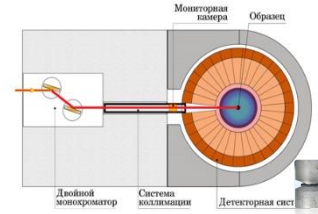
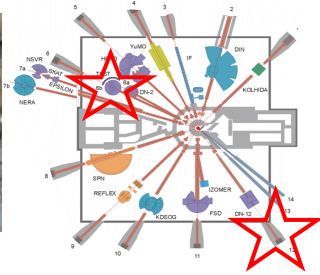
At present, the neutron physics laboratory manages to achieve the following pressure values:

- for sapphire anvils the average maximum pressure is 8 GPa;
- for diamond anvils the average maximum pressure is 35 GPa.

# Experimental techniques under extreme conditions

Neutron diffractometers at IBR-2 reactor, Joint Institute for Nuclear Research, Dubna

Neutron diffractometer DISC at IR-8 research reactor, Kurchatov Institute, Moscow



Maximum pressure ~ 35 GPa

Temperature range 4 -320 K

Maximum pressure ~ 8 GPa =80 000 atm.

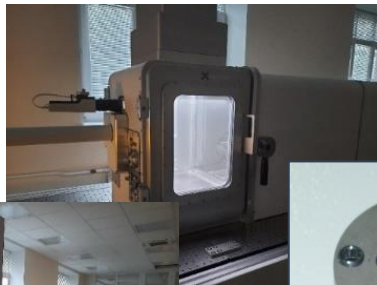
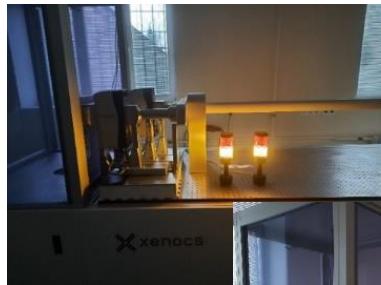
Temperature range 10 -320 K

Maximum pressure ~ 3 GPa

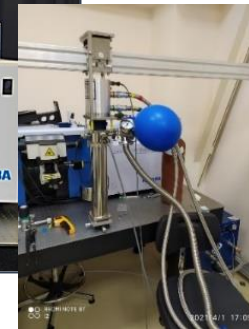
Temperature range 3 -1000 K

X – ray diffractometers Xeuss , FLNP JINR (Dubna, Russia)

LabRAM spectrometer Horiba, FLNP JINR (Dubna, Russia)

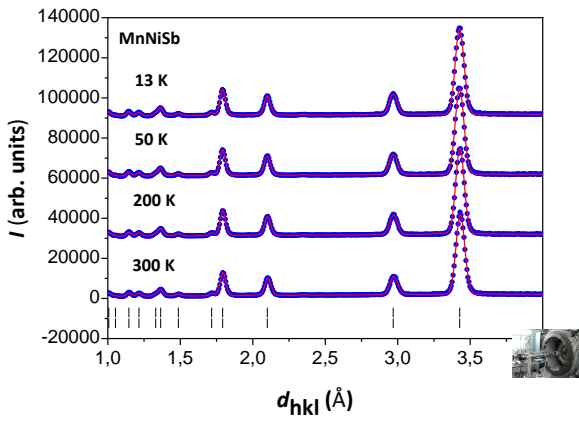


Maximum pressure ~ 35 GPa  
Temperature range - 300 K



Maximum pressure ~ 35 GPa  
Temperature range - 10 -300 K

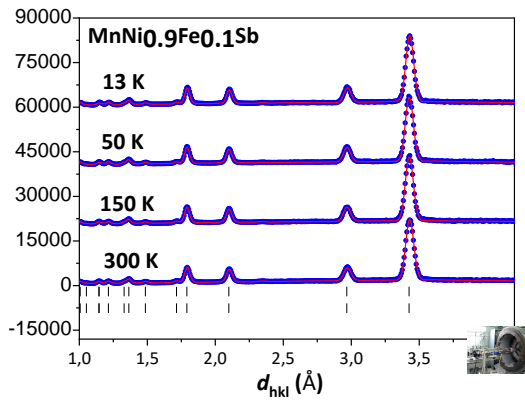
# MnNiSb and MnNi<sub>0.9</sub>M<sub>0.1</sub>Sb (M=Fe, Ti, V) at low temperature



