

## The peculiarities of local structure of YbNi<sub>2</sub> and YbCo<sub>2</sub> intermetallics synthesized at high pressure.

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**Abstract.** Local structure of YbCo<sub>2</sub> and YbNi<sub>2</sub> was investigated by EXAFS and XANES spectroscopy. It was found that the bond Yb-Co(Ni) has the highest static disorder and its length increases with temperature decrease, while all other bonds remain almost unchanged. This phenomenon may be caused by short-range magnetic ordering at temperatures above the phase transition. XANES measurements above  $L_{III}$ -Yb absorption edge in YbCo<sub>2</sub> and YbNi<sub>2</sub> revealed that both compounds have almost the same density of free  $5d$ -states

### 1. Introduction

Unusual magnetic and transport properties of Laves phases YbM<sub>2</sub>, where M – transition metal, are determined in general by hybridization of  $4f$  electron with  $s$ - and  $d$ - conduction band electrons. In the case of magnetic compounds there is also a contribution of rare earth  $5d$  and metal  $3d$  band hybridization [1-3]. Despite intensive study of intermetallic Yb compounds some questions are yet to answer, including influence of temperature and pressure (hydrostatic and chemical), which may change in the local interatomic distances, and hence the magnitude of the exchange interaction [4-7]. Investigation of the local structure of YbCo<sub>2</sub> and YbNi<sub>2</sub> by X-ray absorption spectroscopy may remove contradictions and gaps in the data on properties of these compounds.

### 2. Experiment

Samples were prepared by melting of the constituent materials at a constant pressure of 8 GPa in a chamber of the “Toroid” type [8]. Then samples were rapidly quenched to room temperature, and pressure was released. The resulting material was a homogeneous polycrystal.

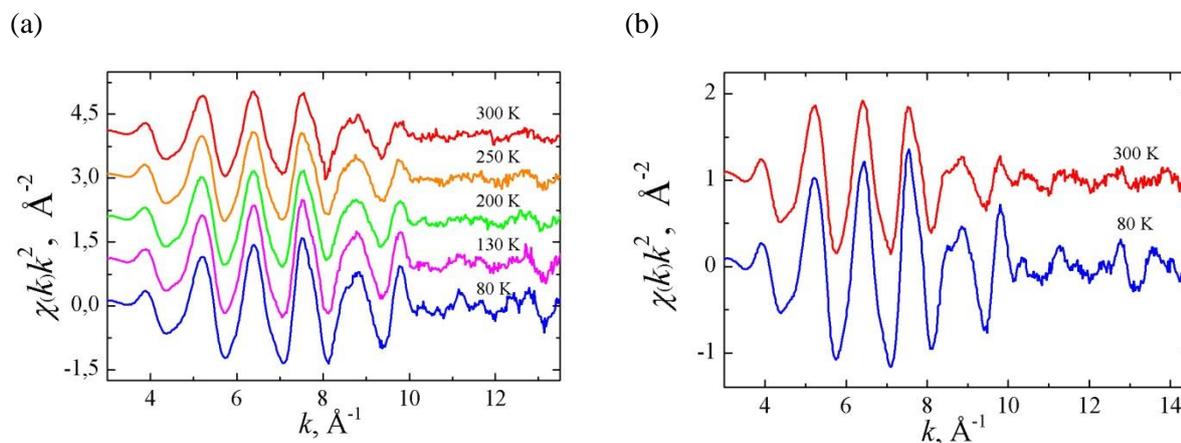
The X-ray absorption measurements were carried out at I811 beamline of MAX IV facility (Lund, Sweden) in the transmission mode at  $K$ -Co and  $L_{III}$ -Yb absorption edges in 80-300 K temperature range with normalized energy resolution of  $1 \times 10^{-4}$ . EXAFS spectra analysis was performed using the VIPER [9] software pack with standard procedure of EXAFS-function  $\chi(k)$  extraction and Fourier-analysis. Fitting of EXAFS-functions was performed in standard harmonic approximation. Back-scattering amplitude and phase shift calculated by FEFF [10] within the framework of structure model of cubic Laves phase C15.

