MS21 O3

Crystal structure of $RbWOP_2O_7$ a new diphosphate W(V) isotypic with $KWOP_2O_7$

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Keywords: W(v)diphosphate, tungstyl ion, mixed framework

Crystal structure of new diphosphate of W(V) $RbWOP_2O_7$ isotypic with $KWOP_2O_7$.

A new W(V) diphosphate $RbWOP_2O_7$ [1]isotypic to the $KWOP_2O_7$ [2] has been synthesized. It crystallises in space group $P2_1/n$ with:

a=5.0988(1)Å b=11.9183(1)Å
c=11.6910(1)Å β=90.632(2)°.

This structure is characterized by mixed framework of corner sharing P_2O_7 groups and WO_6 octahedra forms large tunnels where the Rb^+ ions are located. This study shows that this structure is similar to that with potassium ion.

[1]: D.Mezaoui, S. Belkhiri, R. Belhouas, A. Leclaire, H.Rebbah, J. Soc. Chem., 2006, 16(2), 163.
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MS21 O4

Structural disorder in the $Al_{(1-x)}Ga_xPO_4$ solid solution at high temperature.

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α-Quartz is the most commonly used piezoelectric material. Piezoelectric properties are limited in principle by the α–β phase transition at 846 K, however, piezoelectric measurements show that the properties of α-quartz resonators start to degrade at temperatures above 573 K. This degradation can be linked to increasing structural disorder found by neutron total scattering measurements. Structure-property relationships have been developed for α-quartz homeotypes in order to identify new materials such as $AlPO_4$ and $GaPO_4$ with better intrinsic properties. The thermal stability of the α̃quartz form and the piezoelectric response were found to be a function of the structural distortion of a material with respect to the β̃quartz structure type. Analysis by reverse Monte Carlo modelling of our recent total scattering experiments on quartz and $GaPO_4$ show that the degree of disorder in the instantaneous structure increases well before the phase transition, implying a rapid decrease of the piezoelectric properties.

New materials can also be obtained based on solid solutions between existing α̃quartz homeotypes. Such an approach can in principle enable materials with tunable piezoelectric properties to be obtained by varying the chemical composition as in the case of the $AlPO_4$-$GaPO_4$ system in which the structural distortion varies linearly as a function of composition. Three representative compositions in the $Al_{(1-x)}Ga_xPO_4$ solid solution (x = 0.14, 0.20, 0.63) were investigated on the GEM diffractometer at the ISIS spallation neutron source. Total neutron scattering data were obtained from room temperature up to 873 K in the α̃quartz-type phases and in the β̃quartz-type phase at 1018 K for $x = 0.14$. Rietveld refinement does not support a domain-type model for the latter. In the present study the influence of the existing static Al/Ga disorder on thermally induced disorder is investigated, which can be correlated to their piezoelectric properties at high temperature. This thermally induced disorder is found to be most pronounced for the samples with high Al content, for which α–β transitions are observed.