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Synthesis, structural reinvestigation and physical properties of alkali hexatitanate
Kunimitsu Katoaka,† Mikito Mamiya,† Norihiro Kijima,‡ Kenichi Ohshima,† Junji Akimoto,† †Advance Industrial Science and Technology (AIST, Japan). E-mail: katoaka-kunimitsu@aist.go.jp

The alkali hexatitanate having the tunnel structure form a class of compounds that can exhibit interesting physical properties such as bronze-type TiO2, [1], [2] and Li ion conductor in the alkali-earth titanates [3], [4] as well as their intriguing structural features. In the tunnel-type alkali and alkaline earth hexatitanate A2Ti6O13 (A = H, Li, Na, K, Sr and Ba) systems, several compounds are reported until now. H2Ti6O13 and Li2Ti6O13 is known as metastable form by ion-exchange method. However, crystal structure and physical properties of H2Ti6O13 and Li2Ti6O13 has not been reported. In the present study, we successfully synthesized polycrystalline sample of H2Ti6O13 and Li2Ti6O13 by ion-exchange method from Na2Ti6O13 [5]. The crystal structure was determined ab-initio structure determination by powder X-ray and neutron diffraction data. In addition, the structural validity was confirmed by bond valence sums calculation, and the results of the present first-principles calculation by the FLAPW method. The result of crystal structure on Li2Ti6O13 showed LiO2 plain tetra coordinates. This Li-O coordination is not normal, and different from that in other A2Ti6O13 compounds. On the other hand, the crystal structure of H2Ti6O13 showed OH-O hydrogen bonding, and ordered arrangement of proton is seen in the crystal structure.

Keywords: alkali hexatitanate, structural reinvestigation, physical properties

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The structure and magnetic properties of the solid-solution: Na2(Zn,Co)SiO4
Charles H. Lake,§ William D. Moon,§ Yuan Hu,§ Brian H. Toby,§ John Mitchell,§ Hong Zheng,§ §Indiana University of Pennsylvania, Indiana, PA 15701, (USA).§Argonne National Laboratory, Argonne, IL 60439, (USA). E-mail: lake@iup.edu

Na2ZnSiO4, a homeotype of wurtzite, is of interest as a host structure for the creation of potentially interesting magnetic materials. The solid-solution series Na2(Zn1-x,Co)xSiO4 was synthesized by high temperature ceramic methods. The resulting blue compounds possessed band gaps of ~1.7 eV, independent of Co2+ doping percentage. Initial powder X-ray data were collected on a Rigaku Miniflex II diffractometer with copper Kα radiation and later high resolution data were collected on the 11-BM diffractometer at the Advanced Photon Source, Argonne National Laboratory with a wavelength of 0.41360 Å. The resultant data verified that the Co2+ and Zn2+ ions were randomly distributed forming a single Zn-Co phase from 0 < x < 0.50. Rietveld analysis converged to X2 of 1.89 and R = 2.49 %. All atoms possessed tetrahedral environments, but those associated with the sodium ions were highly distorted. The high resolution data revealed a more complicated structure than predicted with evidence for aperiodicity in the crystal structure. Magnetic moment versus temperature data were collected from 2 K to 350 K under 1000 G field. The data conform to a Curie-Weiss plot (1/χ vs. T), which represents primarily paramagnetic behavior although the positive Y intercept indicates the presence of short-range antiferromagnetic interactions at high temperature. At low temperatures, a paramagnetic-antiferromagnetic interchange occurred with a Néel temperature at 5 K. Keywords: solid-solution, rietveld, antiferromagnetism