

Hypothetical Phase Transitions and soft modes in A₂BX₄-type Dielectrics

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Rubidium selenate, Rb₂SeO₄, and Cesium selenate, Cs₂SeO₄, belong to a family of A₂BX₄-type (X = O, Cl, Br) crystals with the Beta-K₂SO₄ type structure. As the temperature decrease, the crystals transform from a high-temperature phase I to an orthorhombic phase II (Beta-K₂SO₄-type structure) at T₁. At lower temperature, many of the A₂BX₄-type crystals, for example K₂SeO₄, Rb₂ZnCl₄ and Rb₂ZnBr₄, transform into an incommensurate phase with the modulation wavevector along the a-axis at T₂. However, the phase transition could not be found for many A₂BO₄-type (X=O) crystals below T₁, although the calculated dispersion curves contain an unstable Sigma-2 phonon branch whose qualitative and quantitative features are similar to those obtained for the prototype incommensurate crystal K₂SeO₄. Indeed, a softening tendency of the Sigma-2 phonon branch around $0.7a^*$ was observed in Rb₂SeO₄ and Cs₂SeO₄. The estimated hypothetical temperature is below -150 K.

In A₂BX₄-type (X = Cl, Br) crystals, further phase transitions take place at T₃ and T₄. Soft phonon mode which make contribution to the phase transition at T₄ has been observes around T-point (0,1/2,1/2). In order to clarify the mechanism of low-temperature phase transition and the hypothetical one in A₂BO₄-type crystals, we have to obtain additional information about the behavior of the low-energy optical branches around T-point 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 (0 x x) direction for K₂SeO₄. The low-frequency mode softens slightly in the vicinity of $x = 1/2$ as the temperature

approaches T₂ = 131 K from above, and does not vanish, but hardens with further decreasing temperature. In Rb₂SeO₄, the hollow was not observed around T-point. The phonon dispersion frequency was essentially unchanged below room temperature. The inelastic neutron scattering study on other A₂BO₄-type crystals is now in progress.

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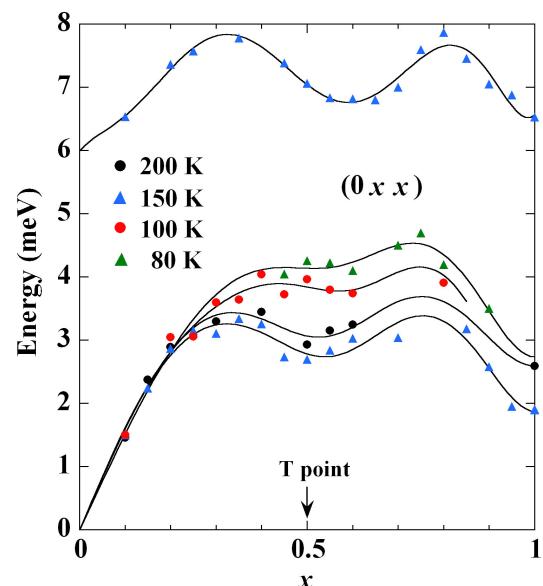


Fig. 1. Phonon dispersion curves in an extended-zone scheme on the (0 x x) for K₂SeO₄.