Origin of the magnetisation enhancement by Zr addition in $(Sm_{1-x}Zr_x)(Fe_{0.8}Co_{0.2})_{12}$ studied using X-ray magnetic circular dichroism

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The scarcity of rare earth elements (RE) categorized as critical raw materials have stimulated the search for new rare earth-free/lean alloys alternatives for Nd-Fe-B based permanent magnets. Some of $REFe_{12}$ compounds with tetragonal $ThMn_{12}$ (1:12) structure show high magnetocrystalline anisotropy [2] and an inherent lean content of rare earths (7.7 at.%) compared with $Nd_2Fe_{14}B$ (11.8 at.%) can induce high magnetisation. However, binary $REFe_{12}$ is not thermodynamically stable and a ternary element in substitution of Fe is needed to obtain the 1:12 structure in bulk, which reduces the saturation magnetisation of the compound [3]. Recently, it has been reported that substitution of Sm with Zr stabilises the 1:12 structure without decreasing magnetisation in the certain range of Zr concentration [4,5].

In this work, we have measured XMCD spectra at the Fe and Co $L_{2,3}$-edges and the Sm $M_{4,5}$-edges in (001) oriented epitaxial $(Sm_{1-x}Zr_x)(Fe_{0.8}Co_{0.2})_{12}$ ($x = 0$, 0.14 and 0.26) films grown on a (001)-oriented V underlayer deposited on a MgO(001) single crystalline substrate, as reported by Hirayama et al. [6]. The magnetisations of these films at room temperature (RT) are summarized in Table 1. The XMCD experiment was performed at BL25SU of SPring-8. The element specific magnetisation was calculated by the sum rule analysis for the XMCD spectra recorded at RT and 20 K, which showed an increase of the magnetisation for the sample with $x = 0.14$. The present results show that the small addition of Zr of 0.14 enhances the magnetic moment of Fe atoms by a 6% while a large change of a 23% of the magnetic moment of Sm is found. The relatively low concentration of Sm in the 1:12 structure compared with Fe makes that the total magnetisation of the alloy is driven mainly by the enhancement of the magnetic moments of Fe, with a total increase of a 6.3%. Since the intensity of the resonant absorption (not shown here), which is proportional to the number of the $3d$ electron, doesn't change significantly, the charge transfer between Fe and Zr can be discarded as a dominant factor for this enhancement. This observation likely suggests that Zr substitution mainly affects the crystal structure such as the increase of local Fe-Fe distances or the weakening of Fe $3d$ – Sm $5d$ hybridisation, which leads to the enhancement of the ferromagnetic coupling.

Table 1.- Summary of the magnetisation measured at RT by SQUID and the magnetisation and magnetic moments of each element calculated by XMCD which was recorded at RT.

Zr content	Magnetisation (T) SQUID	Magnetisation (T) XMCD	Magnetic moment m (μ_B)		Δm (%)
x = 0	1.78	1.75	Fe	2.32	-
			Co	1.53	-
			Sm	-0.42	-
x = 0.14	1.87	1.86	Fe	2.46	6.0
			Co	1.55	1.3
			Sm	-0.32	23.8

Reference
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