TALK for the American Physical Society March Meeting, March 20-26, 2004, Montreal, Canada

Low Temperature Structure of $K_2V_3O_8$. B.C. Chakoumakos[1], K. Oikawa[2], T. Kamiyama[2], B.C. Sales[1], M.D. Lumsden[1], S.E. Nagler[1], [1]Oak Ridge National Laboratory*, Oak Ridge, Tennessee 37831-6393 USA, [2]Institute of Materials Structure Science, KEK, Tsukuba 305-0810 Japan.
$K_2V_3O_8$ is a 2-dimensional $S = 1/2$ antiferromagnet ($T_N \sim 4$K) that exhibits field-induced spin reorientation [1] and enhanced heat transport [2] at low temperature. At 110K, infrared, permittivity, and heat capacity measurements [3] suggest a structural distortion. To elucidate the structural changes below110K, we undertook a neutron powder diffraction study on the t-o-f instrument *Vega* at the KEK. From refinements in the nominal space group *P*4*bm*, the *a* cell edge expands on cooling, then abruptly contracts below 110K. The *c* cell edge contracts monotonically. The displacement parameters of the intralayer oxygen atoms deviate from expected behavior, exhibiting increased positional disorder below110K. The disorder of the apical oxygen of the magnetic V^{+4} ion is greater at all temperatures than for the other oxygen atoms. By analogy with the closely related melilite structure, a modulated structure with rigid rotations of polyhedral units in a 3 x 3 x 1 supercell is inferred for the low temperature structure of $K_2V_3O_8$.
[1] Lumsden et al., Phys. Rev. Lett. 86, 159 (2001).
[2] Sales et al., Phys. Rev. Lett. 88, 095901 (2002).
[3] Choi et al., Phys. Rev. B 65, 054101 (2001).
*Supported by the Division of Materials Sciences, U.S. D.O.E. (contract DE-AC05-00OR22725 with UT-Battelle, LLC).