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Phase formation in the $(1-y)\text{BiFeO}_3-y\text{BiScO}_3$ system under ambient and high pressure

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Abstract

Formation and thermal stability of perovskite phases in the $\text{BiFe}_{1-y}\text{Sc}_y\text{O}_3$ system ($0 \leq y \leq 0.70$) 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, BiFeO_3) 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 BiFeO_3 -like $R3c$ phase and a cubic ($I23$) sillenite-type phase based on $\gamma\text{-Bi}_2\text{O}_3$. Single-phase perovskite ceramics of the $\text{BiFe}_{1-y}\text{Sc}_y\text{O}_3$ 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 $\sqrt{2}a_p \times \sqrt{2}a_p \times 2\sqrt{3}a_p$ superstructure ($a_p \sim 4 \text{ \AA}$ 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 $0.30 \leq y \leq 0.60$, while the monoclinic $C2/c$ phase ($\sqrt{6}a_p \times \sqrt{2}a_p \times \sqrt{6}a_p$) 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 $\text{BiFe}_{1-y}\text{Sc}_y\text{O}_3$ phases prepared under high pressure are metastable regardless of their symmetry. At ambient pressure, the phases with the compositions in the ranges of $0.20 \leq y \leq 0.25$, $0.30 \leq y < 0.50$ and $0.50 \leq y \leq 0.70$ start to decompose above 970, 920 and 870 K, respectively.

Graphical Abstract

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