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Anisotropic peak broadening analysis of a biogenic soil greigite (Fe_3S_4) with Rietveld analysis and single peak fitting

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ABSTRACT

A new approach for modeling anisotropic peak broadening with Rietveld analysis has been tested on a biologically grown soil greigite, whose morphology (as determined by TEM, Stanjek et al. 1994) had a symmetry lower than cubic. The anisotropic morphology of this greigite determined with single peak fitting was more evident than with the Rietveld analysis in the cubic setting, because in Rietveld analysis {*hhh*} reflections are treated as one reflection, although two different peak breadths are required: one for modeling two (*hhh*) reflections perpendicular to the [111] axis of elongation and one for modeling the remaining six (*hhh*) reflections. For assessing the lower morphological symmetry, the cubic structure was transformed into the tetragonal and into the trigonal system. In both crystal systems, the axis of shape anisotropy is [001]. Due to splitting of peaks, the anisotropic morphology became then measurable. Contributions from other likely sources of anisotropic peak broadening, such as stacking faults and chemical inhomogeneities could be ruled out.

The cell-edge length a = 9.868(4) Å agrees with previous values (Stanjek and Murad 1994). The isotropic temperature factors of B (Fe_{8a}) = 1.16(6) Å^2, B (Fe_{16d}) = 1.7(2) Å^2 and B (S_{32e}) = 1.10(8) Å^2 are much smaller than the overall factor B = 3.2(4) Å^2 determined by Skinner et al. (1964), whereas the anion positional parameter u = 0.2535(3) is identical with 0.2505(38).