Phonons in NaNbO3

I. Tomeno, Y. Tsunoda,(1) M. Nishi,(2) and K. Oka (3)
Faculty of Education and Human Studies, Akita University, (1)School of Science and Engineering, Waseda University, (2) ISSP, The University of Tokyo, (3)Nanoelectrics Research Institute, AIST

Sodium niobate NaNbO3 has a simple cubic perovskite structure above 913 K. NaNbO3 shows a complicated sequence of phase transitions as a function of temperature.[1] First, the cubic to a tetragonal phase transition takes place at 913K. Next, three distinct orthorhombic phases are found in the intermediate range between 643 and 848K. Then an antiferroelectric monoclinic phase exists in the range between 193 and 643 K. Below 193 K, NaNbO3 has a ferroelectric orthorhombic structure. First-principles calculations have predicted the coexistence of zone-center and zone-boundary instabilities in cubic NaNbO3.[2]

Diffuse X-ray and neutron scattering experiments for NaNbO3 strongly suggest the zone-boundary phonon instability.[3-4] In addition, infrared reflectivity measurements show that the frequency of zone-center TO phonon in the cubic phase decreases gradually on cooling.[5] Unfortunately, there is no data for the phonon dispersion relations. Here we report preliminary results for cubic NaNbO3.

Inelastic neutron scattering measurements were performed using the triple-axis spectrometer T-11 (HQR) at JRR-3M. Figure 1 shows the TA phonon dispersion relation along the [111] direction determined at 933 K. The essential feature is the R-point softening in the cubic phase. The measurements up to 1223 K indicate that the frequency of the R-point TA phonons in cubic NaNbO3 increases gradually with increasing temperature. In addition, we found out the M-point softening of the TA phonons along the [110] direction with the polarization parallel to the [1 -1 0] direction. The softening at the R and the M points suggests that the rotation of the oxygen octahedra becomes unstable. The zone-boundary phonon softening roughly explains results for diffuse X-ray scattering in the cubic phase.[3-4] Further experiments are necessary to investigate the lattice dynamics of cubic NaNbO3.

References

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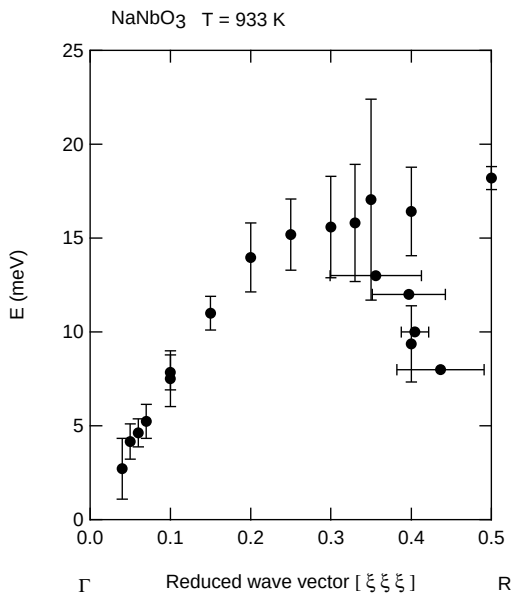

Fig. 1. Phonon dispersion relations for cubic NaNbO3 along the [111] direction.