Phonon modes of beta-Na0.33V2O5

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Introduction

Vanadium bronze,beta-Na0.33V2O5, was recently found to undergo superconducting phase transition at 8K under 8Gpa by Yamaguchi, Ueda and Mori1). Since then, doped vanadium bronze, beta-AxV2O5 with A=Na, Ka, Sr, Cu, Ag etc. and x=0.2-0.6, have been identified as a group of n-type ceramic superconductors in a low temperature range under high pressure. These materials exhibit relatively high negative Seebeck coefficient, e.g., about 100microV/K at 380K for A=Cu and x=0.602). The unit cell of beta-AxV2O53) consists of three different 1D VOn (n=5 or 6) sublattices extended parallel to b-axis, namely, two leg ladders, two rows of corner shared VO6 octahedra and zigzag VO5 square pyramids, respectively. Doped cations sit at roomy interstitial sites situated adjacent to the zigzag VO5 square pyramids. Present neutron inelastic scattering measurment was aimed to elucidate phonon spectra, i.e., DOS and low energy modes related with the spin/charge ordering and structural instabilities which could have connections with 2kf-CDW, superconductivity as well as high Seebeck effect being observed for the doped vanadium bronzes , beta-AxV2O5.

Experimental Procedures

Beta-Na0.33V2O5 powder sample was prepared by the solid sate reaction method. Mixture of appropriate molar ratio of Na2V2O7, V2O3 and V2O5 powders was mixed in an agate mortar, then pelletized and fired at 650 celsius deg. for 12hrs in vacuum. Same pellets were pulverized , mixed and sintered at 650 celsius deg. for a couple of times. Neutron scattering experiment was carried out by the use of a cold neutron spectrometer JRR3M-AGNES at room temperature, 100K, and 10K. For comparison, room temperature run was carried out for the V2O5 reference powder sample. Neutron inelastic intensities observed by 328 He3 gas counters were added in an appropriate way then DOS curves were calculated. Pulsed cold neutron radiation with lambda=4.22 was utilized through out the experiment.

Results

Figure 1 shows phonon-DOS spectra of V2O5, Ca0.26V2O5, and Na0.33V2O5 samples obtained from the anti-Stokes side, i.e., the neutron energy gain side of the inelastic scattering intensities. Phonon-DOS curves of V2O5 and Ca0.26V2O5 were obtained previously. Observed inelastic scattering intensities are mostly due to the vibration of vanadium atoms because of their very large incoherent scattering cross section, σ_i=5.08 barn, relative to oxygen and calcium atoms. Discontinuity of DOS curves from 24meV to 36meV is due to the contamination of lambda/2 incident neutron beam. There are obvious differences in the three DOS curves in the range from 7 to 20meV. V2O5 sample shows a peak intensity at 9meV but the DOS curves of Ca0.26V2O5 and Na0.33V2O5 shows rather flat features. In Na0.33V2O5, some softening feature is seen at around 10meV relative to the calcium system.

References

1)T.Yamauchi, Y.Ueda and N.Mori; Phys. Rev. B 29 (2002) 57002.
2)D.Abe; Master Thesis, Grad. School Eng., Tohoku Univ. 2007.
3)A.D.Wadsley; Acta Crystallogr.8(1955)695

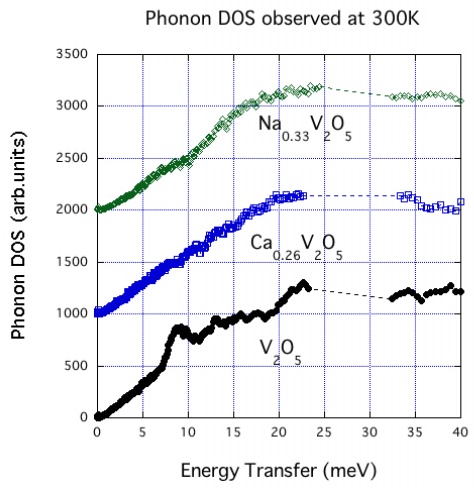

Fig. 1. Observed phonon density of states curves of V2O5, Ca0.26V2O5, and Na0.33V2O5.