American Mineralogist, Volume 94, pages 323–333, 2009

Fukalite: An example of an OD structure with two-dimensional disorder

S. Merlino,[1] E. Bonaccorsi,[1,2,*] A.I. Grabezhev,[3] A.E. Zadov,[4] N.N. Pertsev,[5] and N.V. Chukanov[6]

[1]Dipartimento di Scienze della Terra, University of Pisa, Italy
[2]CNR-Institute for Geosciences and Georesources, Via Moruzzi 1, Pisa, Italy
[3]Institute of Geology and Geochemistry, Ural Branch of Russian Academy of Science, Pochtovyi Lane 7, Ekaterinburg 620151, Russia
[4]"NPP Teplochim" Limited, Dmitrovskoye Highway 71, Moscow 127238, Russia
[5]Institute of Geology of Ore Deposits, Petrography, Mineralogy and Geochemistry, Russian Academy of Science Moscow, Staromonetny Lane 35, Moscow 119017, Russia
[6]Institute of Problems of Chemical Physics, Russian Academy of Science, Chernogolovka, Moscow Region 142432, Russia

Abstract

The real crystal structure of fukalite, $Ca_4Si_2O_6(OH)_2(CO_3)$, was solved by means of the application of order-disorder (OD) theory and was refined through synchrotron radiation diffraction data from a single crystal. The examined sample came from the Gumeshevsk skarn copper porphyry deposit in the Central Urals, Russia. The selected crystal displays diffraction patterns characterized by strong reflections, which pointed to an orthorhombic sub-structure (the "family structure" in the OD terminology), and additional weaker reflections that correspond to a monoclinic real structure.

The refined cell parameters are $a = 7.573(3)$, $b = 23.364(5)$, $c = 11.544(4)$ Å, $\beta = 109.15(1)°$, space group $P2_1/c$. This unit cell corresponds to one of the six possible maximum degree of order (MDO) polytypes, as obtained by applying the OD procedure. The derivation of the six MDO polytypes is presented in the Appendix[1]. The intensity data were collected at the Elettra synchrotron facility (Trieste, Italy); the structure refinement converged to $R = 0.0342$ for 1848 reflections with $I > 2\sigma(I)$ and 0.0352 for all 1958 data.

The structure of fukalite may be described as formed by distinct structural modules: a calcium polyhedral framework, formed by tobermorite-type polyhedral layers alternating along **b** with tilleyite-type zigzag polyhedral layers; silicate chains with repeat every fifth tetrahedron, running along **a** and linked to the calcium polyhedral layers on opposite sides; and finally rows of CO_3 groups parallel to (100) and stacked along **a**.

Keywords: Crystal structure, fukalite, calcium carbonate silicate, OD structure