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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.

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2T and 4T Polytypes of Ca(Gex, Si1-x) O3 Wollastonite

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Three kinds of superstructures of wollastonite whose compositions were Ca(Ge0.15, Si0.85)O3, Ca(Ge0.55, Si0.45)O3 and Ca(Ge0.65, Si0.35)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%.