

m14.p04**An alternative approach for the description of modulated structures using differential geometry**

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Differential geometry is a theory that has been existing for one and a half century and is much solicited in many physical topics, but not a lot in crystallography. In fact, Hans Wondratschek [1] hints at this mathematical topic, when introducing two spaces for the description of the symmetry operations: the *point space* and the associated *vector space*. In our work, we think of \mathbf{R}^n as a differential manifold in which we consider n -dimensional lattices, be they smoothly modulated or not. The focus of our viewpoint is to say that each node of the lattice is linked to an origin point not by a vector, but by a curve belonging to a family $\{c_\lambda \mid \lambda \in M\}$, where M is a \mathbf{Z} -module. If we parametrize each of these curves between 0 and 1, we can see that the extremities of the corresponding velocity vectors at 0 generate a periodic lattice of translations in the tangent space. Using this approach, it seems that the symmetry of modulated structures can be described without erring in a higher dimensional space (superspace) and the diffraction pattern of such structures could be better understood considering the Fourier transform in the tangent space.

[1] H. Wondratschek, *Introduction to space-group symmetry: Basic concepts*, taken from: *International Tables for Crystallography*, Vol. A, pp 720 - 721, Kluwer Academic Publishers, Dordrecht, 2002.

m14.p05**2T and 4T Polytypes of Ca(Gex, Si1-x) O3 Wollastonite**Fumito Nishi^a, Takahiro Kuribayashi^b, Yasuhiro Kudoh^b, Ritsuro Miyawaki^c*^aSaitama Institute of Technology, Saitama. ^bInstitute of Mineralogy, Petrology and Economic Geology, Faculty of Science, Tohoku University, Miyagi. ^cDept. of Geology and Paleontology, Shinjuku Branch of National Science Museum, Tokyo, JAPAN. E-mail: nishi@sit.ac.jp***Keywords: structure analysis, polytypes, wollastonite**

Three kinds of superstructures of wollastonite whose compositions were Ca(Ge_{0.15}, Si_{0.85})O₃, Ca(Ge_{0.55}, Si_{0.45})O₃ and Ca(Ge_{0.65}, Si_{0.35})O₃ were synthesized. In this abstract, they are called 0.15Wo, 0.55Wo and 0.65Wo. The lattice constants of 0.15Wo, 0.55Wo and 0.65Wo are: (angstrom, degree) a=4X7.949(5), 2X8.016(4), 2X8.038(5), b=7.352(1), 7.421(1), 7.451(1), c=7.093(1), 7.157(2), 7.194(1), alpha=90.06(2), 90.08(2), 89.93(1), beta=95.11(1), 94.86(2), 94.85(2), gamma=103.39(1), 103.44(2), 103.34(1), respectively.

0.55 Wo consists of the two units of the basic-wollastonite along *a*-axis. The stacking sequence of 0.55Wo is represented as AA, where A is the unit cell of the basic-wollastonite. The final R-value was 6%.

65Wo consists of the two units of the basic-wollastonite along *a*-axis, too. However, the stacking sequence of 0.65Wo is represented as AB, where A is described above and B is the unit cell of the basic-wollastonite with *b*/2 displacement. The final R-value was 9%.

15Wo consists of the four units of the basic-wollastonite along *a*-axis. There were four possible stacking sequences represented 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 characteristics. The structure AAAA was most reasonable and the final R-value was 13%.