Structural analysis and Observation of Spin-Gap in Vanadium Oxide V_4O_9

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Among various binary systems, a number of binary vanadium oxides are reported. They have been searched for and extensively studied for a long time. However there remains one binary vanadium oxide whose crystal structue is not known yet. Obviously, its physical properties are not reported. That compound is V_4O_9. Here, we present the crystal structure and physical properties of V_4O_9.

V_4O_9 is unstable at high temperature. Hence, it is impossible to obtaion single crystals. Using V_4O_9 powder samples we started structural analysis by means of transmission electron microscopy(TEM) and powder X-ray diffraction(XRD). And then, we determined lattice constants and positions of vanadium atoms. But it was difficult to identify the positions of oxygen atoms, since the diffraction intensity of oxygen atom is too weak in XRD. To get the information about oxygen positions, powder neutron diffraction measurements(ND) were carried out on the Kinken powder diffractometer for high effciency and high resolution measurements, HERMES (T1-3) at JRR-3M of JAERI in Tokai with wave length 1.82646(6) Å. In the result of the experiment, oxygen atomic position was improved. Furthermore, it was clarified that previous our estimation of the space group and the unit cell is wrong. Combined with TEM and ND, we reassingned the space group to *Cmcm* with a doubled unit cell. The precise structural analysis of V_4O_9 is now in progress.

Temperature dependence of magnetic susceptibility of V_4O_9 indicates spin-gap behavior. To elucidate details of spin-gap nature, inelastic neutron scattering mesasuremets were carried out on the ISSP-PONTA triple axis spectrometer (5G) at JRR-3M of JAERI in Tokai. The obtained spin-gap energy is 8.3 meV (see Fig. 1) which is consistent with the χ measurement. Constant-Q scan at 2.3 K with a peak at Q=1.2 Å^{-1} can be fitted by dimer model. From structural point of view , our V_4O_9 model can be regarded as an isolated dimer system. The result is reasonable with our V_4O_9 model.

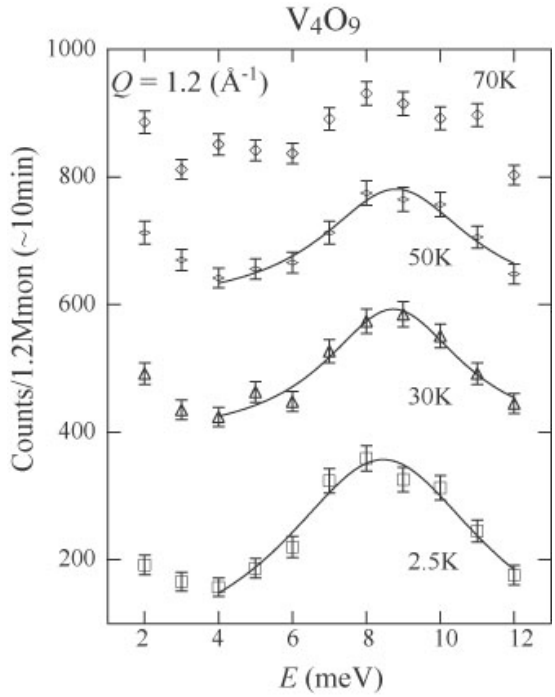

Fig. 1. Neutron scattering profiles at Q=1.2 Å^{-1} at several tempertures.