Two kinds of Superstructures of (Ge, Si) Wollastonite

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Two kinds of superstructures of wollastonite whose compositions were $Ca(Ge_{0.55}, Si_{0.45})O_3$ and $Ca(Ge_{0.65}, Si_{0.35})O_3$ were synthesized. The former is called 0.55Wo and the latter 0.65Wo in this abstract. The lattice constants of 0.55Wo and 0.65Wo are: (angstrom, degree) a=2X8.016(4), 2X8.038(5), b=7.421(1), 7.451(1), c=7.157(2), 7.194(1), alpha=90.08(2), 89.93(1), beta=94.86(2), 94.85(2), gamma=103.44(2), 103.34(1), respectively. Though both of them are twice as large as the basic structure of wollastonite, those structures are different. Basically, 0.55Wo has the two units of the basic-wollastonite along a-axis and has no other partial structures in it. The largest difference between the basic wollastonite and 0.55Wo is the fact that the basic wollastonite has an inversion center but 0.55Wo has not it. Therefore, the basic wollastonite includes only 15 independent atoms but 0.55Wo includes the 60 atoms in the unite cell. The final R-value was 6% after the structure refinement of 0.55Wo. 0.65Wo has the two units of the basic-wollastonite along a-axis, too. However, the X-ray diffracrion pattern of 0.65Wo was largely different from that of 0.55Wo and it showed the extinction rule of the pseudo-C lattice. The structure model having the stacking of the basic-wollastonite unit with b/2 displacement were tried and the R-value was 9% after the structure refinement.
Keywords: structure analysis, superstructure, wollastonite