

## 08-Inorganic and Mineralogical Crystallography

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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  $\text{KSbO}_3$  crystals have shown yet another trigonal phase with  $a = 5.37 \text{ \AA}$ , that gives diffuse diffraction spots.

PS-08.01.28 THE CRYSTAL AND BOND STRUCTURE OF  $\text{C}_{11}\text{A}_7 \cdot \text{CaF}_2$ . By Qi-jun Yu\*, Xiu-ji Feng, Jin-xiao Mi and Jin-chuan Shen, Department of Materials Engineering, Wuhan University of Technology, Wuhan, China.

$\text{C}_{11}\text{A}_7 \cdot \text{CaF}_2$  is an important constituent in Portland cement clinker containing fluorine, but its crystal structure and characteristics have not been profoundly determined so far.  $\text{C}_{11}\text{A}_7 \cdot \text{CaF}_2$  single crystals in a state of trigonal tristetrahedron of  $40\sim 120 \mu\text{m}$  have been prepared for the first time by flux evaporation growth method. A cubic structure, cell dimension of  $11.981(2) \text{ \AA}$ , molecular number of two, theoretical density of 2.72, space group of  $\bar{I}43d$  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  $[\text{AlO}_4]$  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  $\text{C}_{11}\text{A}_7 \cdot \text{CaF}_2$  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  $\text{SiH}_4$  and  $\text{H}_2$ . Only under certain conditions (cell pressure, 200-400Torr; gas flow rates, 80-120 $\text{cm}^3/\text{min}$ ; 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 crystallite with triangle-shape, and the small crystallite size is about  $0.1 \mu\text{m}$ .

The fractal dimensions are calculated by sandox 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 unequilibrium.

Reference:

1. B. B. Mandelbrot, The Fractal Geometry of Nature, New York, 1983.
2. Jens Feder, Fractals, 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<sup>1</sup>, G. Ivaldi<sup>1</sup>, C. Chopin<sup>2</sup>, R. Compagnoni<sup>1</sup>, C. Davidson<sup>3</sup> and A. Davis<sup>4</sup>.

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Magnesiodymortierite 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 (-),  $\alpha = 1.678$ ,  $\beta = 1.700$ ,  $\gamma = 1.701$ ,  $2V = 38.5^\circ$ ,  $D_{\text{calc}} = 3.22 \text{ g/cm}^3$ . An anisotropic refinement of the structure with diffraction data collected from a very small ( $0.07 \times 0.07 \times 0.05 \text{ mm}$ ; 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.