XMCDと第一原理計算から見た $Mn_{3-x}Ga$ の垂直磁気異方性

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Perpendicular Magnetic Anisotropy in $Mn_{3-x}Ga$ studied by XMCD and first-principles calculations

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Introduction

Magnetic ordered alloys have attracted significant attention for use as spintronics materials because they are highly likely to exhibit perpendicular magnetic anisotropy (PMA). Tetragonal $Mn_{3-x}Ga$ alloys are widely recognized as hard magnets which exhibit high PMA, ferromagnetic or ferrimagnetic properties depending on Mn composition, and metallic properties [1]. Two kinds of Mn sites, which couple antiferromagnetically, consist of the $Mn_{3-x}Ga$ with the $D0_{22}$-type ordering. On the other hand, the $L1_0$-type ordered Mn_1Ga alloy possesses the single Mn site. In order to investigate the mechanism of PMA and large coercive fields in $Mn_{3-x}Ga$, site-specific magnetic properties have to be investigated explicitly. X-ray magnetic circular dichroism (XMCD) can become a powerful tool to study them. However, the difficulty in deconvolution of two kinds of Mn sites has prevented the site-resolved detailed investigations. Some assumptions are required for the analysis [2]. First-principles calculations were also performed, resulting in the small orbital moment anisotropy in the Mn compound cases because of the spin-flip contribution of MA [3]. In this study, we perform the deconvolution of each Mn site using the systematic XMCD measurements for different Mn contents in $Mn_{3-x}Ga$. We discuss the site-specific spin and orbital magnetic moments which are deduced from angular-dependent XMCD and compare with the density-functional-theory (DFT) calculations.

Experimental

The samples were prepared by magnetron sputtering on MgO substrates. On the 40-nm-thick Cr and 30-nm-thick CoGa buffer layers [4], 3-nm $Mn_{3-x}Ga$ were deposited at room temperature and capped by the 2-nm-thick MgO layer. We prepared the samples of x=0 (Mn_3Ga), 1 (Mn_2Ga), and 2 (Mn_1Ga) cases. X-ray diffraction peaks originated from $D0_{22}$ and $L1_0$-type orderings were clearly observed. The X-ray absorption spectroscopy (XAS) and XMCD were performed at BL-7A in the Photon Factory (KEK). The total-electron-yield mode was adopted, and all measurements were performed at room temperature.

Results

Mn $L_{2,3}$-edge XAS in $Mn_{3-x}Ga$ showed clear metallic line shapes. XMCD intensities decreased with increasing the Mn contents, resulting in antiferromagnetic coupling. With increasing Mn contents, the fine structures in XMCD line shapes which come from two kinds of Mn sites were clearly detected. Based on the spectrum of Mn_1Ga which consists of single Mn site, the subtraction from Mn_1Ga XMCD spectrum after the normalization of spectral intensities deduces the anti-parallel coupled another Mn site. After the deconvolution processes, the spin and orbital magnetic moments for each site were estimated using magneto-optical sum rules. Furthermore, clear hysteresis curves at Mn L_3-edge XMCD were also detected, which was consistent with the results of magneto-optical Kerr effects. In the presentation, we discuss the site-specific magnetic properties depending on the Mn contents and compared with the DFT calculations.

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