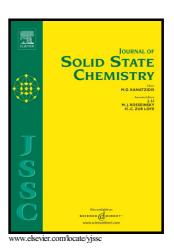
Author's Accepted Manuscript

Determination of Cation Distribution in the Fe[Li $_{1/2}$ Fe $_{3/2}$]O $_4$ -LiFeTiO $_4$ -Li[Li $_{1/3}$ Ti $_{5/3}$]O $_4$ System: Mixed Nature of Solid Solution and Superlattice

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 $\label{eq:continuity} Determination of Cation Distribution in the Fe[Li_{1/2}Fe_{3/2}]O_4-LiFeTiO_4-Li[Li_{1/3}Ti_{5/3}]O_4 \ System: \ Mixed Nature of Solid Solution and Superlattice$

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Abstract

The solid solution technique is one of the oldest but most powerful methods in the search for advanced materials. Hume-Rothery rules regarding solid solutions are well established for alloys, but little is known oxides. spinel about In this study, focused the oxides of Fe[Li_{1/2}Fe_{3/2}]O₄-LiFeTiO₄-Li[Li_{1/3}Ti_{5/3}]O₄ to clarify their cation distribution, which necessitates other rules for substitutionally ordered/disordered solid solutions. Here, the chemical formula of the spinels is represented as $\text{Li}_{1/2+x/2}\text{Fe}_{5/2-3x/2}\text{Ti}_x\text{O}_4$ with $0 \le x \le 5/3$. Synchrotron radiation X-ray diffraction measurements indicated two types of 1:3 cation order at the octahedral site over the wide x range; i.e., the cation order between one Li⁺ ion and three Fe³⁺ ions at $0 \le x \le 1$ and the cation order between one Li^+ ion and three Ti^{4+} ions at $1 < x \le 1.55$. Rietveld refinements indicated that the formation of the cation order at $1 < x \le 1.55$ is achieved by a combination of $1 \times (\text{Li}_{1-x_1-y_1}^+\text{Fe}_{y_1}^{3+}\text{Ti}_{y_1}^{4+})$ and $3 \times$

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