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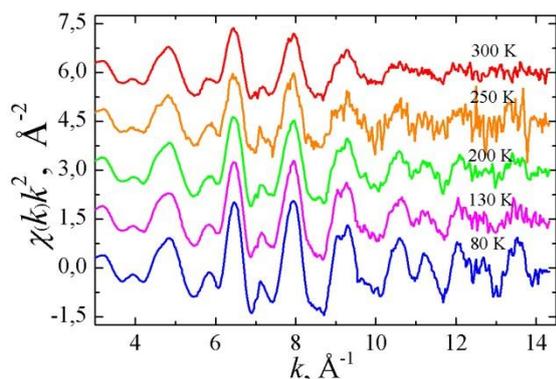
### 3. Results and discussion

EXAFS-functions  $\chi(k)k^2$ , measured above  $K$ -Co and  $L_{III}$ -Yb absorption edges at different temperatures are given in Figures 1 and 2.

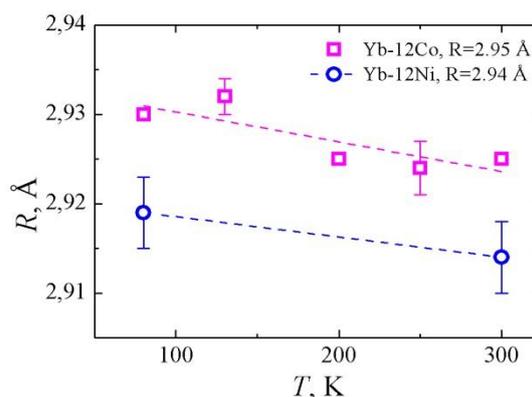


**Figure 1.** EXAFS-functions  $\chi(k)k^2$ , measured above  $L_{III}$ -Yb absorption edge at temperatures 80-300 K for  $\text{YbCo}_2$  (a) and  $\text{YbNi}_2$  (b).

The radii of coordination spheres Yb-M slightly change with temperature. At the same time the other distances stay almost unchanged. Bond lengths are shorter than the values extracted from XRD data for  $\text{YbNi}_2$  and  $\text{YbCo}_2$  intermetallics [11,12], except the bond length Yb-Yb. It is equal to published data for  $\text{YbCo}_2$ , and is 0.03  $\text{\AA}$  greater for  $\text{YbNi}_2$ . The value of the distance between Yb and Co(Ni) atoms is the most significant for the magnetic properties of these compounds (Fig. 3). The radius of the first coordination shell, corresponding to the shortest distance between atoms Yb and Co(Ni), increases with decreasing temperature. Weak Co moments survive far above the phase transition temperature [13], forming the clusters with short-range magnetic order. Therefore, the increase in the unit cell volume can occur when approaching the phase transition temperature [14] leading to a corresponding increase in local distances.



**Figure 2.** EXAFS-functions  $\chi(k)k^2$ , measured above  $K$ -Co absorption edge at temperatures 80-300 K

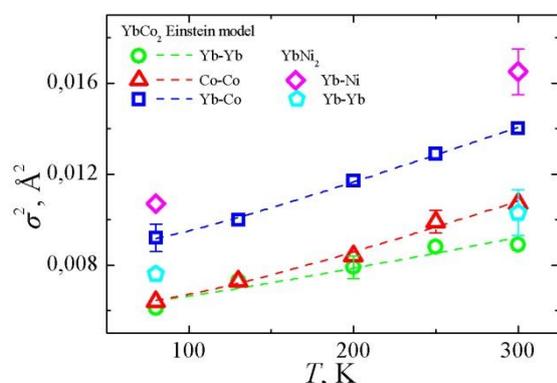


**Figure 3.** Temperature dependence of the distances between Yb and  $d$ -metal atoms in the first coordination sphere. The values in legend were calculated from data [3,23]

