The Effect of Fourier Series Truncation Errors on the Electron Density Distribution of $LiMn_2O_4$

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The effect of Fourier series truncation errors on the electron density distribution (EDD) of $LiMn_2O_4$ has been examined using the single-crystal synchrotron X-ray diffraction data and the molecular dynamics (MD) simulation[1]. The MD crystal structure factors obtained from each MD snapshot taken at 2fs intervals in real space were time-averaged and then reversely Fourier transformed to calculate EDD in a similar way to the X-ray data. The EDD thus obtained in the range $\sin\theta/\lambda < 3.33$ Å^{-1} was scarcely affected by the series truncation errors, indicating unambiguously that a small portion of Li does exist close to interstitial positions near the 16c site of the space group Fd3m. The residual EDD assuming a partial structure with eliminating Li atoms also reproduced a mostly correct picture about the distribution of interstitial Li atoms, even though the value of $\sin\theta/\lambda$ of the MD data was reduced to 0.80 Å^{-1}. The interpretation of EDD obtained from the single-crystal synchrotron X-ray diffraction data was thus verified and reinforced from the MD simulation, not only by looking at the real space distribution of atoms in the snapshots but also by a close examination of their Fourier transform.

[1] Tateishi K. *et al., Annual Report of Ceram. Res. Lab*.,2005, **4**, *in press*.

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