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There are believed to be caused by scattering from the surface layers of the crystal, where loss of potassium to the environment during the high temperature synthesis might cause an increase in consistent with the behaviour of the R3c phase. Weissenberg photographs of other KSB6O3 crystals have shown yet another trigonal phase with \( a = 5.37 \) Å, that gives diffuse diffraction spots.

PS-08.01.28 THE CRYSTAL AND BOND STRUCTURE OF C13A1 • CaF2. By Qi-jun Yu*, Xiu-jing Feng, Jiu-xiao Mi, and Jin-chuan Shen. Department of Materials Engineering, Wuhan University of Technology, Wuhan, China.

C13A1 • CaF2 is an important constituent in Portland cement clinker containing fluorine, but its crystal structure and characteristics have not been profoundly determined so far. C13A1 • CaF2 single crystals in a state of trigonal tristetrahedron of 40–120 μm have been prepared for the first time by flux evaporation growth method. A cubic structure, cell dimension of 11.981 (2) Å, molecular number of two, theoretical density of 2.72 g/cm³, space group of I43d and atomic coordinates were observed as well. The calcium atoms were found to be coordinated either to six oxygen ions in a very asymmetric manner or to six oxygen ions and one fluoride ion in an arrangement similar to distorted octahedral coordination, and the aluminum atoms coordinated to four oxygen ions in an arrangement of [AlO4] tetrahedron which make up a three-dimensional network. The formation mechanism and the strength of Al—O chemical bond were analyzed by approximate quantum chemical calculations. From above results we have determined the relations between the structure and hydration activity of C13A1 • CaF2 from the understanding of crystal structure and chemical bond.


Since the concept of fractal was proposed by Mandelbrot[1], this concept has been applied to a lot of disciplines[2]. In this article the fractal phenomenon in laser-induced chemical vapor deposition(LICVD) of Si powder is reported. The Si powder was synthesized by LICVD of SiH4 and H2. Only under certain conditions(cell pressure 200–400 Torr; gas flow rate 50–120 cm³/min; and silane concentration, 5–10%) the fractal phenomenon can occur. The fractal structure is observed by transmission electron microscopy(TEM). Fig. 1 is the typical picture of the fractal structure. Fig. 2 gives the corresponding transmission electron diffraction(TED) diagram. It can be seen clearly that the Si sample is crystalline. Fig. 1 indicates that the fractal structures with fingering-like are composed of small crystallite with triangle-shape, and the small crystallite size is about 0.1 μm.

The fractal dimensions are calculated by sandbox method[3], and the fractal dimension is 1.75. The experimental results showed that the fractal structure was grown during the initial stage of LICVD of Si powder, where the thermodynamic condition was nonequilibrium.

Reference:

Fig. 1

Fig. 2

PS-08.01.50 MANGNESIODUOMORPHITE: A NEW MINERAL FROM DORA-MAIA MASSIF (ITALY): ITS CRYSTAL STRUCTURE AND VERY-HIGH-PRESSURE METAMORPHOSIS.

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Magnesioduomorphite is the magnesium analogue of duomorphite with an orthorhombic site (o of the independent one), which is AI-free and is occupied by Mg as the most abundant cation. It occurs as rare inclusion within pyrope of coesite-bearing uvcotects (Dora-Maira Massif, western Alps, Italy). Pink to red; biserial (-), \( a = 1.678 \), \( b = 1.002 \), \( c = 1.001 \), \( V = 38.5 \) cm³ g⁻¹, \( \rho = 3.22 \) g/cm³. An anisotropic refinement of the Structure with diffraction data collected from a very small (0.07 x 0.07 x 0.05 mm), singlerystal diffractometer, HKL radiation converted to \( a / b = 0.031 \) for 1087 independent reflections and 447 parameters, including occupancy factors for two tetrahedral (T) and four octahedral (S) sites.
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The structure is based on a framework built up by connecting [001] double chains of octahedra; wide [001] channels in the framework are occupied by a single chain of face-sharing octahedra (M1 sites) and by the Si-tetrahedra.

