Maximum Entropy and Fourier Study on Electron Density of MnO, $LaCoO_3$ and $MgSiO_3$

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The maximum entropy method (MEM) gives us the deduced electron-density distribution without the use of any structure model [1]. On the other hands, the difference-Fourier (D-FR) method is well known to estimate the accurate electron-density through the Fourier transform. We have examined the validity to apply the MEM for electron-density studies in physically meaningful and relatively complicated structures. In this study, the MEM and D-FR maps derived from single-crystal X-ray diffraction data were compared for three materials, i.e. MnO, $LaCoO_3$ and $MgSiO_3$, after optimizing MEM parameters such as resolution and constraint condition.

MnO gave the anisotropic distribution of Mn 3*d*-electrons in the NaCl structure, although Mn^{2+} ions should be spherically distributed in the regular-octahedral coordination. $LaCoO_3$ has a maximum of susceptibility in the temperature range of 100 K, where Co^{3+} ions may have an intermediated spin-state. The temperature dependence of electron density was examined in this study. In a chain of SiO_4 tetrahedra in $MgSiO_3$, two Si-O bridging bonds and the other two non-bridging bonds had different covalent characters. It is conclusive that electron-density distributions deduced by the MEM are well compared with those estimated from the D-FR calculation.

[1] Sakata M., Sato M., *Acta Crystallogr.*, 1990, **A46**, 263.

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