Anomalous Structural Behavior in the Magnetic and Structural Transition of FeRh Thin Films from a Local Viewpoint

The antiferromagnetic-to-ferromagnetic (AFM-to-FM) transition of FeRh thin films was investigated by Fe and Rh K-edge X-ray absorption fine structure spectroscopy (XAFS) in order to clarify the correlation between its global magnetism and local electronic/geometrical structures. A strong Fe-Rh hybridization, which decreases from AFM to FM phases, was revealed. Moreover, only the Fe-Fe Debye-Waller factor in the AFM phase was observed to be enhanced in comparison with that in the FM phase. This behavior suggests the importance of the interplay between the local spin and Fe-Fe distance fluctuations near the phase transition.

Recently, CsCl-type ordered FeRh alloy near the equimolar stoichiometry is attracting renewed interest in view of its potential application to various magnetic devices. Upon increasing its temperature, it shows an antiferromagnetic-to-ferromagnetic (AFM-to-FM) phase transition accompanied with a nearly 1% volume expansion at -350 K [1]. Owing to this magnetic and structural phase transition occurring at mild temperature, FeRh is a promising material for thermally-assisted magneto-recording, antiferromagnetic memory, and electric-field-induced magnetism switching [2-4]. Therefore, it is important to elucidate the origin of the phase transition in FeRh not only from the viewpoint of basic research, but also for device development. Despite many studies on its phase transition, the origin of this interesting phenomenon and the essential interactions involved are still hot topics. Especially, the relationship between spin, structure, and electronic state, which all change through the phase transition, is a key issue. In this study, FeRh thin film was investigated by using X-ray absorption fine structure (XAFS) spectroscopy. XAFS spectroscopy is a powerful tool for detecting both atomic-dependent and bond-dependent local structures. According to the change in the X-ray absorption near-edge structure (XANES) and Debye-Waller factors of Fe-Rh and Fe-Fe, we consider that the local Fe-Fe distance and the spin fluctuations act as precursors. These fluctuations play an important role in driving the phase transition.

100-nm-thick Fe₉₀Rh₃₀ thin film was epitaxially grown on a single crystal MgO(001) substrate by magnetron sputtering and annealing process [5]. Figure 1 shows the XANES spectra at Fe and Rh K edges of FeRh at 300 K (AFM) and 450 K (FM), respectively, in fluorescence yield mode by using a multi-element Ge solid state detector. According to a recent theoretical study, the AFM exchange interaction between two neighboring Fe atoms depends more strongly on volume change than the FM exchange interaction between Fe and Rh atoms [6]. The balance of these exchange interactions is expected to determine the global magnetic state. At a small volume the AFM state is exclusively favored, whereas the FM state is expected to allow for the spin fluctuations more easily because of the weakening of the Fe-Rh Fe-Fe exchange interaction due to a longer Fe-Fe distance [6], resulting in a rather small Fe-Fe Debye-Waller factor. Therefore, the anomalous behavior found in the Fe-Fe Debye-Waller factor indicates that the local Fe-Fe distance and spin fluctuations play an important role in driving the phase transition.