

**Experiment title:**Local structure dependence upon doping in $Y_{2-x}Mg_xRu_2O_7$ pyrochlores**Experiment****number:**

MA-2948

Beamline:

BM25A

Date of experiment:

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Shifts:

15

Local contact(s):

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We used extended X-ray absorption fine structure (EXAFS) spectroscopy to investigate the local order and the distribution of interatomic distances in Mg-doped $Y_2Ru_2O_7$ pyrochlore samples. Experiments were carried out in transmission geometry at beamline BM25A as a

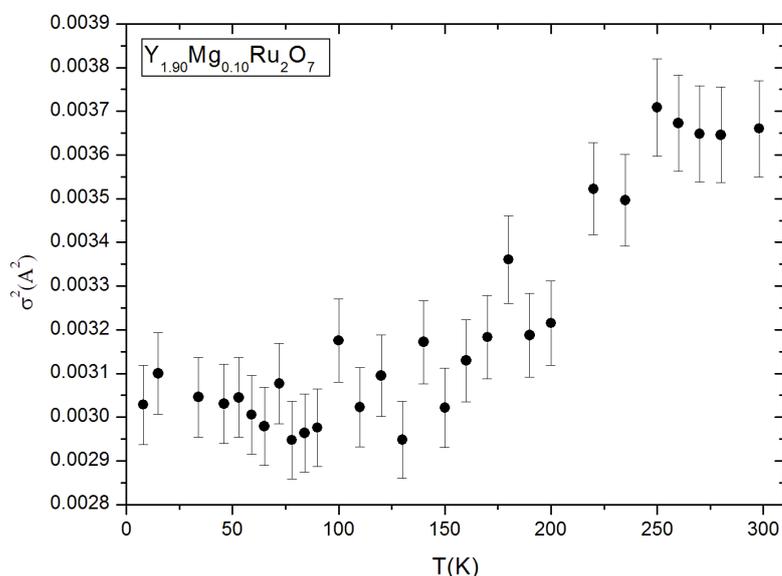


Figure 1: Debye-Waller factor as a function of temperature for the sample with $x = 0.10$

function of temperature at the Ru K edge. We performed measurements by both increasing and then decreasing the temperature, but found no particular hysteresis effect between the different cycles. Results presented hereafter refer to the cooling cycle at 31 different temperatures between 298 K and 8 K for the three samples $Y_{2-x}Mg_xRu_2O_7$ with $x = 0.10, 0.15, \text{ and } 0.20$.

We report in Figure 1 the Debye-Waller σ^2 (\AA^2) factor for the sample with $x = 0.10$ as an example. At variance with what we observed on the undoped

compound (experiment no. MA-2162), no clear peaks appear around the magnetic transition temperature, which should lie between 50 and 100 K for such compounds. We should remark here that an anomaly in the σ^2 behavior would be the fingerprint of the presence of a magneto-elastic coupling or of an additional local disorder. A peak was well visible in the Debye-Waller factor of the undoped compound [1], a slight peak was still visible for the Zn-doped one, with doping level $x = 0.10$, while no features were observed for higher doping levels [2]. In the present case of Mg-doping, no particular feature is observed even for the lowest doped sample (see Figure 1). At variance with the Zn case, however, a bimodal distribution of distances in the first shell did not prove to be effective in fitting experimental data. Indeed, for the Zn-doping, we found that all samples (including the undoped one) were best modeled with a distortion in the RuO_6 octahedra, with the four basal distances shorter (~ 2.00 Å) than the two apical ones (2.04 Å).

Here, the best fits were obtained by maintaining the six first shell distances all equal to each other. In Figure 2, we report first and second shell distances for the three Mg-doped samples.

The dashed lines represent the distances retrieved from diffraction experiments (1.99 Å for Ru-O, and 3.59 Å for Ru-Y and Ru-Ru): while in the first shell the local behavior of oxygen atoms (as seen by EXAFS) corresponds, within the error bars, to the long-range one (as seen by diffraction), this is not true for the second shell distances. Here, distances are splitted, being the Ru-Ru ones always slightly greater than the Ru-Y. This latter finding is, however, not in contradiction with the fact that part of Y^{3+} atoms are replaced by Mg^{2+} , which exhibits a smaller ionic

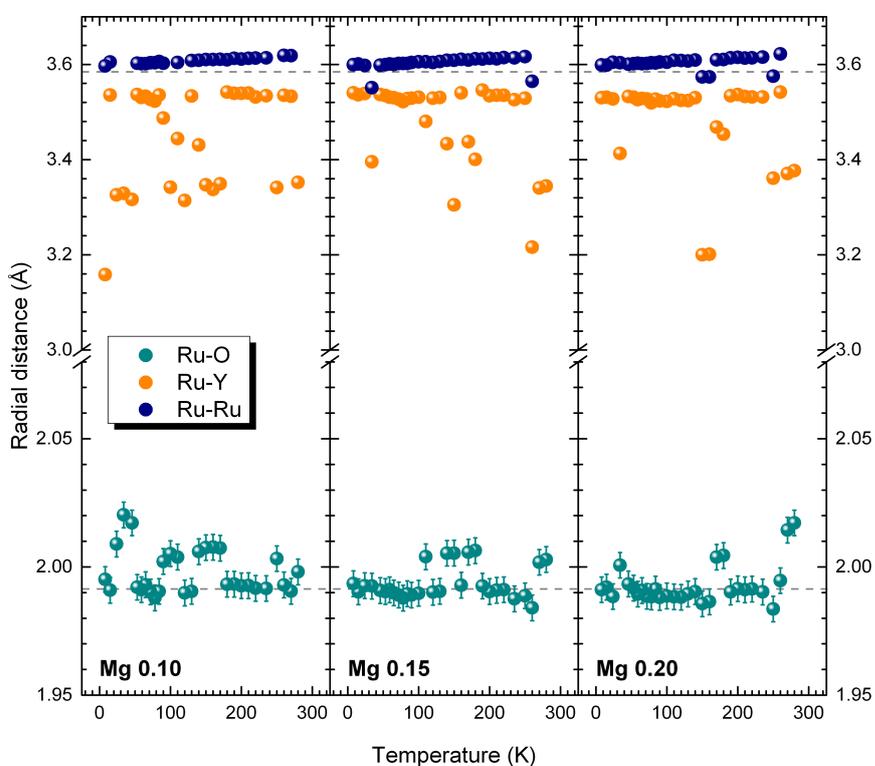


Figure 2: Interatomic distances as a function of temperature for the three Mg-doped samples

radius, and could then be the cause of the observed shrinking of second shell Ru-Y distances.

In the proposal at the basis of this experiment, we stated that the Mg^{2+} dopant, due to a completely different electronic configuration with respect to Zn^{2+} , could influence the magneto-elastic and local structural properties. Looking at the results reported herein, both the huge magneto-structural coupling on the local scale and an additional local order-disorder phase transition at a critical temperature are not observed. The reason might be found in the different chemico-physical properties of these Mg-doped ruthenium pyrochlores.

[1] C. Castellano, G. Berti, S. Sanna, R. Ruiz-Bustos, J. van Duijn, A. Brambilla, A. Muñoz-Noval, P. Carretta, L. Duò, F. Demartin, *Phys. Rev. B* **91** (2015) 224101

[2] G. Berti, S. Sanna, R. Ruiz-Bustos, J. van Duijn, A. Brambilla, A. Muñoz-Noval, F. Demartin, L. Duò, C. Castellano, *RSC Advances* **5** (2015) 100809