These 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 c consistent with the behaviour of the $R3c$ phases. Weissenberg photographs of other $KSbO_3$ 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 $C_{11}A_7 \cdot CaF_2$. By Qi—jun Yu*, Xiu—ji Feng, Jin—xiao Mi and Jin—chuan Shen, Department of Materials Engineering, Wuhan University of Technology, Wuhan, China.

$C_{11}A_7 \cdot CaF_2$ is an important constituent in Portland cement clinker containing fluorine, but its crystal structure and characteristics have not been profoundly determined so far. $C_{11}A_7 \cdot CaF_2$ single crystals in a state of trigonal tristetrahedron of $40 \sim 120$ 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, space group of $I\bar{4}3d$ and atoms coordinates were observed as well. The calcium atoms were found to be coordinated either to six oxygens in a very asymmetric manner or to six oxygens and one fluorine in an arrangement similar to distorted octahedral coordination, and the aluminium atoms coordinated to four oxygens in an arrangement of $[AlO_4]$ 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 $C_{11}A_7 \cdot CaF_2$ from the understanding of crystal structure and chemical bond.

PS-08.01.29 FRACTAL IN LASER-INDUCED CHEMICAL VAPOR DEPOSITION OF SILICON POWDER By W.X. Wang*, D.H. Li, Anhui Institute of Optics and Fine Mechanics, Academia Sinica, Hefei 230031, P.R. China and Structure Research Lab. of University of Science and Technology of China, Hefei 230026, P.R. China, Z.C. Liu, Anhui Institute of Optics and Fine Mechanics, Academia Sinica, Hefei 230031, P.R. China, J.Y. Xing, Z.H. Wan, Structure Research Lab. of University of Science and Technology of China, Hefei 230026, P.R. China.

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, 200-400Torr; gas flow rates, 80-120cm³/min; and silane concentration, 5-10%) the fractal phenomenon can occur. The fractal structure is observed by transmission electron microscope(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 crysallite with triangle-shape, and the small crystallite size is about 0.1 μm.

The fractal domensions are calculated by sandox method[3], and the fractal domension 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 unequilibrium.

Reference:

1. B.B. Mandelbrot, The Fractal Geometry of Nature, New York, 1983.
2. Jens Feder, Fratals, Plenum Press, New York, 1988.
3. S.R. Forrest and T.A. Witten, Jr. J. Phys. A.12(1979)L109.

Fig.1   Fig.2

PS-08.01.30 MAGNESIODUMORTIERITE: A NEW MINERAL FROM DORA-MAIRA MASSIF (ITALY), ITS CRYSTAL STRUCTURE AND VERY-HIGH-PRESSURE METAMORPHISM. G.Ferraris*[1], G.Ivaldi[1], C.Chopin[2], R.Compagnoni[1], C.Davidson[3] and A.Davis[4].

1 Dip. Sci. Mineral. Petrol., Univ. Torino, Italy
2 Lab. Géol., Ecole normale supérieure, Paris, France
3 Geol. Inst. Univ. Basel, Switzerland
4 The Enrico Fermi Inst., Univ. Chicago, U.S.A.

Magnesiodumortierite is the magnesium analogue of dumortierite with an octahedral site (out of 4 independent ones) which is Al-free and is occupied by Mg as the most abundant cation. It occurs as rare inclusion within pyropes of coesite-bearing whiteschists (Dora-Maira Massif, western Alps, Italy). Pink to red; biaxial (-), $\alpha = 1.678$, $\beta = 1.700$, $\gamma = 1.701$, 2V = 38.5°, $D_{calc} = 3.22$ g/cm³. An anisotropic refinement of the structure with diffraction data collected from a very small (0.07 x 0.07x 0.05 mm; single-crystal diffractometer, $MoK\alpha$ radiation) converged to R = 0.031 for 1107 independent reflections and 147 parameters, including occupancy factors for two tetrahedral (T) and four octahedral (M) sites.

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 [M(1) site] and by the Si-tetrahedra.

By putting 2.88 Si + 0.02 P in the T sites, the cell with a = 12.02(3), b = 20.22(3), c = 4.732(2)Å (s.g. Pmcn) contains four f.u. with composition

$[(Mg_{0.49}Ti_{0.19}Fe_{0.01}\square_{0.31})(Al_{0.71}Mg_{0.25}\square_{0.04})_2$

$(Al_{0.95}\square_{0.05})_4][Si(Si_{0.94}P_{0.01}\square_{0.05})_2O_{15.04}(OH)_{2.96}]B$

in agreement with electron- and ion-microprobe analyses. Only one hydrogen atom has been found in the difference Fourier. The further two hydrogens required by the chemical formula are disordered over more than two oxygens; their presence is confirmed by calculations of the charge distribution.

Smaller Al-free tetrahedra 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 magnesiodumortierite under the Dora-Maira metamorphic conditions.

The following general formula for the minerals of the dumortierite group is proposed

$[M'(M'')_2(M'")_4O_{18-x-y}(OH)_x]T'_{3-x}T"_yB$
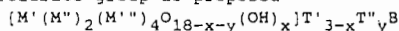
where: M' = Al, Mg, Ti, Fe, RE(?) [M(1) site]; M" = Al, Mg [M(4) site]; M'" = Al [M(2) and M(3) sites]; T'= Si, Al, P [T(1) and T(2) sites]; T" ≈ Sb occurs in holtite (Hoskins, Mumme and Pryce, 1989, Min. Mag., 53, 457-463) and forms a pyramidal group with three oxygen atoms [T(1) and T(2) sites]. In all sites, particulary in M(1), vacances can occur.

