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Electronic and Magnetic Properties of NpNi$_5$

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The physical properties of binary actinides and transition metal alloys are of great importance for the safety assessment of nuclear fuels. Since transition metals are major components of the cladding material of fuel rods (stainless steel, HT-9 etc.), the physical properties of those compounds formed by accidental fuel-cladding interactions could have limiting factors on the fabrication, life time operation and disposal of nuclear fuels. Binary compound of the form ReT$_5$ (Re = rare earth, T = Transition metal) has been in the focus of interest mainly because of their magnetic properties (small Re to T stoichiometric ratio, large spontaneous magnetization and high Curie temperature) and their ability to store large amount of hydrogen per formula unit (f. u.)

Reported in 1997 [1], NpNi$_5$ was synthesized and identified to have hexagonal (D$_2$d) CaCu$_5$ crystallographic structure, with room-temperature lattice parameters a = 8.3107(1) Å and c = 8.1058(1) Å. In the present study, NpNi$_5$ has been synthesized and characterized by means of powder x-Ray diffraction (**Fig.** 2 left panel), Superconducting – Quantum – Interference – Device magnetometry (SQUID, **Fig. 2** right panel), ^{237}Np Mössbauer spectroscopy [2] (**Fig. 3** left panel) and specific heat measurements (**Fig. 3** right panel).

Magnetization curves indicate that NpNi$_5$ is a ferromagnet (T$_C$ ~ 16 K), fit of the paramagnetic part to the Curie–Weiss law (C~1.7 emu·K/mol, θ_P ~ 14.6 K) gives an effective moment μ_{eff} ~ 3.7 μ_B per f.u. – no magnetization hysteresis was observed. The isomer shift ($\delta_{IS} \approx$ -11.1 mm/s vs. NpAl$_2$) observed in Mössbauer spectra suggests a tetravalent Np state, but considering the influence of conduction electrons we determine a Np^{3+} (5f^4 configuration) oxidation state. The hyperfine field determined by fitting of the spectra (~439T) gives an ordered moment at the Np site μ_{Np} ~ 2 μ_B per Np ion (1 μ_B = 215 T [3]). The magnetic transition is clearly visible in the temperature dependence of the specific heat, and a magnetic phase diagram as a function of temperature and external magnetic field was generated.

In this communication we will present the results obtained and discuss them in the light of theoretical considerations.
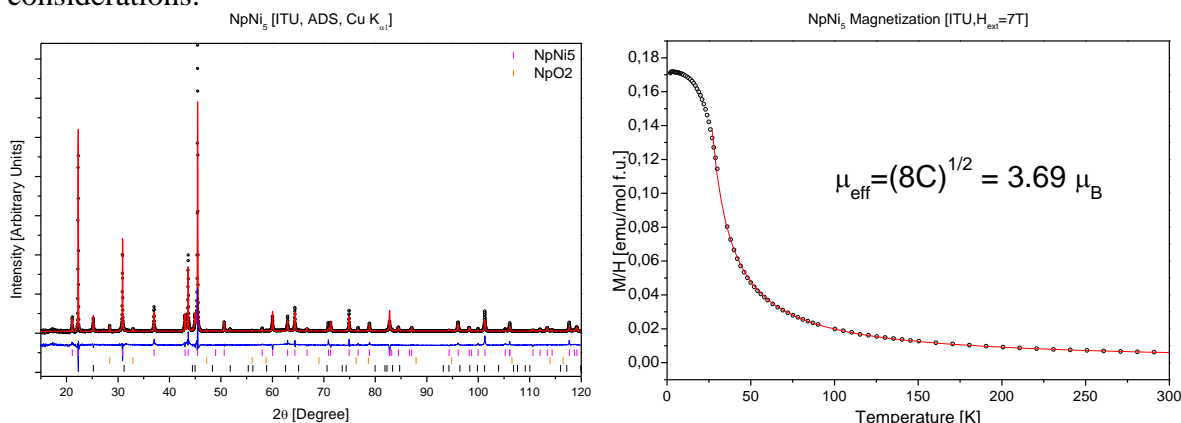

Fig. 2 <u>Left</u>: Powder x-ray diffraction pattern of NpNi$_5$, black dot – measured data, red line – fitted profile, blue line – difference profile, vertical tick – angular position of Bragg peaks. <u>Right:</u> Temperature dependence of the magnetic susceptibility, red line – fit to the Curie-Weiss law.
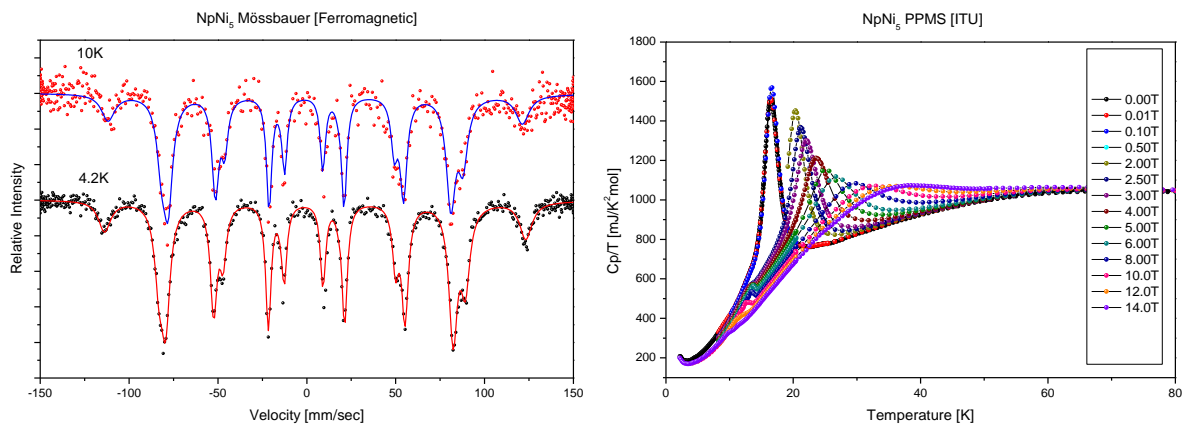
Fig. 3 <u>Left:</u> Mössbauer spectra taken in the ferromagnetic region, dots – measured data, lines – fits of hyperfine fields to the measured data, spectrum is composed of one hyperfine field as expected from the crystallography.

<u>Right:</u> Normalized heat capacity as a function of temperature in various external magnetic fields.

REFERENCES
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