Type of presentation: Poster

IT-9-P-1450 Sr25Fe30O77 : A complex layered and modulated structure solved by electron diffraction

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These past few years, many new structures have been solved using electron diffraction methods. Zone axis precession electron diffraction (PED) and tomography in reciprocal space are two methods enable to reduce importantly the multiple scattering of the electron beam, so that the reflection intensities can be used for structure determination by direct methods.

The ferrite $Sr_{25}Fe_{30}O_{77}$ belongs to a family of phases whose structures consist of an intergrowth of m perovskite layers with complex rocksalt type layers [1-2]. Our compound of interest is the member m = 4 of this family and its structure has been solved by combining both electron diffraction methods cited above. This oxide crystallizes in an orthorhombic system with the sub-cell parameters a ≈ b ≈ 5.4 Å and c ≈ 42 Å. The structure exhibits modulation along axis with a modulation vector . Due to the commensurate nature of the modulation, the structure can be described in a supercell with the parameters a ≈ 27 Å, b ≈ 5.4 Å and c ≈ 42 Å. PED patterns were recorded in zone axis with a Spinning Star unit using a precession angle of 2°. The intensities were extracted with CRISP software [3] in “shape fitting” or “integer” modes. The data were then implemented in SIR2008 software[4] and many trials were made with or without application of geometrical Lorentz correction to obtain the structure. The tomography data collection, recorded by tilting manually every 0.5 degree from -30 to +30 degrees, was inserted in EDT (Electron Diffraction Tomography) software [5], which reconstructs the 3D reciprocal space and integrates automatically the reflection intensities. The resulting intensity file was then used on SIR2008 for structure resolution. The solved structure, by combining both methods, consists of four consecutive layers with Fe in octahedral environment alternating with one complex layer containing Fe in three different environments. The oxygen atoms in this last layer are responsable of the modulated nature of the structure.

References:

[1]Pérez, O., Mellenne, B., Retoux, R., Raveau, B. & Hervieu, M. (2006). Solid State Sciences. 8, 431-443, [2]Grebille, D., Lepoittevin, C., Malo, S., Pérez, O., Nguyen, N. & Hervieu, M. (2006). J.Solid State Chem. 179, 3849-3859, [3]Hovmöller S., www.calidris-em.com, [4]Il milione II suite http://wwwba.ic.cnr.it/content/sir2011-v10, [5]Oleynikov P.www.edt3d.com.

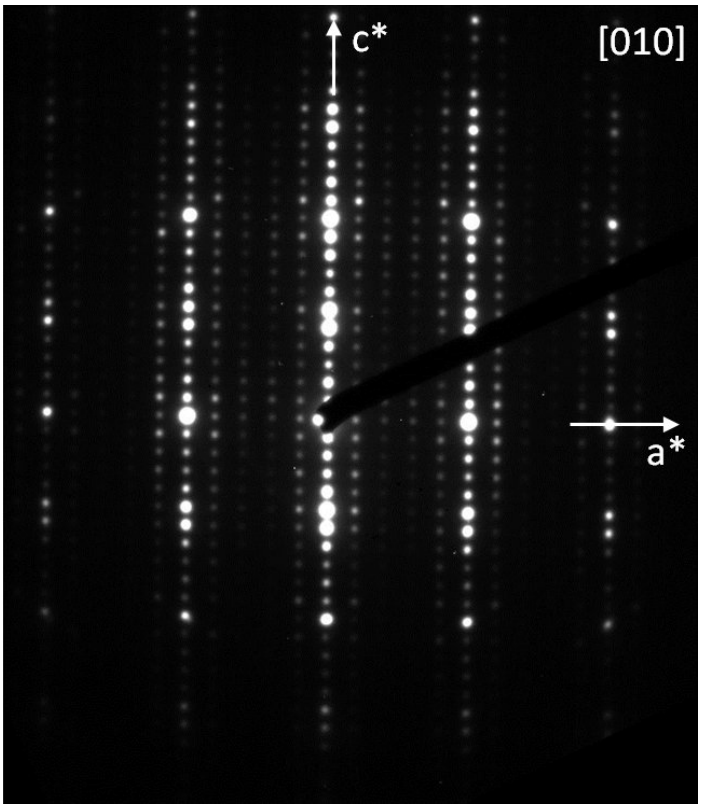

Fig. 1: [010] electron diffraction pattern of $Sr_{25}Fe_{30}O_{77}$

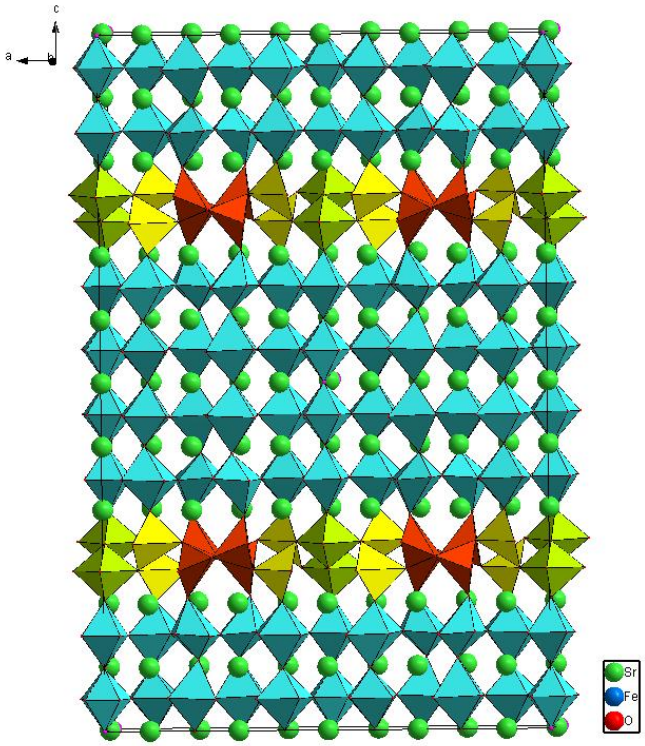

Fig. 2: solved structure of $Sr_{25}Fe_{30}O_{77}$