Pyrrhotites Revisited in Superspace with *ab-initio* Calculations Insights

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Superspace formalism has been used to describe families of compounds with flexible composition [1] with a unique structural model. A superspace model for the Pyrrhotite (Fe1-xS) family is proposed in this work.

Pyrrhotites have metal-deficient NiAs structures. S atoms form a hexagonal sublattice with Fe atoms in the octahedral interstices. Fe-deficient layers alternate regularly with full Fe layers to form superstructures with different composition, symmetry and c parameter [2].

In the common superspace construction, the atomic domains representing the Fe and S atoms are crenel functions. The only parameters which change with the composition are the size of the crenels for the Fe atoms and the modulation weave vector. The structure of a particular composition is obtained through a 3D cut of the superspace construction. For different compositions, distinct stacking sequences are obtained, in agreement with the reported 3D structures.

Ab-initio calculations have been used to study the stability of the different stacking sequences.

[1] Pérez-Mato J.M., Zakhour-Nakhl M., Weill and Darriet F., *J. Mat. Chem.* , 1999, **9**, 2795. [2] Yamamoto A., Nakazawa H., *Acta Cryst.*, 1982, **A38**, 79.

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