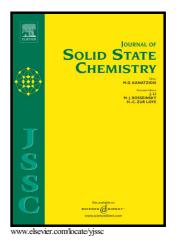
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ACCEPTED MANUSCRIPT Phase formation in the (1-y)BiFeO₃-yBiScO₃ system under

ambient and high pressure

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Abstract

Formation and thermal stability of perovskite phases in the BiFe_{1-v}Sc_vO₃ system ($0 \le y \le 0.70$) were studied. When the iron-to-scandium substitution rate does not exceed about 15 at.%, the single-phase perovskite ceramics with the rhombohedral R3c symmetry (as that of the parent compound, BiFeO₃) can be prepared from the stoichiometric mixture of the respective oxides at ambient pressure. Thermal treatment of the oxide mixtures with a higher content of scandium results in formation of two main phases, namely a BiFeO₃-like R3c phase and a cubic (I23) sillenite-type phase based on γ -Bi₂O₃. Single-phase perovskite ceramics of the $BiFe_{1-\nu}Sc_{\nu}O_{3}$ composition were synthesized under high pressure from the thermally treated oxide mixtures. When y is between 0 and 0.25 the high-pressure prepared phase is the rhombohedral R3c with the $\sqrt{2a_p} \times \sqrt{2a_p} \times 2\sqrt{3a_p}$ superstructure $(a_p \sim 4 \text{ Å} \text{ is the pseudocubic})$ perovskite unit-cell parameter). The orthorhombic *Pnma* phase $(\sqrt{2}a_p \times 4a_p \times 2\sqrt{2}a_p)$ was obtained in the range of $0.30 \le y \le 0.60$, while the monoclinic C2/c phase $(\sqrt{6a_p} \times \sqrt{2a_p} \times \sqrt{6a_p})$ is formed when y=0.70. The normalized unit-cell volume drops at the crossover from the rhombohedral to the orthorhombic composition range. The perovskite $BiFe_{1-\nu}Sc_{\nu}O_{3}$ phases prepared under high pressure are metastable regardless of their symmetry. At ambient pressure, the phases with the compositions in the ranges of $0.20 \le y \le 0.25$, $0.30 \le y \le 0.50$ and $0.50 \le y \le 0.70$ start to decompose above 970, 920 and 870 K, respectively.

Graphical Abstract

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