## PS-08.01.31 STRUCTURAL MODEL AND POLYTYPISM IN TUNGUSITE.

G.Ferraris[1], A. Pavese[2], S. Soboleva[3].
1 Dip. Sci.Miner.Petr., Univ. Torino, Italy.
2 Dip. Sci.Terra, Univ. Milano, Italy.
3 IGEM, Russian Acad.Sci., Moscow, Russia.

Tungusite is a light green hydrous silicate of Ca and Fe reported from different localities of the Siberian Platform and described the first time by V.I. Kudriashova (1966, Dokl. Akad. Nauk SSSR, 171, 1167-1170).

On the basis of X-ray (powder patterns) and electron diffraction studies (selected area and oblique texture patterns) and of comparison with the crystal structures of reyerite (Merlino, 1989, Min. Mag., 52, 247-256) and gyrolite (Merlino, 1989, Min. Mag., 52, 377-387) new data on tungusite have been obtained.

No single crystals suitable for X-ray structural studies have been found and the electron diffraction shows a widespread stacking disorder along the c* axis. The most ordered sample shows a metrically monoclinic C-centred cell, with a = 9.66, b = a√3, c = 21.86 Å, α ≈ 100, ß = 90, γ= 90°. By analogy with gyrolite, the structural model is based on a triclinic (P$\bar{1}$) cell with a ≈ b = 9.66, c = 21.86 Å, α ≈ 98.6, ß = 90, γ = 120°. The proposed model maintains the $S_1OS_2X\bar{S}_2\bar{O}S_1$ sequence of tetrahedral (S), octahedral (O) and complex (X) sheets reported in gyrolite by Merlino; it differs from this structure pratically only for the contents of the

complex sheet X. While in gyrolite the X sheet contains only one Na and two Ca octahedra plus water molecules, in tungusite this sheet is completely filled by nine octahedra. The following ideal crystallochemical formula is derived for tungusite:

$(Ca_{14}Mg_9{}^{2+})[T_8O_{20}(OH)_6][T'_8O_{20}(OH)_8]_2,$
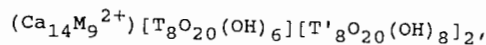
where M is mainly a bivalent with minor monovalent and trivalent cation (Fe^{2+} ≈ 6, Na$^+$ ≈ 2, Fe^{3+} ≈ 1, in our samples); T and T' are mainly Si with, in our samples, a maximum of 2Al which should stay in T' (S_2 sheet). This type of substitutions in M requires that some OH are replaced by H_2O. Some of our samples ("white tungusite") show clearly a composition which is intermediate between tungusite and gyrolite.

With reference to the C-centred cell, possible polytypes can be derived by shifts only along the b axis (±1/9, ±2/9, ±4/9; monoclinic cells) and along a axis as well (±1/3, ±1/2, ±1/6; triclinic cells). The shifts are referred to the O sheets with respect to the S_1 and S_2 sheets.

PS-08.01.32 CRYSTAL STRUCTURE OF Sr(ReO₄)₂.H₂O

T. Todorov and J. Macicek*, Institute of Applied Mineralogy, Bulg. Acad. Sci., Rakovski str. 92, 1000, Sofia, Bulgaria.

The existence of strontium perrhenate monohydrate was mentioned for the first time by Smith & Maxwell (J. Am. Chem. Soc., 1951, 73, 658-660) and proven by means of X-ray powder data and TGA analysis by Wassilopulos (Über Polinare Oxide des 4 and 7 wertigen Technetium mit Erdaklialien. Karlsruhe. Kernf. Inst. Radiochem., 1965, S. 67)

Our STA analysis of fresh Sr(ReO₄)₂.2H₂O prepared according to Smith & Maxwell (1951) supported the existence of the monohydrate in the temperature range of 66 - 155°C. Complete powder data were evaluated (PDF 42-682; Macicek). We managed to grow single crystals of Sr(ReO₄)₂.H₂O from absolute CH₃OH. Crystal data: M_r = 606.03, orthorhombic, Pbca (61),

a = 11.594(2), b = 12.304(1), c = 23.885(4)Å, V = 3407 Å³, Z = 16, D_x = 4.73 g.cm^{-3}, R = 0.042 for 2151 reflections with I > 2σ(I).

Coordination polyhedron of Sr(1) consists of nine oxygen atoms from eight ReO₄ tetrahedra and one water molecule at 2.548(16) - 2.686(15)Å. Sr(2) is coordinated to eight oxygen atoms from seven ReO₄ groups and the second H₂O molecule [2.507(15) - 2.814(20)Å]. Sr(1) atom participates in seven double [Sr...Sr 6.175(3) - 6.530(3)Å] and one single Sr-T-Sr [Sr...Sr 6.818(3)Å] bridges, while Sr(2) forms six double [Sr...Sr 6.325(3) - 6.558(3)Å] and three single [Sr...Sr 6.632(3) - 6.818(3)Å] bridges. The ReO₄ tetrahedra have irregular geometry with Re-O distances and [O-Re-O] angles within 1.702(15)-1.742(15)Å and [106.7(8)-111.8(7)°]. Three of the ReO₄ groups are linked to four Sr ions, and the fourth one only to three. The non-coordinated oxygen from Re(4)O₄ has three closest neighbours: O(22) at 3.233(22)Å, O(23) at 3.282(23)Å and O(13) at 3.368(22)Å.

PS-08.01.33 STRUCTURES OF CALCIUM AND LEAD PERRHENATE UREA HYDRATES.

By J. Macicek*, R. Petrova, O. Angelova, Bulgarian Academy of Science, Rakovski str. 92, 1000, Sofia, (Bulgaria)

Preliminary investigation of the system M(ReO₄)₂-Urea-H₂O, M = large divalent cations, indicate formation of 1:1:1 addition compounds. Single crystals of lead and calcium species have been studied on an Enraf-Nonius CAD4/SDP44 diffractometric system.