Structural studies on the antigorite polysomatic series

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Antigorite is a 1:1 layer silicate of the serpentine group with a complex waved structure. The structure can be conveniently thought as a polysomatic series of lizardite and talc modules alternating along *a* in different proportions [1]. The most recurring polysome may be described as $S^{+8}\ T\ S^{-7}$, ($a \approx 43.5$ Å) where *S* and *T* are serpentine and talc modules, respectively, and S^{+} and S^{-} refer to the polarities of the tetrahedral sheet in two adjacent half-waves (Fig. 1).

Reliable structural data for antigorite are difficult to obtain with conventional X-rays sources because natural crystals are frequently faulted and disordered. On the other hand, electron crystallography suffers the sensitiveness of the mineral to the strong electron/matter interaction. Only recently, thanks to an exceptionally good suite of crystals from Val Malenco (Italian Alps) characterized by a relatively low density of defects we have been able to refine the $S^{+8}\ T\ S^{-7}$ antigorite structure down to $R_{obs} \approx 5.8\%$ [2].

Known polysomes range from $S^{+6}\ T\ S^{-5}$ to $S^{+12} T\ S^{-11}$ ($a \sim 33.0 \div 63.5$ Å). Theoretical speculation and recent papers [3] suggest that polysomes with even number of *S* modules might have different structural topology and thus different properties. Unfortunately, these polysomes do not occur in nature ordered at a suitable scale for conventional X-ray structural analysis - saying 10^5 cube microns – then we have been pointing to the brilliant synchrotron X-rays sources in order to achieve structural information from smaller, and hopefully defect-free crystals – saying as smaller as 10^3 cube microns.

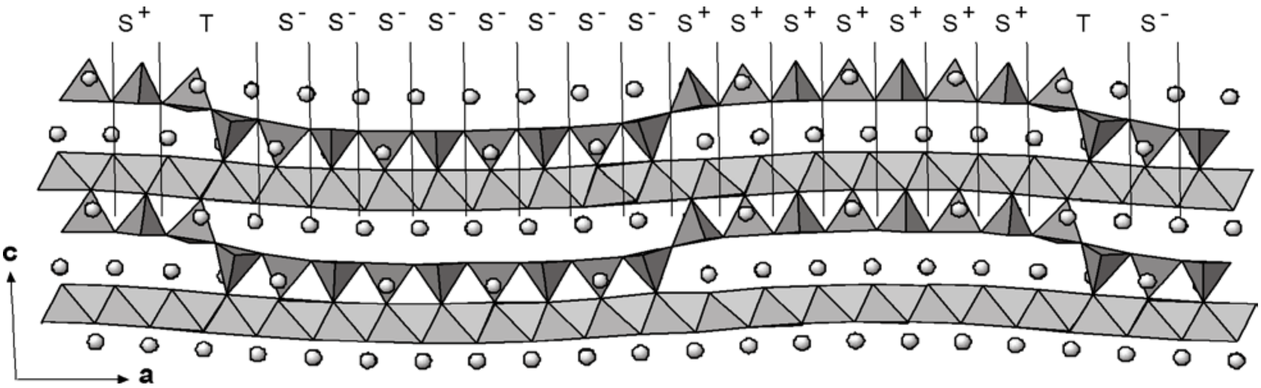

Fig. 1. Antigorite structure as seen down [010].

So far, our experiments at Desy have covered the following steps:

1. Collection of a reference crystal (with know structure refined from conventional data) in order to compare results.
2. Collection of $S^{+8}\ T\ S^{-7}$ antigorite crystals of reduced size and, hopefully, reduced density of defects, with the aim to get better results. Some fine details, such as H-bonding, minor cation substitution and so on, need better data in order to be fully understood.
3. Collection of a crystal with apparent geometry other than $S^{+8}\ T\ S^{-7}$.

4. Collection of a lizardite crystal (one of the building blocks of the antigorite polysomatic series) with apparent geometry that do not fit the know T1 and $2H_1$ known structures. This could introduce interesting implication in the polysomatic series formulation.

These data are currently under study. In the following table are summarized some data collection information and some preliminary results.

Table 1. Collection data set and preliminary results.

Sample	Mineral	λ (Å)	xx/CCD distance (cm)	Symmetry											
				Conventional						Synchrotron					
				a (Å)	*b*	*c*	*α* (°)	*β*	*γ*	*a* (Å)	*b*	*c*	*α* (°)	*β*	*γ*
A1	antigorite	0.7	12	43.30	9.20	7.23	90	91.4	90	43.60	9.27	7.27	90	91.3	90
A11	antigorite	0.7	10	-	-	-	-	-	-	41.10	9.26	7.26	90	88.6	83.5
A97	antigorite	0.7	8	-	-	-	-	-	-	43.48	9.25	7.26	90	91.3	90
L73	lizardite	0.56	4.5	-	-	-	-	-	-	5.39	5.39	7.29	90	90	120

These results are encouraging because match quite well our expectations about the metrics of the investigated samples and also indicate that we are faced probably with new antigorite (A11) and a new lizardite (L73) polymorphs.

At the same time we are working on these data, we are also planning new synchrotron experiments on additional antigorite samples with expected new structures.

References

[1] Ferraris G., Mellini M., and Merlino S. Rend. Soc. It. Min. Petr. **41**, 181 (1986)
[2] Capitani G.C. and Mellini M., Am. Mineral., in press (2004).
[3] Dódoni I., Póstfai M., and Buseck P.R., Am. Mineral. **87**, 1443 (2002).