XRD and XAFS Study of Co-Fe-Ga Heusler Nanoparticles

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Recently, we reported the first chemical synthesis of Heusler Co_2FeGa nanoparticles using a modified impregnation method [1]. We extend this approach to carbon-encapsulated Co-Fe-Ga nanoparticles and studied long and short range order structure by XRD and XAFS measurements. From TEM observations, particle size decrease with increasing silica template amount. Synchrotron XRD measurements were performed at SP12B1 and BL17A1 with photon energy of 7120 eV and 9297 eV, respectively. Figure 1 shows the XRD patterns of Co-Fe-Ga nanoparticles as a function of silica amount. (220), (311) and (222) reflection peaks verify the formation of cubic phase. While the presence of (111) and (200) reflection peaks of the 1g silica sample signify the formation of L_{21} Heusler phase. Impurity phase including cubic Fe and Co are identified. With increasing silica template from 1g to 2g, the intensity of diffraction peaks (crystallinity) decrease due to decreasing nanoparticle amount examined. Under condition of silica amount more than 1.5g, both (111) and (200) diffraction peaks vanish with increasing broadening of (220) peak concurrently indicating smaller crystal size. XRD result is consistent with TEM data.

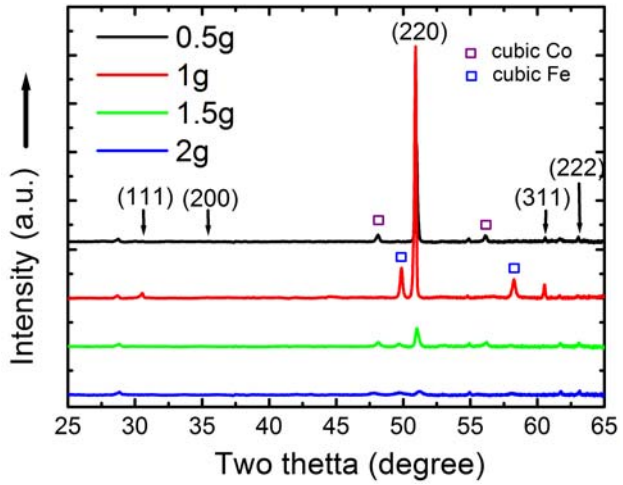

Fig. 1: XRD patterns of Co-Fe-Ga nanoparticles with various amounts of silica template.

The local atomic environment around Fe and Co was investigated by performing NEXAFS and EXAFS measurements at Fe and Co K-edges. XAFS data were collected at BL17C1 beamline using transmission mode and the Co-Fe-Ga nanopowders were pressed to form pellets to reach transmission depth more than 5 mm. As shown in Fig. 2, by comparing the edge position, white line, major shape resonances with metallic standards and bulk reference, Co-Fe-Ga nanoparticles resembled with bulk Co_2FeGa. The absence of metal oxide and possible presence of metallic Co in Co-Fe-Ga nanoparticles with silica amount more than 1g were indicated. The broadening shape resonances due to size effect were also observed.

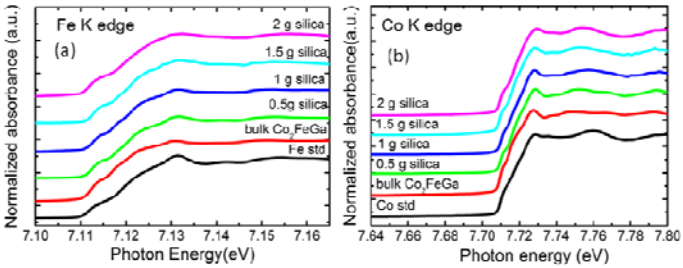

Fig. 2: Normalized NEXAFS spectra of Co-Fe-Ga nanoparticles as a function of silica template: (a) Fe K-edge; (b) Co K-edge.

Fourier transformed k^3 weighted χ magnitude (EXAFS) at Fe and Co K-edges for Co-Fe-Ga nanoparticles with various silica amounts are described in Fig. 3. Compared with bulk Co_2FeGa and metallic Fe/Co references, short range geometry of Co-Fe-Ga nanoparticles with silica amount less than 1g resemble bulk Co_2FeGa. Increasing geometric disordering occur for Co-Fe-Ga with silica more than 1.5g, especially within local atomic environment surrounding Co.

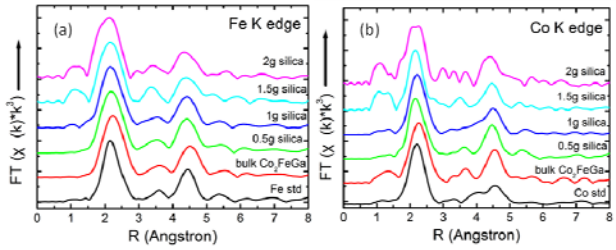

Fig. 3: Fourier transformed k^3 weighted χ magnitude (EXAFS) at K-edges of Fe (a) and Co (b).

The correlation between crystal structure and magnetic behavior of the Co-Fe-Ga nanoparticles of various sizes provides insights on size effect of ternary alloyed nanoparticles. Furthermore, short range order structured information derived from XAFS analysis complement the magneto-structural information obtained from Mößbauer spectroscopy.

Reference

[1] L. Basit *et al.*, J. Phys. D **42**, 084018 (2009).