Structures and Phase Transitions in A2BO4-type Dielectrics

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Among a lot of A2BX4-type ferroelectrics (X = O, Cl, Br), a typical soft phonon-mode was observed in K2SeO4 clearly both above and below the normal-incommensurate (N-INC) phase transition point by neutron scattering. That is to say, the transition in K2SeO4 is interpreted as a displacive-type one. On the other hand, since the soft mode above the N-INC transition point in Rb2ZnBr4, Rb2ZnCl4 and K2ZnCl4 was not observed, it was thought that the transition type was an order-disorder one. For many A2BO4-type crystals such as K2SO4, K2CrO4, Rb2SeO4 and Cs2SeO4, the N-INC transition has never been reported. However, in the case of K2CrO4 and Rb2SeO4, the calculated dispersion curves contain an unstable sigma2 phonon branch whose qualitative and quantitative features are similar to those obtained for prototype incommensurate material K2SeO4. Indeed, a softening tendency of the sigma2 phonon branch around 0.7a* was observed in K2CrO4 and Rb2SeO4 [1]. The estimates hypothetical temperature in Rb2SeO4 is below -150 K.

In order to clarify the mechanism of low-temperature incommensurate phase transition and the hypothetical one in A2BO4-type crystals, we have to obtain additional information about the behavior of the low-energy sigma2-sigma3 optical branches in various A2BO4-type crystals. Therefore, we performed inelastic neutron scattering experiments by use of the triple-axis spectrometers (4G and T1-1) at JRR-3M of JAERI.

Figure 1 shows the phonon dispersion curves in an extended-zone scheme along the (x 0 0) direction for K2Se0.5Cr0.5O4. Two modes, which were anticrossed to each other around x ~ 0.7, were observed. It is clear that low-frequency mode softens slightly in the vicinity of x = 1 with decreasing temperature, although the frequency will remain finite at 0 K. The estimated hypothetical temperature is about -160 K, which is lower than the calculated hypothetical temperature.

In Cs2SeO4, whose calculated hypothetical transition temperature was -151 K, the phonon dispersion frequency was essentially unchanged below room temperature. Our experimental results show that the plausible hypothetical temperature will be lower. The inelastic neutron scattering study on Rb2MoO4 is now in progress, because we found a new N-INC transition at 223 K.

References

[1] H. Shigematsu et al., J. Korean Phys. Soc. 46 (2005) 235.

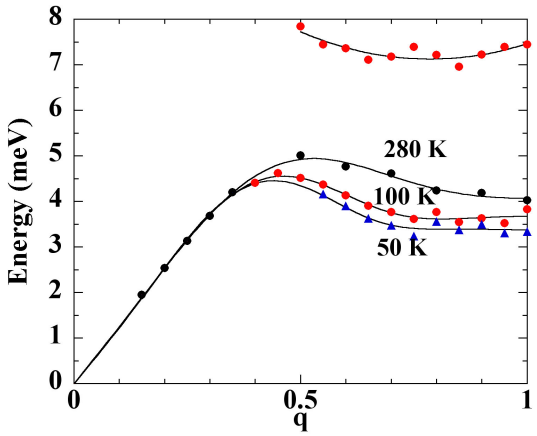

Fig. 1. Phonon dispersion curves in an extended-zone scheme on the (x 0 0) for K2Se0.5Cr0.5O4.