Structural Studies of Two-Dimensional Ferromagnets A_2CuF_4 (A=K, Rb, Cs) at High Pressure and Low Temperature

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The layered compound K_2CuF_4 is a well-known example of a two-dimensional Heisenberg ferromagnet. The origin of the ferromagnetic interaction between neighboring Cu spins is the alternative ordering of dx^2-z^2 and dy^2-z^2 orbitals, resulting from the antiferrodistortive (AFD) arrangement of Jahn-Teller distorted CuF_6 octahedra in the basal plane. Recent magnetic susceptibility measurements revealed a drastic change of the magnetism at about 8-9 GPa, suggesting a rearrangement of the octahedra from AFD order to a more compact one like the ferrodistortive (FD) order in La_2CuO_4.[1] High-pressure x-ray diffraction experiments were subsequently made at room temperature and showed a structural phase transition at 9.5-11.3 GPa, above which all the elongated axes of the CuF_6 octahedra align parallel to the *b*-axis.[2] A theoretical study has shown a possibility of the occurrence of a pressure- induced ferro-to-antiferromagnetic transition in K_2CuF_4 without distortive change from AFD to FD order in the basal plane.[3]

In the present study, we have made high-pressure powder x-ray diffraction experiments at 10 K using synchrotron radiation so as to verify the correspondence of the magnetic and structural changes. A diamond anvil-cell was used and the pressure was generated by loading the membrane with ^4He gas. Pressure was changed at low temperature and was determined by the ruby fluorescence technique. A 4:1 mixture of methanol and ethanol was used as the pressure medium. Figure 1 shows the diffraction patterns of K_2CuF_4 at 10 K under various pressures up to 14 GPa. As shown in the figure, new peaks corresponding to the high pressure phase observed at room temperature appear at 8.3 GPa and grow with increasing pressure. It becomes evident that the transition pressure P_T shifts to a lower value at low temperature and the magnetic change corresponds to the structural transition since the values of P_T and the width of P_T are exactly the same as those for the magnetic change.

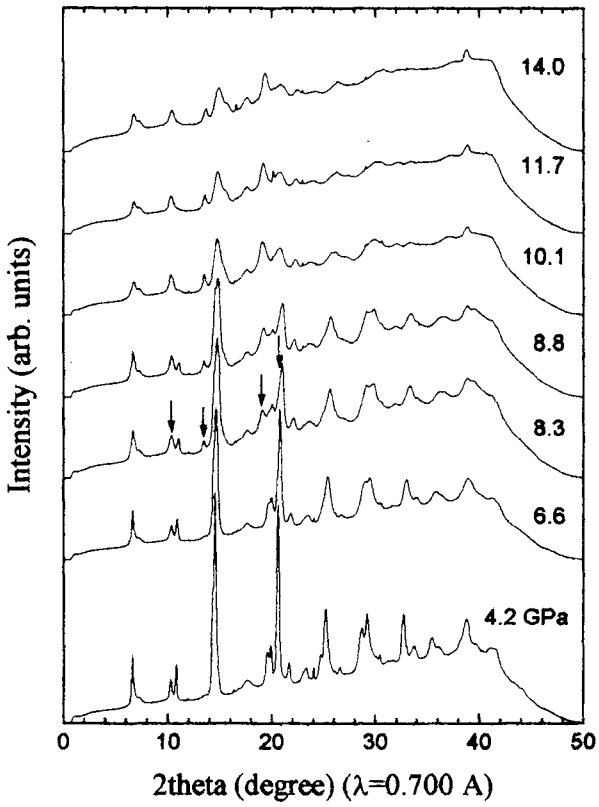

Fig. 1. X-ray diffraction patterns of K_2CuF_4 up to 14 GPa at 10 K. Arrows show new peaks.

1) M. Ishizuka *et al.*, J. Phys. Soc. Jpn. **65**, 1927(1996).
2) M. Ishizuka *et al.*, Phys. Rev. B**57**, 64(1998).
3) T. Kawamoto and N. Suzuki, J. Phys. Soc. Jpn. **66**, 2487(1997).