The temperature dependences of Debye–Waller factors  $\sigma^2(T)$  for coordination shells around ytterbium and cobalt atoms were also obtained. Here Debye-Waller factor is defined as a standard deviation of the interatomic distance from the mean value  $\sigma^2 = \sigma_s^2 + \sigma_d^2$  and consists of the temperature independent contribution  $\sigma_s^2$  due to the statistical disordering of atoms and dynamic contribution  $\sigma_d^2$  due to thermal vibrations. The temperature dependence of the dynamic contribution can be calculated using Einstein model:  $\sigma_d^2 = (\hbar/2\omega\mu) \text{cth}(\Theta_E/2T)$

Here  $\omega$  – the frequency of longitudinal oscillations,  $\mu$  – the reduced mass of the atomic pair,  $\Theta_E = \hbar\omega/k_B$  - Einstein temperature. Experimental results are shown in Figure 4 and Table 1.

One can see that Einstein temperature and hence bond rigidity is the highest for Co-Co bond (Table 1) that correlates with the fact that this bond is the shortest. The greatest static disorder corresponds to Yb-Co bond. Magnetic ordering is determined by the exchange interaction between sublattices of Co and Yb. The spread of distances between the atoms and the corresponding change in the overlap of the wave functions affect the density of states in 3*d*-band of Co and magnetic moment of Co atoms.



**Table 1.** Einstein temperatures and Debye-Waller factors for YbCo<sub>2</sub> interatomic bonds.

Bond	$\Theta_E$ , K	$\sigma_s^2(\text{\AA}^2)$
Yb-Yb	190	0,005
Co-Co	260	0,003
Yb-Co	207	0,006

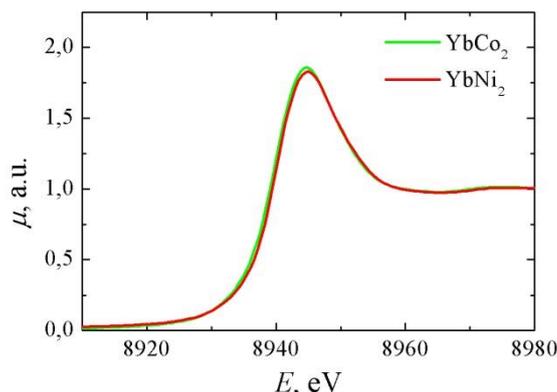
**Figure 4.** Temperature dependence of Debye–Waller factors for Yb-Co, Yb-Yb, Yb-Ni bonds

For YbNi<sub>2</sub> it was not possible to distinguish the static and dynamic contribution since only two temperature points were available. However, we can say that in YbNi<sub>2</sub> the atoms have a higher degree of disorder than in YbCo<sub>2</sub> and Debye-Waller factor of Yb-Ni bond is also the largest.

The normalized experimental *L*<sub>III</sub>-Yb XANES spectra for YbCo<sub>2</sub> and YbNi<sub>2</sub> measured at the temperature of 8 K are shown in Figure 5. Energy position of the absorption edge indicates that Yb atom is in Yb<sup>3+</sup> valence state. The shape and intensity of the white line are almost identical for both samples and do not vary with temperature. XANES spectroscopy above *L*<sub>III</sub>-absorption edge is based on the excitation of an electron from an internal 2*p*<sub>3/2</sub> level on the *d*-valence orbitals and carries information about the density of unoccupied electron states, therefore, the density of free 5*d*-states of these two compounds is almost the same.

#### 4. Conclusion

The distance between Yb and Co (Ni) atoms increases with decreasing temperature. Perhaps this is due to the presence of clusters with short-range magnetic ordering at temperatures above the phase transition. The same bond has the greatest static disorder. The shape and intensity of the *L*<sub>III</sub>-Yb absorption edge white line is practically identical for YbCo<sub>2</sub> and YbNi<sub>2</sub> samples, which indicates almost the same value of the density of free 5*d*-states in these two compounds.



**Figure 5.** XANES spectra of YbCo<sub>2</sub> and YbNi<sub>2</sub> compounds measured above L<sub>III</sub>- Yb absorption edge.

### Acknowledgments

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