Neutron Diffraction and Mössbauer studies on Ca_2FeMoO_6

Sung Baek Kim[1*], **Chul Sung Kim**[2]

[1]Department of Biomedical materials, Konyang University, Daejeon, Republic of Korea
[2]Department of Physics, Koomin University, Seoul, Republic of Korea
[*]E-mail: physics@konyang.ac.kr

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In recent years, the series of ordered double perovskite oxides A_2FeMoO_6(A=Ba, Sr), which exhibits spin polarization giant tunneling magnetoresistance at room temperature, have been studied with the interest of many scholars. In general, it is known that the magnetic properties of the perovskite oxides depend on the crystallographic properties due to the tolerance factor, even if the non-magnetic ions at the A-site are not directly involved in magnetism. Therefore, a Ca_2FeMoO_6 sample in which A-site ions have an ionic radius smaller than Sr was prepared, and the magnetic properties according to the crystal structure were studied by neutron diffraction and Mössbauer spectroscopy.

The single phase polycrystalline Ca_2FeMoO_6 powder was prepared by a solid-state reaction method, and chemical composition of the sample was confirmed to be stoichiometric by Rutherford backscattering spectrometer(RBS). Neutron diffraction data for the powder sample were collected at various temperatures ranging from 10 to 360 K using a high resolution powder diffratometer in HANARO reactor.

The crystal structure of the Ca_2FeMoO_6 at room temperature is found to be monoclinic with lattice constants a_0=5.5729 Å, b_0=5.5170 Å, c_0=7.6971 Å, and β=89.92 °. The unit cell parameter of a_0 increases linearly with increasing temperature,but b_0 and c_0 increase rapidly above Curie temperature(T_C). The T_C is determined to be 350 K in the Mössbauer zero velocity counts technique. The Mössbauer spectrea have been taken at various temperatures ranging from 17 to T_C. Figure 1 shows that the Mössbauer absorption lines are 6 in number and are sharp at 17 K. It can be understood that Fe ions occupy a single crystallographic site. The isomer shift value at room temperature is 0.43 mm/s relative to the Fe metal that are consistent with the Fe^{3+} valence state. We analyzed the hyperfine parameters of the Mössbauer spectra as a function of temperature and observed the magnetic properties with crystallographic changes through neutron diffraction experiments.

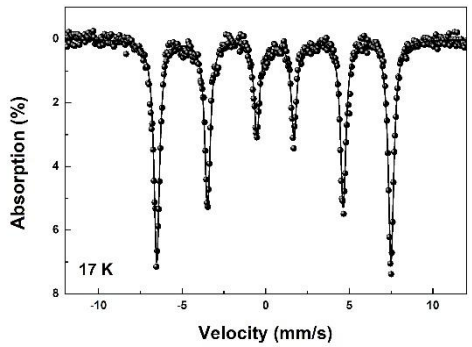

Fig. 1. Mössbauer spectrum of Ca_2FeMoO_6 at 17 K.

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