Neutron diffraction, magnetic and transport studies of $NdNi_4Al$ compound

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The RNi_4Al compounds crystallize in the hexagonal $CaCu_5$-type structure. R occupies the 1a site and Ni(1) the 2c site, whereas Ni(2) and Al are statistically distributed on the 3g position. Diffraction patterns have been collected on the neutron powder diffractometer SV7-a at the FRJ-2 reactor in the Forschungszentrum Jülich, Germany. The neutron wavelength was 1.0957 Å and temperature was varied between 4.2 K and RT. The experiment was performed with external magnetic fields up to 5T perpendicular to the horizontal diffraction plane. Additionally, in time-of-flight technology was employed between 1.8 and 10 K using the diffractometer ROTAX at the spallation source ISIS in Chilton, U.K.

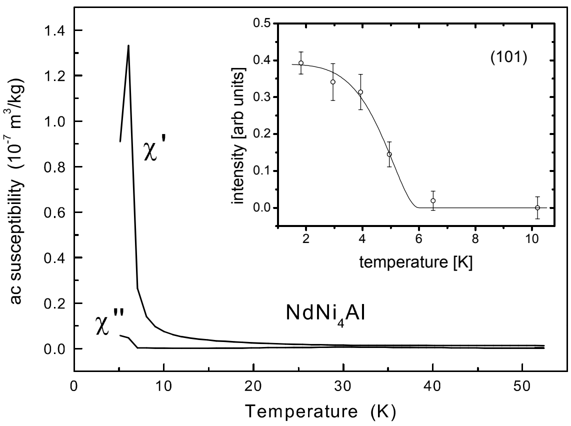

Fig. 1. The real, χ', and the imaginary, χ'', part of the a.c. susceptibility for $NdNi_4Al$. Inset: Temperature dependence of the (101) reflection measured by ROTAX.

The ferromagnetic ordering temperature T_C and magnetic moment at $H = 6$ T for $NdNi_4Al$ are 6 K and 1.52 μ_B/f.u., respectively [1]. Fig. 1 shows the real, χ', and the imaginary, χ'', part of the a.c. susceptibility for $NdNi_4Al$ compound and, as an inset, the temperature dependence of the (101) reflection measured by ROTAX (after the subtraction of the nuclear contribution obtained at RT). Both methods provide the evidence of the para- ferromagnetic phase transition at this same temperature of 6 K.

The neutron diffraction experiments on $NdNi_4Al$, using the diffractometer SV7-a, have been also carried out in external magnetic fields. Fig. 2 presents the neutron diffraction patterns at 4.2 K for H in the range from zero to 5 T. Increase of some peaks being the effect of magnetic contributions to the intensities is well visible.

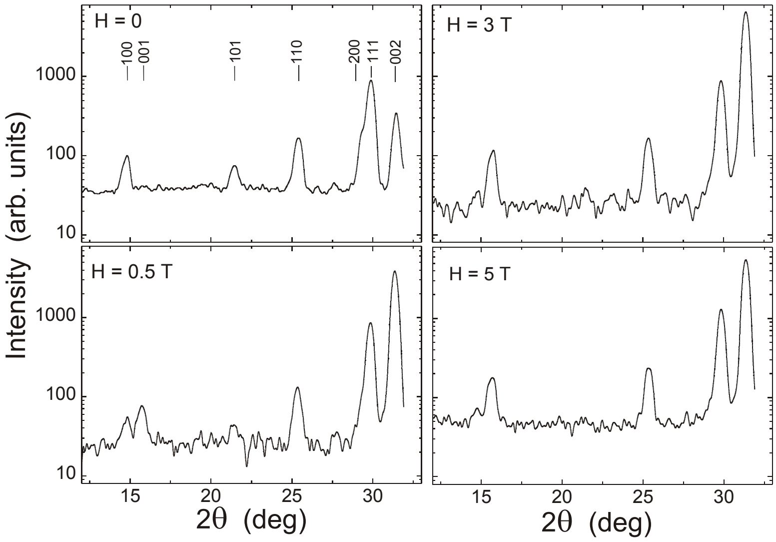

Fig.2. Low angle part of the neutron diffraction patterns collected at various external magnetic fields indicating the appearance of a long-range ferromagnetic order

