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Crystal structure refinement of an axinite specimen from synchrotron tts-μDiffraction data

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Synchrotron through-the-substrate microdiffraction (tts-μXRD) allows the study of polycrystalline samples included in polished thin sections [1]. In a tts-μXRD experiment the primary beam passes first through the glass substrate before reaching the thin section where the target material is embedded. This technique has now been extended to the study of crystal microvolumes [2]. A polished thin section (30μm) cut out of an epidote-pyroxene-axinite pneunomatolitic outcrop from Pont de Suert (Catalonia, Spain) has been studied and intensity data of microvolumes of triclinic axinite crystals were directly collected. The basic steps of this new tts-uXRD application include:

- Collection of 2D patterns (frames) for each randomly-oriented crystal microvolume.
- Determination of the reciprocal lattice orientation for each randomly-oriented crystal microvolume which allows assigning the *hkl* indices of the crystal dataset. Previously the metric has been refined from angular peak positions or from circularly averaging the sum of collected patterns.
- Merging of the individual crystal datasets to produce an extended dataset suitable for structure solution and refinement.

Axinite is a triclinic complex silicate with unit cell formula Ca₄X₂Al₄\Si₈B₂O₃₀\₂ (space group P-1) with X being Fe²⁺, Mn²⁺ and even Mg²⁺. The resulting dataset from 7 axinite microvolumes (614 unique reflections, 65% data completeness for 1.08Å resolution) allowed the crystal structure solution using Patterson-function direct methods [3] and an accurate single-crystal least-squares refinement. From the combination of an electron microprobe analysis and μXRD information, the cationic distribution in the unit cell of this axinite specimen was determined.

References

[1] J. Rius, A. Labrador, A. Crespi, C. Frontera, O. Vallcorba, C. Melgarejo. *J. Synchrotron Rad.*, **2011**, 18, 891-898.

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[3] J. Rius. *IUCrJ*, **2014**, 1, 291-304.

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