## [MS15-04] $Sr_{25}Fe_{30}O_{77}$ : A 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 [1-5]. Both 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 [6-8]. The 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 Åand c ≈ 42 Å. The structure exhibits modulation along a→axis with a modulation vector q→ = 2/5 a→. 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 [9] in "shape fitting" or "integer" modes. The data were then implemented in SIR2008 [10] with or without application of geometrical Lorentz correction. The tomography data collection, recorded by tilting manually every 0.5 degree from -30 to +30 degrees, was inserted in an automated "3D Electron Diffraction Tomography" software [11], which reconstructs the 3D reciprocal space and integrates automatically the reflection intensities. The resulting intensity file was then used on SIR2008 software for structure resolution.

[1] Gemmi, M., Klein, H., Rageau, A., Strobel, P. & LeCras, F. (2010). Acta Cryst. **B66**, 60-68.
[2] Hadermann, J., Abakumov, A.M., Turner, S., Hafideddine, Z., Khasanova, N.R., Antipov, E.V. & Van Tendeloo, G. (2011). Chem. Mater. **23**, 3540–3545.
[3] Klein, H. (2011). Acta Cryst. **A67**, 303-309.
[4] Gemmi, M., Campostrini, I., Demartin, F., Gorelik, T.E. & Gramaccioli, C.M. (2012). Acta Cryst. **B68**, 15-23.
[5] Mugnaioli & E., Kolb, U. (2013).Microporous and Mesoporous Materials. **166**, 93-101.
[6] Pérez, O., Mellenne, B., Retoux, R., Raveau, B. & Hervieu, M. (2006). Solid State Sciences. **8**, 431-443.
[7] Grebille, D., Lepoittevin, C., Malo, S., Pérez, O., Nguyen, N. & Hervieu, M. (2006). J.Solid State Chem. **179**, 3849-3859.
[8] Lepoittevin, C., Malo, S., Nguyen, N., Hebert, S., Van Tendeloo, G. & Hervieu M. (2008). Chem.Mater. **20**, 6468-6476.
[9] Hovmöller S., www.calidris-em.com
[10] Il milione II suite http://wwwba.ic.cnr.it/content/sir2011-v10.
[11] Oleynikov P.www.edt3d.com.

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