sectional groups of the two individuals, in their respective orientations, obtained across a plane which corresponds to the composition plane of the twin.

The second case needs the use of *lattice complexes*, which are types of crystallographic orbits generated by atoms in a crystal structure under the action of the symmetry operations of the space group.

When part of the atoms of an individual of a twin have a continuation across the twin interface, the individuals have a substructure in common, which corresponds to a lattice complex. If a crystal structure is composed of lattice complexes some of which have an eigensymmetry higher than the space group, these can be invariant under the action of the twin operation(s) and govern thus the formation of the twin.

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# Keywords: lattice complexes; subperiodic groups; twinning

#### FA2-MS01-P13

Non-MDO 4-layer Ferrophlogopite from Ruiz Peak (New Mexico). <u>Massimo Nespolo</u><sup>a</sup>, Isabella Pignatelli<sup>a</sup>. *aCRM<sup>2</sup> UMR-CNRS 7036, Institut Jean Barriol, Nancy-Université, France.* E-mail: <u>Massimo.Nespolo@crm2.uhp-nancy.fr</u>

In this study we investigated a crystal of ferrophlogopite from a rhyodacite lava flow at Ruiz Peak (New Mexico), belonging to the same rock hand specimen previously investigated by Ross et al. [3]. The analysis of the singlecrystal X-ray diffraction pattern, obtained with an Oxford SuperNOVA microsource using CuKa radiation, shows four reflections in the 1/10 Å<sup>-1</sup> period of the 1M basic structure along the non-family rows: the crystal is thus a non-MDO 4-layer polytype. The cell parameters are a =5.3194(3) Å, b = 9.2107(5) Å, c = 39.828(5) Å,  $\alpha = 90^{\circ}$ ,  $\beta = 92.537(5)^{\circ}$ ,  $\gamma = 90^{\circ}$ . The stacking sequence has been obtained by PID analysis [4] and it can be expressed by RTW symbols 2 2 22 [3], Z symbols 1353 [7] and OD symbols 2040 [2] in the homo-octahedral approximation. It is the first time that this polytype is found in the Ruiz Peak sample, although it was discovered in a Ti-biotite by means of oblique-texture electron diffraction [6] and indicated with the  $4M_3$  Ramsdell symbol. The atomic coordinates of the structural model have been obtained from those of the 1M polytype from the same sample, by applying the PID stacking vectors. The space-group type, as obtained from the stacking sequence, would be C2/c, but the intensities distribution reveals a triclinic structural symmetry. This lower symmetry can be due to the desymmetrization of the OD layers and/or to the cation ordering in the octahedral sheets [1]. C2/c is therefore the maximal space-group type for this polytype whereas the correct space-group type is a triclinic translationengleiche subgroup of it. Consequently the Ramsdell symbol  $4M_3$  previously used to indicate this stacking sequence [3, 5, 6], should actually be modified

25<sup>th</sup> European Crystallographic Meeting, ECM 25, İstanbul, 2009 *Acta Cryst.* (2009). A**65**, s 179 in 4*A* to take into account the structural symmetry. The structural refinement is in course and the preliminary results confirm the stacking sequence obtained by PID analysis.

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# Keywords: mica polytypes; OD structures; X-ray diffraction

### FA2-MS01-P14

**The Misfit Layer Structure of Franckeite.** <u>Emil</u> <u>Makovicky</u><sup>a</sup>, Václav Petříček<sup>b</sup>, Michal Dušek<sup>b</sup>, Dan Topa<sup>c</sup>. <sup>a</sup>University of Copenhagen. <sup>b</sup>Czech Academy of Sciences Prague. <sup>c</sup>University of Salzburg. E-mail: <u>emilm@geol.ku.dk</u>

Franckeite from San Jose, Bolivia, nominally Pb46Ag02Sn25  $Sb_2Fe_{0.8}S_{12.6}$ , consists of alternating pseudohexagonal (H) and pseudotetragonal (Q) layers. The triclinic crystal structure has a pronounced one-dimensional transversal wave-like modulation and a non-commensurate layer match in two dimensions. The Q layer is an MS layer (M=Pb, Sn<sup>2+</sup>, Sb..), four atomic planes thick, with a 5.820 Å, b 5.872 Å, and the layer-stacking vector c 17.367 Å. The lattice angles are  $\alpha$  94.98°,  $\beta$  88.43°,  $\gamma$  89.97°; the modulation vector  $\mathbf{q} = 0 a^*$ + 0.1286  $b^*$  - 0.0284  $c^*$ . The H layer is a single-octahedral MS<sub>2</sub> layer (M = Sn<sup>4+</sup>, Fe..) with a 3.672 Å, b 6.275 Å, c 17.447 Å,  $\alpha$  95.25°,  $\beta$  95.45°,  $\gamma$  89.97°; the modulation vector is  $q = 0 a^* + 0.1374 b^* - 0.0304 c^*$ . Length of the modulation vector is 45.67 Å; the match of centred (sub)cells in this bdirection, 15.5 Q : 14.5 H, occurs at 91.00 Å, a double of the modulation vector plus a structurally important difference  $\Delta = 0.34$  Å. The *a* and *b* vectors of both subsystems are parallel; the c vectors diverge. 5D superspace refinement was performed in the superspace group C-1, using 7260 observed reflections. It resulted in the overall R(obs) value equal to 0.113. The Q layers are composed of two tightlybonded double-layers, separated by an interspace hosting lone electron pairs. Average composition of cations on the outer surface was refined as Pb<sub>0.9</sub>(Sn,Sb)<sub>0.1</sub> whereas that of cations covering the interspace with lone electron pairs, with a typical configuration analogous to that observed in orthorhombic SnS, corresponds to Sn(Sb)<sub>0.64</sub>Pb<sub>0.36</sub>. Iron is dispersed over Sn<sup>4+</sup> sites in the H layer. Franckeite does not form cylindrical aggregates (as does related cylindrite) because of the increased thickness of the Q layer.

#### Keywords: modulated structure; misfit layer structure; Pb-Sn-Sb-Fe sulphide; franckeite