A Complex $PbMnO_{2.75}$ Phase solved by Electron Crystallography

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When a crystalline structure has one small cell parameter, a high resolution electron micrograph (HREM) obtained in a transmission electron microscope (TEM) can give valuable information on the crystalline structure. Such an image can be seen as the convolution of the projection of the crystal potential and the microscope inherent contrast transfer function (CTF). After deconvolution a projected potential map is obtained. Especially in cases where the other cell parameters are very large and X-ray powder diffraction is not able to solve the structure this method is valuable.

In this contribution we will present the structure determined by the above method of a complex phase of approximate stoichiometry of $PbMnO_{2.75}$. Its unit cell is monoclinic of space group *A2/m* (a = 32.232 Å, b = 3.831 Å, c = 35.671 Å, β = 130°) [1].

Image treatment was done using the Visual Electron Crystallography software [2]. The images were first Fourier filtered, then deconvoluted from the contrast transfer. The obtained projected potential map allowed to distinguish the Pb and Mn cations and to place them in the projection onto the **ac** plane. Due to the small b parameter and the space group, atoms can only be located at y = 0 or y = 0.5. Taking into account the usual distances between cations in the same system allows to distinguish between the two values.

The final atomic coordinates differ little from the positions given in [1]. The mean distance between the atoms is 0.3 Å, which is comparable to the standard deviation of the positions in [1].

[1] Bougerol C., Gorius M.-F., Grey I.E., *JSSC*, *to be published*. [2] http://cryst.iphy.ac.cn/VEC/

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