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System: Mixed Nature of Solid Solution and
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Determination of Cation Distribution in the $\text{Fe}[\text{Li}_{1/2}\text{Fe}_{3/2}]\text{O}_4\text{--LiFeTiO}_4\text{--Li}[\text{Li}_{1/3}\text{Ti}_{5/3}]\text{O}_4$ 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 about oxides. In this study, we focused on the spinel oxides of $\text{Fe}[\text{Li}_{1/2}\text{Fe}_{3/2}]\text{O}_4\text{--LiFeTiO}_4\text{--Li}[\text{Li}_{1/3}\text{Ti}_{5/3}]\text{O}_4$ 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 $0 \leq x \leq 5/3$. 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 Fe^{3+} ions at $0 \leq x \leq 1$ and the cation order between one Li^+ ion and three Ti^{4+} ions at $1 < x \leq 1.55$. Rietveld refinements indicated that the formation of the cation order at $1 < x \leq 1.55$ is achieved by a combination of $1 \times (\text{Li}_{1-x1-y1}^+ \text{Fe}_{x1}^{3+} \text{Ti}_{y1}^{4+})$ and $3 \times$

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