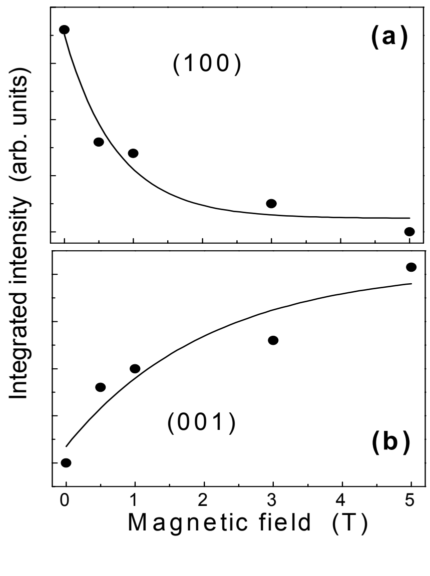

Fig. 3. The field dependence of the (001) and (100) reflection intensities

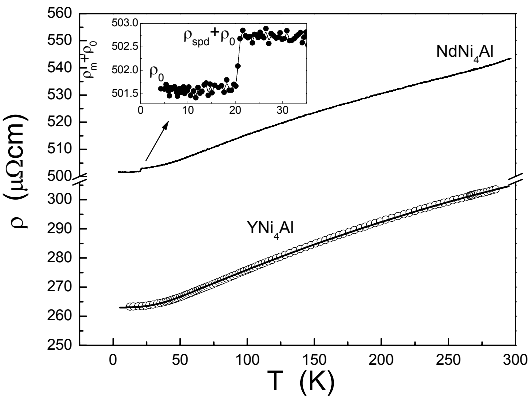

Fig. 4. Electrical resistivity of the $NdNi_4Al$ compound. The ρ(T) dependence of the non-magnetic isostructural YNi_4Al compound is also shown (bottom curve) together with a fit to formula (1). Inset shows the magnetic part (ρ_m + ρ_0) of the $NdNi_4Al$ resistivity in the vicinity of the phase transition.

From the appearance of the (001) and the disappearance of the (100) peak it is evident that the ferromagnetic alignment is perpendicular to the hexagonal axis, i.e., the moments are ordered in the hexagonal basis plane (Fig. 3). The field dependence of the (001) reflection intensities resembles a typical magnetization curve.

The $\rho(T)$ dependence of $NdNi_4Al$ illustrated in Fig. 4 consists both of the magnetic and phonon contributions. To display only the magnetic contribution within the transition area the phonon part of the isostructural nonmagnetic YNi_4Al compound was subtracted, i.e., $\rho_m(NdNi_4Al) + \rho_0 = \rho(NdNi_4Al) - \rho_{ph}(YNi_4Al)$, where $\rho(T)$ of YNi_4Al was fitted with the modified Bloch-Grüneisen relation for metal-like compounds:

$$\rho(T) = \rho_0(\mathrm{NdNi_4Al}) + \rho_{ph} - kT^3 \tag{1}$$

with

$$\rho_{ph} = 4R\Theta_D\left(\frac{T}{\Theta_D}\right)^5 \int_0^{\theta_D/T} \frac{x^5 dx}{(e^x-1)(1-e^{-x})} . \tag{2}$$

From the fit (solid line for YNi_4Al in Fig. 4) the residual resistivity is $\rho_0 = 263$ μΩcm, the constant $R = 0.165$ μΩcm/K, the Debye temperature $\Theta_D = 204$ K and the parameter describing the scattering of the conduction electrons into a narrow d band near the Fermi level $K = 2.25\times10^{-7}$ μΩcm/K^3. The inset of Fig. 4 enables the estimation of the spin-disorder resistivity as $\rho_{spd} = 1.14$ μΩcm.

Below T_C a quadratic dependence of resistivity on temperature is usually observed related to the magnon excitations, which may be modified by a presence of an energy gap. It stem from the inset of Fig. 4 that below T_C the resistivity ρ_m is nearly independent on temperature, which implies a very large energy gap for magnons excitations in the studied $NdNi_4Al$ compound. Hence, only high energy magnons may appear leading to the destruction of the long-range ferromagnetic order in zero or small magnetic fields. Moreover, a large value of the residual resistivity (~ 500 μΩcm) is visible. We have observed it also for other RNi_4Al compounds, while in the case of RNi_4B [2,3] this value was usually below 50 μΩcm. The explanation may be based on the difference in crystallographic structures. In the case of RNi_4B the B atoms occupy the well-defined (2d) sites of the $CeCo_4B$ structure, whereas the Al atoms in RNi_4Al are statistically distributed on the (3g) sites of the $CaCu_5$ type structure. Therefore, the lattice disorder in the case of $NdNi_4Al$ may be responsible for the increased residual resistivity.

The present magnetic and neutron diffraction studies reveal that:

1) The ferromagnetic ordering temperature T_C and magnetic moment at $H = 6$ T for $NdNi_4Al$ compound are 6 K and 1.52 μ_B/f.u., respectively.
2) In the ferromagnetic phase the magnetic moments are ordered in hexagonal basis plane.
3) The neutron diffraction experiments support the assumption from earlier studies that the Ni atoms do not provide a ferromagnetic contribution.

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[3] T. Toliński, A. Kowalczyk, V. Ivanov, *phys. status sol.* (b) **240** (2003) 153.

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