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Ionic conductivity and crystal structure for the $Li_{3-2x}Cr_{2-x}Ta_x(PO_4)_3$ system

Abstract

The monoclinic phase ($P2_1/n$) was formed for $0 \le x \le 0.6$ and the NASICON-type rhombohedral phase ($R\bar{3}c$) was obtained for the region $0.8 \le x \le 1.2$ in the $Li_{3-2x}Cr_{2-x}Ta_x(PO_4)_3$ system. The activation energy for Li^+migration was ca. 0.45 eV for the monoclinic structure and ca. 0.36 eV for the rhombohedral structure. The maximum conductivity of 8.4×10^{-6} S cm^{-1} at 298 K was obtained for x=0.8 of the $Li_{3-2x}Cr_{2-x}Ta_x(PO_4)_3$system. The conductivity of $LiCrTa(PO_4)_3$ was enhanced about three to five times by the addition of the lithium salt due to the improvement of the sinterablity. The maximum conductivity was 2.4×10^{-5} S cm^{-1} at 298 K for $LiCrTa(PO_4)_3$–$0.2Li_3BO_3$.

Keywords — Li^+ ionic conductor, solid electrolyte, $LiCrTa(PO_4)_3$, NASICON, conductivity.