ESRF	**Experiment title:** EXAFS study of decagonal superstructure $Al_{71}Ni_{13}Co_{16}$ and basic decahonal phase $Al_{75}Ni_{14.5}Co_{10.5}$	**Experiment number:** HS-1074
Beamline: BM29	**Date of experiment:** from: 9.11.99 to: 12.11.99	**Date of report:** 21.02.2001
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Report:

The structure of quasicrystals (QCs), crystals having quasiperiodic long-range order and non-crystallographic symmetry, is a subject of considerable interest. We used local and chemical selectivity of Extended X-ray Absorption Fine Structure (EXAFS) to determine the local atomic structure around Co and Ni in single crystals of decagonal AlNiCo. The X-ray Absorption Spectra (XAS) of two single crystals with nominal compositions $Al_{71.5}Ni_{15.5}Co_{13}$ and $Al_{75}Ni_{14.5}Co_{10.5}$ have been measured at the BM29 beamline at ESRF in total electron yield geometry with the 10-fold **c** axis oriented along ($\mathbf{E} \parallel \mathbf{c}$) and normal ($\mathbf{E} \perp \mathbf{c}$) to the electric field vector **E**. Samples were cooled down to 70 K to reduce the effects of thermal motion on the structure. EXAFS data analysis was performed using the theory developed in Ref. [1] and implemented in the GNXAS package [2]. Important details of the local environment of the transition metal atoms in *d*-AlNiCo are found.

Firstly, we observe different local environments for Co and Ni (fig. 1). Nickel has a bimodal nearest-neighbour surrounding with Al atoms at the distance of about 2.46 Å and T (Ni) about 2.67 Å. For cobalt such bimodal distribution cannot be excluded, but it is less evident: the model with only Al atoms in the first shell at around 2.42 Å agrees better with the experiment (fig. 2). These conclusions are in a good agreement with the assumption that Co atoms are surrounded only by Al.

Secondly, our data depict a higher degree of order along the **c** axis compared to the decagonal plane due to the periodic and quasiperiodic long-range order, respectively.

Thirdly, the absence of the T-T correlations around 4 Å in the **E** ∥ **c** measurements confirms the effective absence of the 4 Å periodicity along the decagonal axis in these QCs and gives some indications about its reasons. Our results are compatible with the effective periodicity of 8 Å which is revealed by interlayer diffuse scattering.

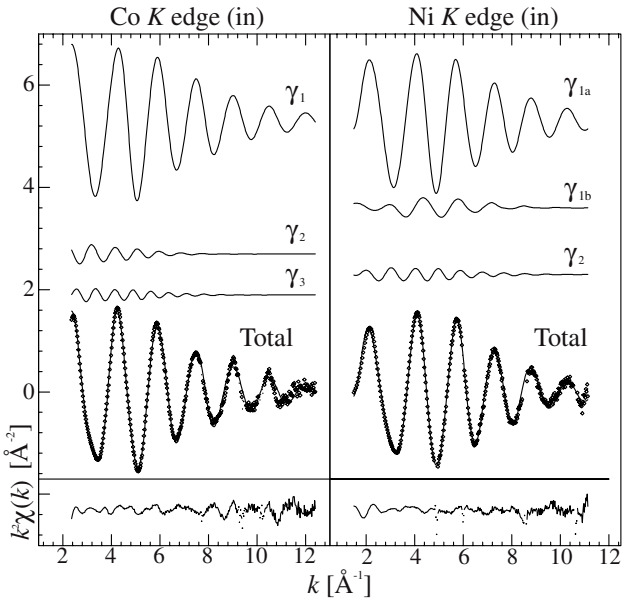

Fig.1 The experimental signal, total model EXAFS signal and their difference for Co (left) and Ni (right) for the **E** ⊥ **c** geometry.

For more details see Ref. [3].

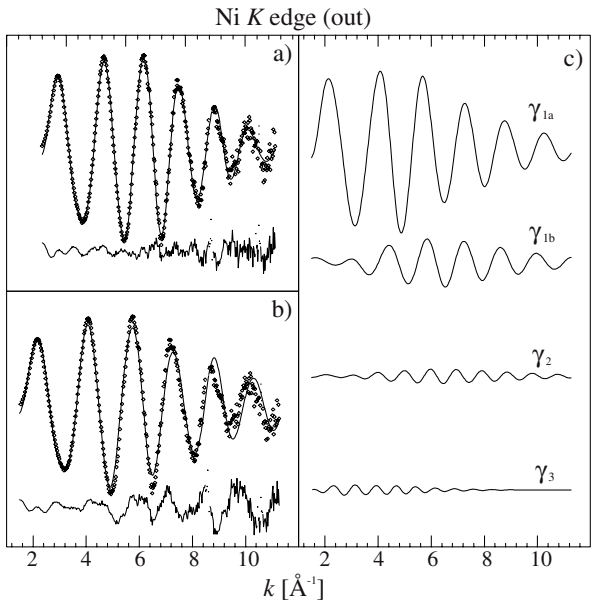

Fig.2 The experimental and calculated Ni **E** ∥ **c** EXAFS signals. The model with the bimodal first shell (a) fits the observations significantly better than the model with the one-component first shell (b). The individual contributions of the next-neighbour shells are presented in (c).

References

[1] Benfatto M., Natoli C. R., Bianconi A., Garcia J., Marcelli A., Fanfoni M., Davoli I., *Phys. Rev.* **B34**(1986)5774

[2] Filipponi A., Cicco A. D., *Phys. Rev.* **B52**(1995)15135

[3] Zaharko O., Meneghini C., Cervellino A., Fischer E., *Eur. Phys. Jour. B* **19**(2001)207