By putting 2.88 Si 1 0.02 p in the T sites, the cell with a = 12.02(3), b = 20.22(3), c = 4.732(2)Å (e.g. FeMn) contains four f.u. with composition

\[ \text{[Fe}_{\text{25}}\text{Mn}_{\text{75}}\text{O}_{\text{16}}\text{]}.\]

\[ \text{[Al}_{\text{2}}\text{Si}_{\text{2}}\text{O}_{\text{5}}\text{]}.\]

In agreement with electron- and ion-microprobe analyses, only one hydrogen atom has been found in the framework. The further two hydrogens required by the chemical formula are disordered over more than two oxygen sites, their presence is confirmed by calculations of the charge distribution. Smaller Al-free tetrakaidecahedrons and lower contents of high-charge cations in the face-sharing octahedra under compression, are proposed to be the crystallochemical basis for the formation of magnesiowustite under the Drobe-Maia metamorphic conditions.

The following genera of formulas for the minerals of the manganowustite group are proposed:

\[ \text{[M}^{\text{II}}\text{]}\text{M}^\text{III}\text{O}_{\text{6}}\text{H}_{\text{2}}\text{]}.\]

where: \( \text{M}^\text{II} = \text{Al, Mg, Ti, Fe}^{\text{II}}\text{(M1 sites)}; \text{M}^\text{III} = \text{Al, Mg (M4 sites)}; \text{M}^\text{IV} = \text{Al (M2 and M3 sites)}; \text{T}^\text{+} = \text{Si, Al, Fe}^{\text{III}}\text{(T1 and T2 sites)}; \text{T}^\text{2+} = \text{Si} \text{occurs in holite (Newkie, Numma and Peys, 1989, Min. Mag., 51, 457-463) and forms a pyramidal group with three oxygen atoms (T(1) and T(2) site). In all sites, particularly in M(1), replacement can occur.}

PS-08.01.32 STRUCTURAL MODEL AND POLYTYPEISM IN TUNGSTATE.

T. I. Popov and J. Malicie.

The existence of strontium parahexahydrogen tungstate (Sr(HO)\textsubscript{2}WO\textsubscript{6}) was mentioned for the first time by Smith & Maxwell (1951) supported the existence of the hydroxy tungstate in the temperature range 48-200°C. Complete powder data were evaluated (JCPDS 28-866, Malicie). We managed to grow single crystals of Sr\textsubscript{2}WO\textsubscript{6} from plasticine clay. Crystalline data: \( a = 6.58.03, b = 12.30.41, c = 23.22.4(4)\text{Å}, V = 340.7\text{Å}^3, \) \( R = 0.042 \) for 215 reflections with \( l < 25(1)\).

Coordination polyhedron of Sr\textsuperscript{2+} consists of nine oxygen atoms from eight WO\textsubscript{6} tetrahedra and one water molecule at 2.548(15)Å, Sr(WO\textsubscript{6})\textsubscript{2} (Sr(2)) is coordinated to eight oxygen atoms from seven WO\textsubscript{6} and one HO\textsubscript{3} molecule (2.557(15)Å, 2.555(15)Å). Sr(1) atom participates in seven double discs - Sr 3.153(15) - 3.350(9)Å and one single Sr-2-Sr (3.409(13)Å, 3.431(13)Å, 3.490(13)Å, 3.497(13)Å). Three single Sr-W 3.614(3) - 3.635(3)Å and three bridges of two Sr-W 3.633(3) - 3.652(3)Å. The Sr(WO\textsubscript{6})\textsubscript{2} tetrahedron have irregular geometry with 20-20 angles at Sr-W distances 3.409(13)Å and (3.431(13)Å, 3.490(13)Å, 3.497(13)Å). The four coordination groups are linked to Sr or W, the fourth one only to three. The non-coordinated oxygen from Sr(WO\textsubscript{6})\textsubscript{2} has three closest neighbours: 1.20 Å at 3.333(2)Å, 0.133 Å at 3.867(2)Å, 0.133 Å at 3.867(2)Å.

