EUROPEAN **S**YNCHROTRON **R**ADIATION **F**ACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

ESRF

	Experiment title: Study of the Origin of Giant Magnetostriction in RE-Fe	**Experiment number**:
Beamline: ID24	**Date of experiment**: from: 25-4-07 to: 30-4-07	**Date of report**: 26/9/07
Shifts: 18	**Local contact(s)**: M. Ruffoni	*Received at ESRF:*

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Report:

The huge anisotropy of the 4f electron cloud and high Curie temperature in rare-earth-Fe_2 ($REFe_2$) compounds, which crystallize in the Laves or C15 phase, lead to large magnetostriction at room temperature. In these systems, when the orientation of the magnetic moment of the 4f shell is rotated with respect to the crystallographic axes by the application of a strong external magnetic field, it is assumed that the anisotropic 4f charge density is rigidly co- rotated. The surrounding atoms will attain new equilibrium positions when changing the orientation of the 4f shell in order to minimize the total energy, and this will result in important local strains.

In the framework of a collaboration between the INRIM (Torino) and the ESRF, we have been trying to apply Differential XAS techniques to detect such strains in thin amorphous films of $REFe_2$. The aim of the present experiment was to confirm previous measurements on thin amorphous films of $TbFe_2$ (see exp report HS2942 – HS2946) and give us additional input concerning the effect of the RE, by looking at other similar systems where only the RE is substituted. In particular, we expected to measure similar "large" differential XAS at the L_3 edge of the RE in other $REFe_2$ Laves phase systems, such as $DyFe_2$. The comparison of this signal for different RE embedded in the same structure, together with the ab – initio simulations, will help clarify the role of the asymmetry of the RE in the generation of such large magnetostrictive strain.

During these shifts, we succeded in measuring differential XAS signals at the RE L_3 edge on thin amorphous films of $Fe_{73}Tb_{27}$, $Fe_{62}Dy_{38}$ and, $Fe_{59}Tb_8Dy_{33}$ at both the Tb and Dy L_3 edges. Figure 1 shows examples of raw X-ray absorption spectra on the different samples at the two edges, and Figures 2 and 3 report the Differential Signals normalized to the edge jump. The data is not energy calibrated and is plotted as a function of pixel number. Also, the signal to noise ratio on the differential signals can be further improved by averaging data over several runs that have been aquired but are not shown. It is interesting to note that the intensity of the normalized differential signal for a specific absorption edge is different for samples having different chemical environment. Also, the normalized differential signal measured at the Tb L_3 edge is larger than that measured at the Dy L_3 edge on the same sample.

