

Size-structure relationship of β -akaganeite

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Akaganeite is believed to exist primarily in the monoclinic phase (Post, 2003). Older work has also suggested the possibility of a tetragonal structure (Murad, 1979). Previous research on akaganeite was mainly concentrated on the crystal structure but the relation between structure and particle size was not elucidated.

The objective of this study is to investigate the size-structure relationship by analyzing synthetic akaganeite samples using powder XRD ($\text{CuK}\alpha$) and 16 KeV synchrotron diffraction (LBNL ALS beamline 11.3.1). Rietveld refinement was carried out using Materials Studio software (Accelrys Inc., 2004). A simulated annealing procedure was employed to determine the positions and orientation of ions within a crystal (Engel et al., 1999).

It is found that the bulk samples have the tetragonal structure, as reported by Murad (1979), but as the particle size is reduced, the unit cell becomes distorted and can no longer be described as tetragonal. The lattice becomes progressively monoclinic. The most probable reason is the surface energy increases as the particle size decreases. A distinct trend is also observed in the thermodynamic properties depending on structure.

References

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Elastic and structural behaviour of analcite at high pressure

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Analcite (ANL), $\text{NaAlSi}_2\text{O}_6 \cdot \text{H}_2\text{O}$, is a natural zeolite (or feldspathoid). The crystal structure is based on a Secondary Building Unit (SBU) consisting of four-member tetrahedral rings, which are joined to form a complex tetrahedral framework with two different systems of channels: highly distorted 8-rings and regular 6-ring channels. Na and H_2O lie into the structural voids. Two H_2O and four framework oxygens coordinate the Na-atoms. Elastic and structural behaviour of a natural cubic ANL from Sardinia (Italy) was investigated at HP by *in situ* single-crystal X-ray diffraction. A first-order phase transition was observed at $P = 0.98(7)$ GPa. Lattice parameters and reflection conditions confirm that the HP-polymorph has a $P\bar{1}$ space group. The experiment is in progress but no further phase-transition has been observed at least up to 6.3 GPa. Fitting the volume data of the cubic polymorph with a BM-EoS we obtain: $V_0 = 2571.2(4)\text{\AA}^3$, $K_{T0} = 56(3)$ GPa and $K' = 4$ (fixed). For the triclinic polymorph: $V_0 = 2618(13)\text{\AA}^3$, $K_{T0} = 17(1)$ GPa and $K' = 7(1)$. Tetrahedral tilting produces the relevant structural variations in response of the cubic \rightarrow triclinic phase transition. The SBU distortion gives rise to a change of the 8- and 6-ring channels ellipticity and of the extra-framework content topological configuration: it appears in fact that the coordination number of part of the Na atoms is 7 ($2\text{H}_2\text{O} + 5$ framework oxygens) instead of 6.