Relationship between Magnetic Structure and Ferroelectricity of LiVCuO4

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LiVCuO4 has one-dimensional (1D) chains of the edge-sharing CuO4 squares along b, which are separated by the nonmagnetic Li+ and V5+ ions. For this system, the antiferromagnetic transition was found at TN = 2.4 K, where the dielectric susceptibility epsilon measured along a also exhibits an anomaly, indicating that the ferroelectric transition takes place almost simultaneously with the magnetic transition. This simultaneous occurrence of the two transitions or their coexistence is called the multiferroic phenomenon [1]. While almost all multiferroic systems ever reported have the magnetic moments with spin S>1 and/or have more than two magnetic sites, LiVCuO4 has spins S=1/2 of Cu2+ in the 3d x2-y2 orbital and only one crystallographically distinct Cu site. It is considered to be the first example of spin 1/2 multiferroic systems, which does not bring about any complications due to the multi-orbital and multi-site effects in the study of the mechanism of the multiferroic nature.

Neutron scattering studies as well as measurements of the dielectric susceptibility epsilon and ferroelectric polarization P have been carried out in various magnetic fields H for single-crystal samples of LiVCuO4, and the relationship between the magnetic structure and ferroelectricity has been studied [2]. Neutron scattering measurements were carried out using the triple axis spectrometer HQR(T1-1), where the double axis condition was adopted. For H = 0, the neutron scattering intensities were measured at Q = (h, k, 0) and (0, k, l) in the reciprocal space at 1.6 K (<TN) and 5 K (>TN). At 1.6 K, we observed magnetic superlattice reflections at Q = (h, k+-delta, 0) and (0, k+-delta, l) (h and l = odd, k = even) with delta=0.466. The magnetic structure that can reproduce the observed magnetic scattering intensities, is the ab-plane helical one shown schematically in the figure. It is consistent with the structure reported by Gibson et al.[3]. Considering the ferroelectric polarization P observed along a, we have found that the relation P=Q*e3 holds, which is consistent with the existing theories. The ferroelectric polarization along a, Pa at H=0 is found to be proportional to the neutron magnetic scattering intensity, indicating that the magnetic order is closely related to the appearance of the ferroelectricity.

The behaviors of epsilon and Pa drastically change with the applied magnetic field. Neutron diffraction measurements were carried out in the (0kl) scattering plane under the applied field H (//a) and the magnetic structure has been determined, where the spins have the bc-plane helical structure at least in the region H > 2 T. These results are consistent with the observed suppression of Pa by the applied field H along a above 2 T.

According to the existing theories, the ferroelectricity is expected to be along c for the bc-plane helical structure. However, we have not observed the ferroelectricity along c under the field H>2 T applied along a, where the bc-plane helical structure is actually realized. (Note that Schrettle et al.[4] have reported in the recent paper that they observed the weak ferroelectric polarization along c for the bc-plane helical structure.) To understand the origin of this discrepancy remains as a future problem.

References

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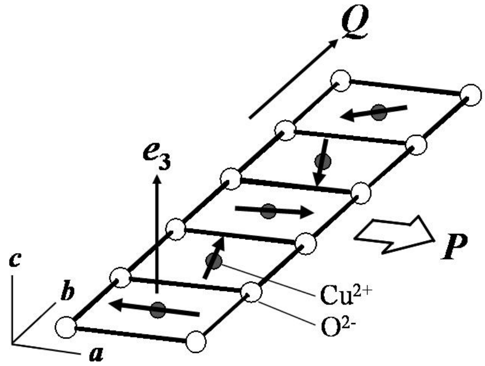

Fig. 1. The magnetic structure and ferroelectric polarization P of LiVCuO4 (Q and e3 are modulation vector and helical axis, respectively)