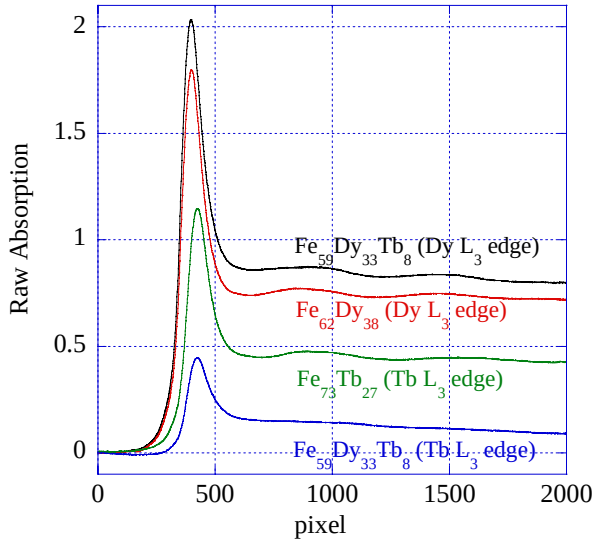

Figure 1

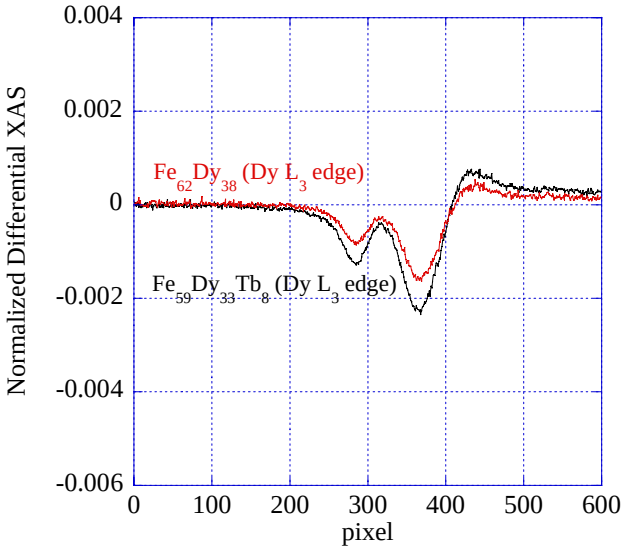

Figure 2

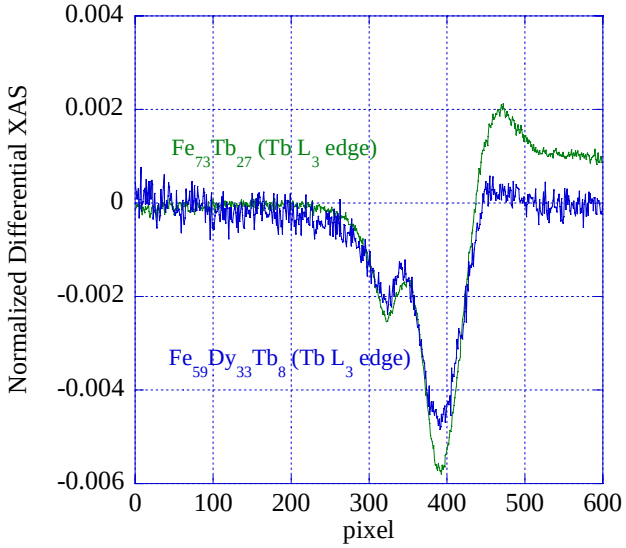

Figure 3

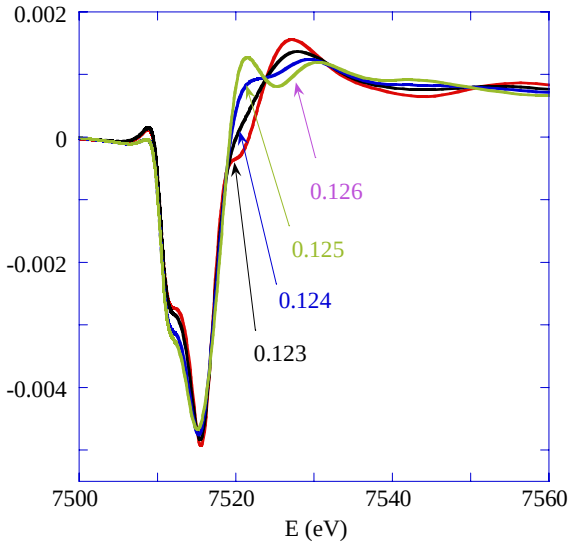

Figure 4

In the attempt to shed light into the local distortions around the RE atoms using the shape and intensity of these signals, we have started a collaboration with Y. Joly, from the Institut NEEL in Grenoble, who has carried out ab-initio calculations of the absorption spectra using a mono-electronic, Muffin Tin potential, fully relativistic multiple scattering theory (FDMNES code). Figure 4 shows examples of calculated differential signals for different positions of the Tb atom within the unit cell (0.125 corresponds to the " undistorted" equilibrium position) in a polycrystalline Fe_2Tb compound. The large signal is seen to have its origin in the polarization of the Tb orbitals due to the very strong spin-orbit interaction. The small lobe at lower energies arises from the 2p→4f quadrupolar transition, whether the main feature is due to the 2p → 5d dipolar transition. The shape of the signal at high energies is seen to be very sensitive to the displacement of the Tb atom from its equilibrium position.

The general agreement in shape and intensity between the calculation and the experiment is excellent, considering the crudeness of the potential used. A more quantitative data analyis is on the way.