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Phonon Dispersions of Ca-doped BaTiO3 Studied by Inelastic X-ray and Neutron Scatterings

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Recently, BaTiO3(BT)-based compounds have received much attention as Pb-free piezo-electric materials. It has been reported that Ca-doping is effective in enhancing the piezo-electric performance of BT, which was confirmed in several compounds such as (Ba, Ca)(Zr, Ti)O3, (Ba, Ca)(Sn, Ti)O3, and (Ba, Ca)(Hf, Ti)O3 [1]. Therefore, it is important to investigate the effect of Ca-doping on the atomic dynamics of BT in order to understand the origin of their high piezo-electricities at the atomic level.
In this study, we performed inelastic x-ray and neutron scattering (IXS and INS) experiments on (Ba,Ca)TiO3 (BCT) to elucidate the effect of Ca-doping on the phonon dispersion of BT. The IXS and INS experiments were performed at BL35XU in SPring-8 and BL01 in J-PARC in Japan. Ba–O optical modes in BT and BCT were clearly observed by both IXS and INS experiment. Furthermore, Ti–O soft modes in these compounds were detected by INS, which is sensitive to lighter elements. In the presentation, effects of Ca-doping on these modes will be discussed in relation to the piezo-electricity.

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