

Phonons in tetragonal BiVO₄

I. Tomeno(A), N. Sato(A), K. Oka(B)

(A)Akita Univ., (B) AIST

Bismuth vanadate BiVO₄ undergoes a second-order ferroelastic phase transition at $T_C=525$ K. The high-temperature paraelastic phase has a tetragonal scheelite structure with space group $I4_1/a$ (C_{4h}^6). In the scheelite structure, the isolated VO₄ tetrahedra are separated by the Bi³⁺ ions. The low-temperature ferroelastic phase has a monoclinic distorted scheelite structure with $I2/a$ (C_{2h}^6). Brillouin scattering studies revealed a dramatic softening of transverse acoustic (TA) modes polarized on the (001) plane at T_C . [1-2] We studied the lattice dynamics of BiVO₄ in the paraelastic phase. Inelastic neutron scattering measurements were performed using the triple-axis spectrometer T-11 (HQR) at JRR-3M.

We performed transverse constant-Q scans at $q = [\sqrt{2}\xi \cos \theta, \sqrt{2}\xi \sin \theta, 0]$ polarized in the (001) plane, where θ is an absolute value of the angle from [100] in the (001) plane. The angular dependence of the TA phonon energy corresponds reasonably to the results of Brillouin-scattering studies. Figure 1 shows that a difference in the TA phonon energy between $q = [\sqrt{2}\xi \cos 35^\circ, \sqrt{2}\xi \sin 35^\circ, 0]$ and $q = [\xi, \xi, 0]$ becomes large with increasing ξ . These results demonstrate that the acoustic symmetry axes in a tetragonal scheelite structure deviate from the crystallographic high-symmetry $[\xi, \xi, 0]$ direction. We measured the phonon dispersion relation along the $[\sqrt{2}\xi \cos 35^\circ, \sqrt{2}\xi \sin 35^\circ, 0]$ direction at $T=533$ and 773 K. The results plotted in Fig.1(b) indicate that the softening of the TA mode along $[\sqrt{2}\xi \cos 35^\circ, \sqrt{2}\xi \sin 35^\circ, 0]$ occurs in the small ξ region. Brillouin-scattering measurements revealed that the frequency of the TA phonon propagating along the $[\sqrt{2}\xi \cos 35^\circ, \sqrt{2}\xi \sin 35^\circ, 0]$ direction becomes small toward T_C . Thus we expect

that the TA phonon branch at $T=533$ K have a relatively flat slope in the vicinity of zone center. We also found a central peak associated with the softening of TA modes. Further experiments are necessary to investigate the lattice dynamics of tetragonal BiVO₄ in a wide temperature range.

References [1]G. Benyuan, M. Copic and H. Z. Commins, Phys. Rev. B24, 4098 (1981). [2]H. Tokumoto and H. Unoki, Phys. Rev. B27, 3748 (1983).

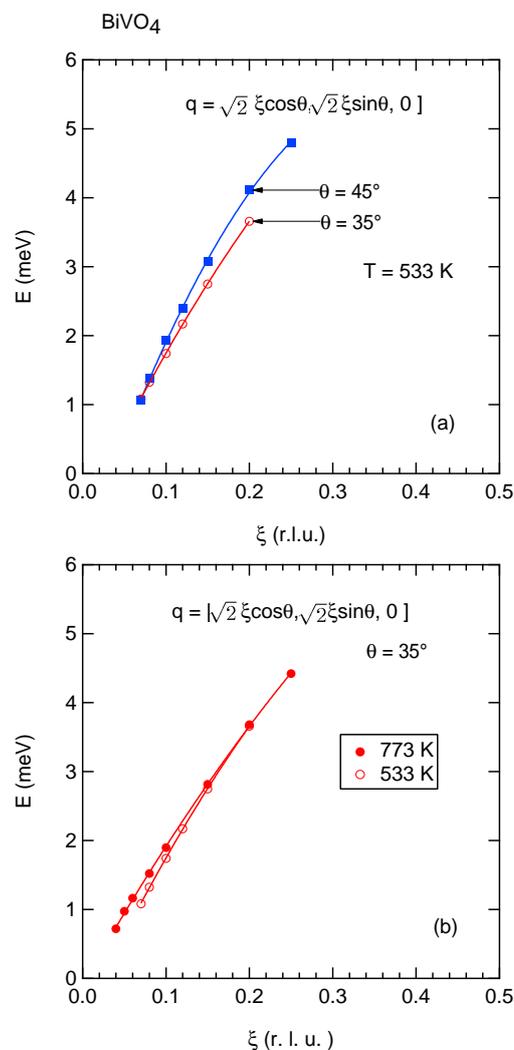


Fig. 1. The TA phonon dispersion curves in tetragonal BiVO₄.