T = 300 K M = 3,8  $\mu_B$



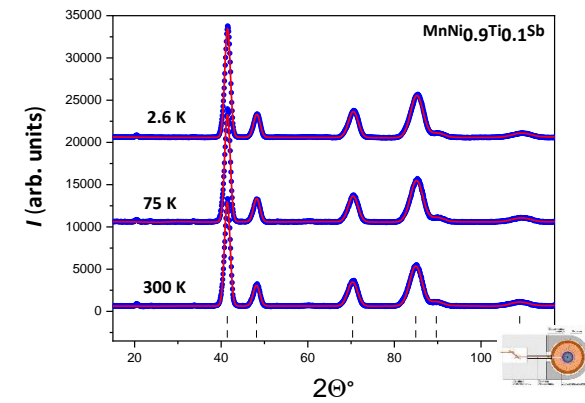
T = 13 K M = 4,1  $\mu_B$



T = 300 K M = 3,5  $\mu_B$



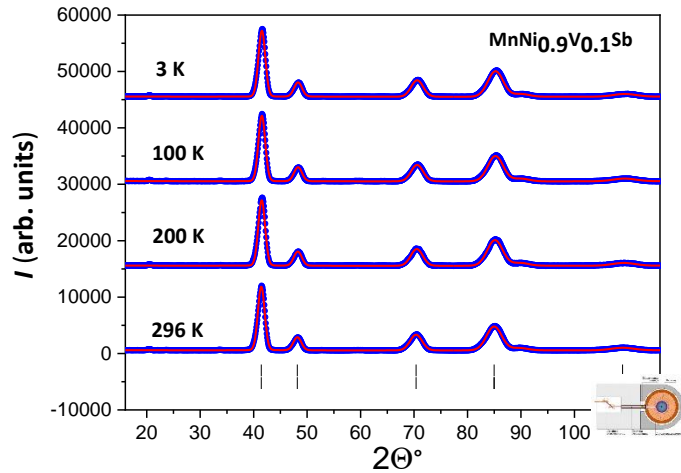
T = 13 K M = 4,0  $\mu_B$



T = 300 K M = 3,4  $\mu_B$



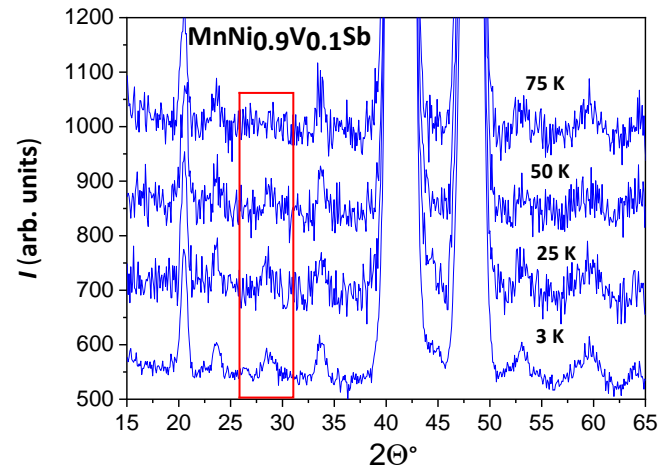
T = 2,6 K M = 3,7  $\mu_B$



T = 300 K M = 3,5  $\mu_B$

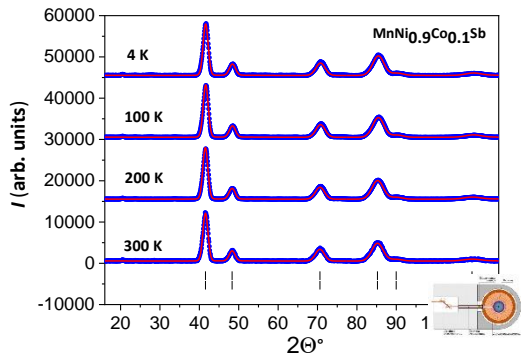


T = 3 K M = 3,8  $\mu_B$





