

2a and 4a Polytypes of (Ge, Si)- Wollastonite

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Three kinds of superstructures of wollastonite whose compositions were $\text{Ca}(\text{Ge}_{0.65}, \text{Si}_{0.35})\text{O}_3$, $\text{Ca}(\text{Ge}_{0.50}, \text{Si}_{0.50})\text{O}_3$ and $\text{Ca}(\text{Ge}_{0.15}, \text{Si}_{0.85})\text{O}_3$ were synthesized. In this abstract, they are called 65Wo, 50Wo and 15Wo. The lattice constants of 65Wo, 50Wo and 15Wo are: (angstrom, degree) $a=2X8.038(4)$, $2X7.995(2)$, $4X7.949(5)$, $b=7.451(1)$, $7.400(1)$, $7.352(1)$, $c=7.194(2)$, $7.148(2)$, $7.093(1)$, $\alpha=89.93(2)$, $90.05(2)$, $90.06(2)$, $\beta=94.85(2)$, $94.97(2)$, $95.11(1)$, $\gamma=103.34(2)$, $103.43(1)$, $103.39(1)$, respectively.

65Wo consists of the neighbouring two units of the basic-wollastonite along the a -axis. The X-ray diffraction pattern showed a pseudo- C lattice. Therefore, the stacking sequence of 65Wo can be represented as AB, where A is the unit cell of the basic-wollastonite and B is the unit cell of the basic-wollastonite with $b/2$ displacement. The final R-value was 12%.

50Wo consists of the neighbouring two units of the basic-wollastonite along the a -axis, too. However, the X-ray diffraction pattern was different from 65Wo. Judging from the characteristics of the X-ray diffraction, the stacking sequence of 55Wo is represented as AA. The final R-value was 13%.

15Wo consists of the four units of the basic-wollastonite along the a -axis. There were four possible stacking sequences described as AAAA, ABAB, AABB and AAAB. The structure having the sequence AAAA will show the strong intensity on the $h=4n$ diffraction. The structure ABAB will show the strong intensity on the $h=2n$ diffraction. The structure AABB will show the extinction rule of the pseudo- C lattice. The last structure AAAB will not show any characteristic rules on the X-ray diffraction. As the result of the observation of the X-ray diffraction of 15Wo, it was clear that the stacking sequence AAAA was most reasonable. The final R-value was 14%.

In common with 65Wo, 50Wo and 15Wo, each tetrahedral site has the statistical distribution of Ge and Si atoms.

References

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