Materials Science

16A2/2001G063

Evidence for d-f Coulomb mechanism in the resonant x-ray scattering of DyB_2C_2

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Introduction

Resonant x-ray scattering (RXS) has now become a powerful technique to observe orderings of orbital and quadrupolar moments. However, there have been a criticism that RXS do not observe the orderings directly. For example, in the K-edge resonance in d-electron systems, RXS utilizes the p-state as the intermediate state of the E1 process. Although we expect the p-state contains information on the d-shell, it can also be influenced by the surrounding ions. The same criticism also applies to f-electron systems if the L_{III}-edge is utilized. The present study on the antiferroquadrupolar (AFQ) order in DyB_2C_2 shows that the d-f Coulomb interaction is responsible for the resonance.

Results and Analysis

Figure 1 shows the energy dependence of the (0 0 2.5) resonant reflection of DyB_2C_2 for σ- σ' and σ-π' polarization channels. The peak at 7.792 and 7.782 keV corresponds to the E1 (2p-5d) and E2 (2p-4f) resonance, respectively. These resonances have been considered to be caused by the AFQ order of the 4f electrons. However, since the surrounding B and C atoms are also distorted below T_Q, the 5d state could be influenced by the B and C atoms; this means that the E1 resonance do not necessarily reflect the AFQ order of the 4f state, but the displacements of B and C atoms.

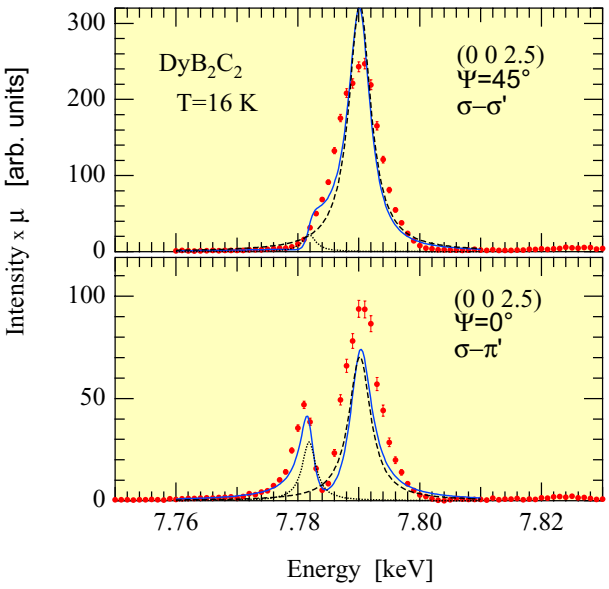

Figure 1: Energy dependence of the (0 0 2.5) resonant reflection originating from the AFQ order.

One mystery in this experimental result is that the E2 resonance is well separated in the σ-π' channel but is hidden in the tail of the E1 resonance for σ-σ'. In order to solve this mystery, we have analyzed the data by utilizing a theory developed by Lovesey *et al.*, which directly connects the atomic tensors with the scattering amplitude.

The calculation described in Refs. 1 and 2 shows that the structure factors for the E1 and E2 resonances have opposite sign for σ-σ' and same sign for σ-π', respectively. Furthermore, it is shown that this difference in sign is caused by the fact that the rank 2 atomic tensors for the 4f and 5d shells have opposite signs. This means clearly that the charge distributions of the 4f and 5d electrons are orthogonal to each other because of the Coulomb interaction. This is the direct evidence for the Coulomb mechanism in RXS for an AFQ system.

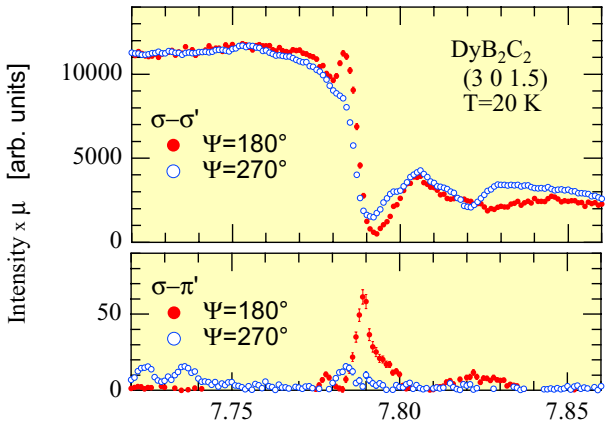

Figure 2: Energy dependence of the (3 0 1.5) resonant reflection. For σ- σ', there is a contribution of Thomson scattering from the lattice distortion.

Analysis of another reflection at (3 0 1.5) also confirm the above interpretation. In addition, it is concluded that the displacement of B and C atoms prefer to avoid the charge distribution of 4f, and not that of 5d.

References

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