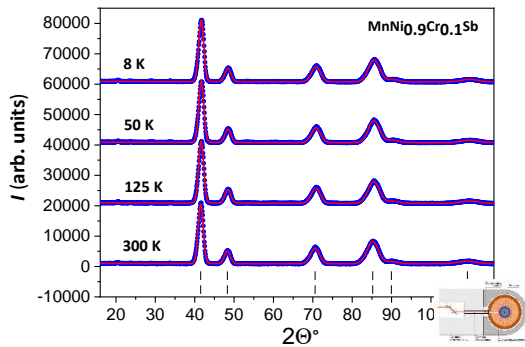
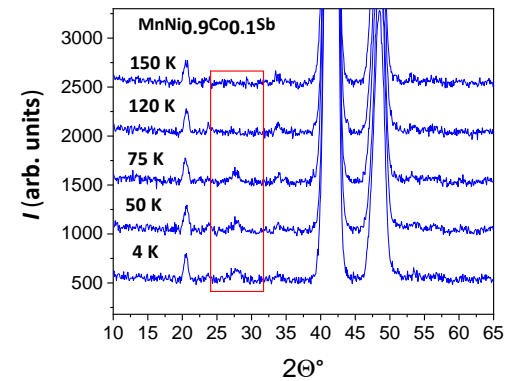
# MnNi<sub>0.9</sub>Co<sub>0.1</sub>Sb and MnNi<sub>0.9</sub>Cr<sub>0.1</sub>Sb at low temperature



$T = 300 \text{ K}$     $M = 3,6 \mu_B$



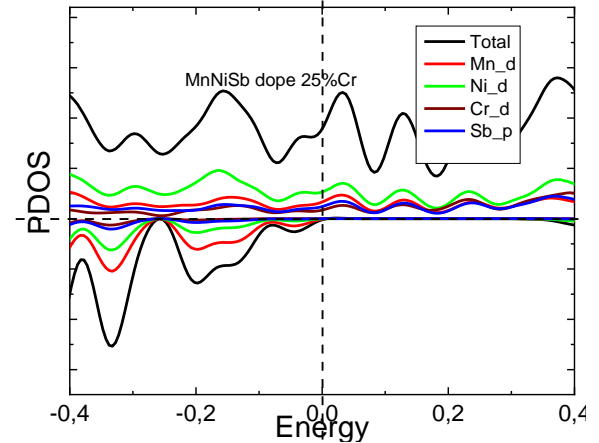
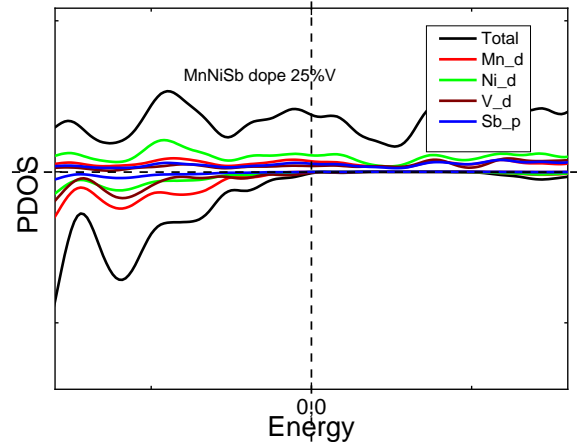
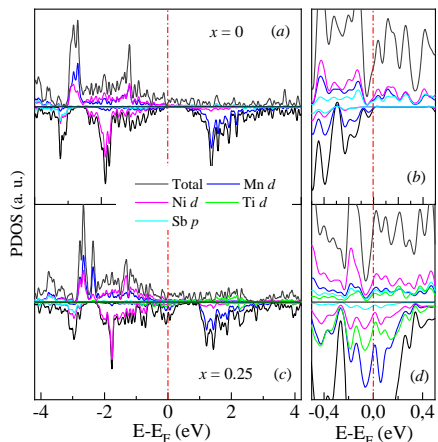
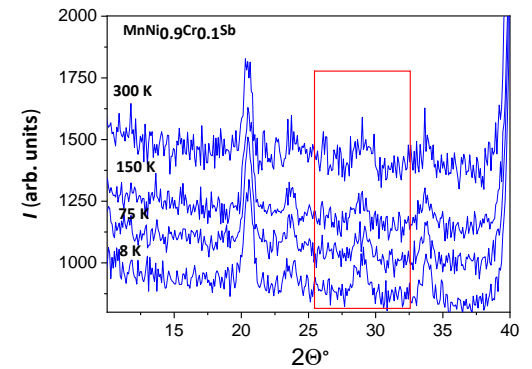
$T = 4 \text{ K}$     $M = 4,1 \mu_B$