PS-08.01.33 STRUCTURAL STUDIES OF CALCIUM AND LEAD PHOSPHATE UREA MICTRATES.

V. V. Vasiliev and E. V. Petriu.

Preliminary investigation of the system (Ca,Fe\textsubscript{3}-)\textsubscript{2}PO\textsubscript{4}-\textsubscript{2}H\textsubscript{2}O shows a large divalent content, insignificant location of 1111 position of the peaks. Single crystals of urea, calcium and calcium phosphate have been studied on an Enraf-Nonius CAD4 diffractometric system.

Complex sheet X. While in pyroline the X sheet contains only one Na and two Ca octahedra plus water molecules, in turgoite this sheet is completely filled by nine octahedra. The following ideal crystal-chemical formula is derived for turgoite:

\[ \text{[(Ca}_{25}\text{Mg}_{24}\text{)}\text{Fe}_{2}\text{O}_{20}>(\text{OH})_{2}]\text{[Si}_{2}\text{O}_{6}>(\text{OH})_{2}].\]

where M is mainly a bivalent with minor monovalent and trivalent cation (Fe\textsuperscript{3+} = 2, Na\textsuperscript{+} = 2, Fe\textsuperscript{2+} = 1, Si\textsuperscript{4+} = 4) in some samples. T(1) and T(2) are mainly Si with, in our samples, a maximum of 2Al which should stay in T' (3a sheet). This type of substitution in the c-axis is similar to pyroline. One or two samples (white turgoite) show clearly a composition which is intermediate between turgoite and pyroline. With reference to the C-centred cell, possible polytypes can be derived by shifts only along the b axis (11/2, z/2, 1/2; 11/2, z/2, 1/2; 11/2, z/2, 1/2; 11/2, z/2, 1/2; triclinic cell) and along a axis as well (11/2, 11/2, 1/2; 11/2, 11/2, 1/2; 11/2, 11/2, 1/2; 11/2, 11/2, 1/2; triclinic cell). The shifts are referred to the O sheets with respect to the 3a and 3a sheets.

PS-08.01.32 CRYSTAL STRUCTURE OF Sr\textsubscript{2}WO\textsubscript{6}·2H\textsubscript{2}O.

T. I. Popov and J. Malicie.

We managed to grow single crystals of Sr\textsubscript{2}WO\textsubscript{6} from plasticine clay. Crystalline data: \( a = 6.58.03, b = 12.30.41, c = 23.22.4(4)\text{Å}, V = 340.7\text{Å}^3, \) \( R = 0.042 \) for 215 reflections with \( l < 25(1)\).

Coordination polyhedron of Sr\textsuperscript{2+} consists of nine oxygen atoms from eight WO\textsubscript{6} tetrahedra and one water molecule at 2.548(15)Å, Sr(WO\textsubscript{6})\textsubscript{2} (Sr(2)) is coordinated to eight oxygen atoms from seven WO\textsubscript{6} and one HO\textsubscript{3} molecule (2.557(15)Å, 2.555(15)Å). Sr(1) atom participates in seven double discs - Sr 3.153(15) - 3.350(9)Å and one single Sr-2-Sr (3.409(13)Å, 3.431(13)Å, 3.490(13)Å, 3.497(13)Å). Three single Sr-W 3.614(3) - 3.635(3)Å and three bridges of two Sr-W 3.633(3) - 3.652(3)Å. The Sr(WO\textsubscript{6})\textsubscript{2} tetrahedron have irregular geometry with 20-20 angles at Sr-W distances 3.409(13)Å and (3.431(13)Å, 3.490(13)Å, 3.497(13)Å). The four coordination groups are linked to Sr or W, the fourth one only to three. The non-coordinated oxygen from Sr(WO\textsubscript{6})\textsubscript{2} has three closest neighbours: 1.20 Å at 3.333(2)Å, 0.133 Å at 3.867(2)Å, 0.133 Å at 3.867(2)Å.