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Structure Behavior of Monoclinic Boroleucite $KBSi_2O_6$ under Temperature and K-Na Substitution

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Leucite family $R_{16}X_{24}(T,T^{/})_{48}O_{96}$ is characterized by an extremely wide range of isomorphic substitutions:R =K, Rb or Cs in leucite and pollucite, molecule H_2O in analcime, T=Si, T$^{/}$= Al and X=Na in analcime. Al can be replaced by B, Fe, Ga, etc. If Al atoms are replaced by B it could be expected that K may be substituted by Na in R position. For the boroleucite $KBSi_2O_6$ synthetic cubic modification (Ihara, Kamei, 1980) and naturally occurring orthorhombic polymorph lisitzynite (Sokolova et al, 2001) are known.

Present work is focused on the study of thermal transformations and expansion of hydrothermally prepared $KBSi_2O_6$. The result of preparation and XRD study of series $K_xNa_{1-x}BSi_2O_6$ (x = 0, 0.25, 0.5, 0.75, 1) are discussed.

Powder sample of monoclinic modification of $KBSi_2O_6$ boroleucite was obtained by hydrothermal synthesis (T = 600 ˚C, P = 5 kBar, 3 weeks, gold capsules). The crystal structure of monoclinic $KBSi_2O_6$ was first described using single crystal in (Belokoneva et al, 2010). $K_xNa_{1-x}BSi_2O_6$ precursors for glass preparation were prepared by solid-state reactions at 650 ˚C for 29 hours. Glasses were obtained at 1300 ˚C for 1 hour. $K_xNa_{1-x}BSi_2O_6$ powder samples were obtained by crystallization of glasses at 700 ˚C for 36 hours. Thermal behavior has been studied *in-situ* by high-temperature X-ray powder diffraction (Rigaku/Ultima IV, 20-1100 ˚C) and differential scanning calorimetry and thermogravimetry (NETZSCH STA 429, 20-1200 ˚C).

On heating and cooling 20-900-20 ˚C monoclinic $KBSi_2O_6$ transfers to cubic modification reversibly at about 640 ˚C according to HTXRD and dilatometry data. At further heating up to 1100 ˚C cubic modification decomposes at 1050 ˚C with trydimite formation.

DSC study of glasses $K_xNa_{1-x}BSi_2O_6$ (x_K = 0, 0.25, 0.5, 0.75) showed that glass transition temperature is practically constant for all compositions, mass losses increase with increasing of heaver atom content same as it was noted for other alkali boroleucite series (Bubnova et al 2004; 2007; etc.). The melting temperature decreases for Na-rich samples: T=1115 ˚C (x_K = 1.0), 1087 (0.75), 973 (0.25). According XRD data of polycrystalline $K_xNa_{1-x}BSi_2O_6$ in the sample with $_K$ = 0.75 monoclinic $KBSi_2O_6$ crystallizes mixed with cubic modification. Na does not enter the monoclinic modification whereas the cell parameter of cubic modification decreases from 12.60 for pure $KBSi_2O_6$ to 12.55 Å for $K_{0.75}Na_{0.25}BSi_2O_6$ sample. In the samples with $x_K < 0.5$ the reflections of cubic $KBSi_2O_6$ and amorphous phase are registered.

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