$T = 300 \text{ K}$     $M = 3,7 \mu_B$



$T = 8 \text{ K}$     $M = 4,1 \mu_B$



$\text{Ti} = 12,5 \%$     $M = 0,7 \mu_B$

$\text{Ti} = 25 \%$     $M = 0,8 \mu_B$

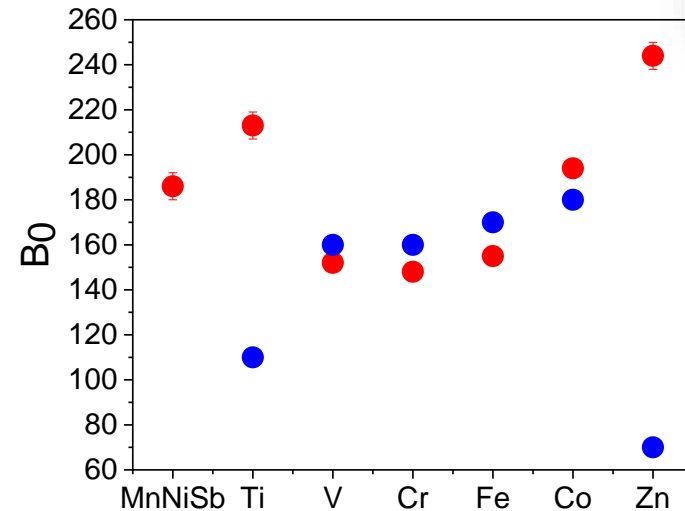
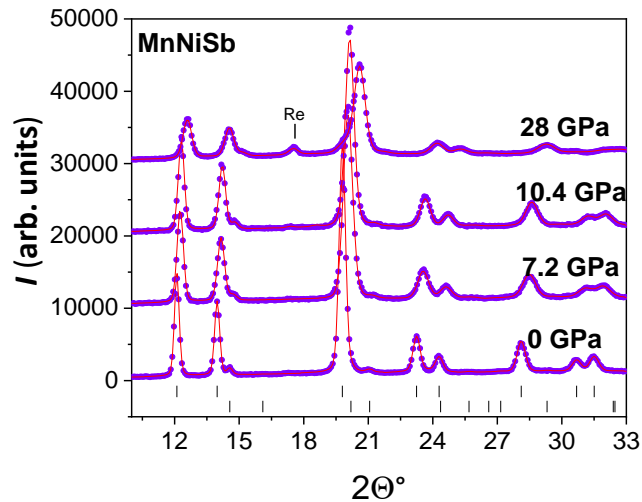
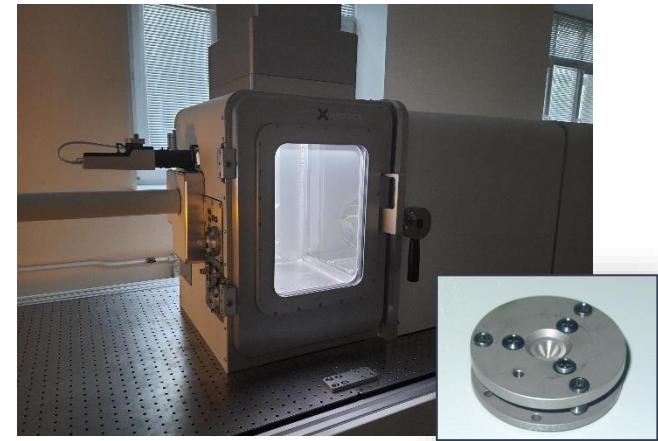
$\text{V} = 12,5 \%$     $M = 1,7 \mu_B$

$\text{V} = 25 \%$     $M = 1,8 \mu_B$

$\text{Cr} = 12,5 \%$     $M = 2,5 \mu_B$

$\text{Cr} = 25 \%$     $M = 2,5 \mu_B$

# MnNiSb and MnNi<sub>0.9</sub>M<sub>0.1</sub>Sb (M – Ti, V, Cr, Co, Fe, Zn) under high pressure



- The experiments under high pressure have been performed on the X-ray diffractometer. The average maximum pressure was 25 GPa.
- We have not found any structural transitions. All the compounds have preserved their original cubic structure.

- In the right graph, the red dots demonstrate the dependence of the bulk module on the substitution of Ni with another element, and the blue dots show the value of the bulk module for pure elements.
- If we dope our systems with a hard element, we obtain a softer compound.

**Thank you for your attention!**