Effect of p-d interaction on circularly polarized Kα emission

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X-ray emission spectroscopy is a useful tool to obtain information of local electronic structure. Although polarization of incident x-rays has been considered, that of emitted x-rays has not been paid attention. Recently, Inami has observed circular dichroism of circularly-polarized Kα emission from a magnetized BCC iron [1]. The new dichroism is substantially larger than typical K-edge x-ray magnetic circular dichroism (XMCD). One of the differences from the K-edge XMCD is 2p-3d interaction, which is larger than np-3d interaction in K-edge XMCD. Here, we estimate intensity of the p-d interaction in BCC iron by using the circularly-polarized Kα emission spectra.

Our idea is fitting of the observed spectra by using a fitting function, which shall be briefly explained as the following. In order to describe the two-photon process including the x-ray emission, the Kramers-Heisenberg formula can be used as a starting point to discuss the emission spectra [2]. We adopted an independent particle approximation which could be partially justified by a calculated result for $L_{2,3}$-edge x-ray photoelectron spectroscopy [3], providing a simplification to describe the emission process. Since an incident x-ray energy is substantially higher than the threshold energy of 1s core state excitation, interaction between the excited photoelectron and the rest system can be neglected. From these approximations, we obtained relative intensity of the emission from each $2p_{3/2}$ and $2p_{1/2}$ sublevel. Next, we adopted a mean-field approximation for 2p-3d exchange interaction in order to describe splits of $2p_{3/2}$ and $2p_{1/2}$ sublevels by an effective magnetic field on 2p states. This enables us to fit relative peak positions of the sublevels by the magnetic field as a fitting parameter.

We fitted observed circularly-polarized Kα emission spectra of a BCC iron by using our fitting function. The p-d interaction of 0.25 eV is estimated with the obtained effective magnetic field and a typical reported magnetic moment of 2.0 μ_B on a Fe ion [4, 5]. The value of the p-d interaction is consistent with the one evaluated from $L_3M_{2,3}M_{2,3}$ Auger electron emission spectroscopy [5]. Moreover, the obtained p-d interaction is strongly reduced from an atomic calculated value of 0.98 eV [6]. These indicate that the emission spectra can provide information for screening of exchange interactions in various magnetic materials.

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