08-Inorganic and Mineralogical Crystallography

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 c consistent with the behaviour of the R3c phase. Weissenberg photographs of other KSBaO₃ 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 CaF₂. By Qi—jun Yu*, Xu—jil Feng, Jin—xiu Mi and Jin—chuan Shen, Department of Materials Engineering, Wuhan University of Technology, Wuhan, China.
CaF₂ is an important constituent in Portland cement clinker containing fluosilicate, but its crystal structure and characteristics have not been profoundly studied so far. CaF₂ single crystals in a state of trigonal tristetrahedron of 40–120 µm have been prepared for the first time by flux vapor growth method. A cubic structure, cell dimension of 11.981 (2) Å, molecular number of two, theoretical density of 2.72, space group of I43d and atoms coordinates were observed as well. The calcium atoms were found to be coordinated either to six oxygen in a very asymmetric manner or to six oxygen and one fluorine in an arrangement similar to distorted octahedral coordination, and the aluminum atoms coordinated to four oxygen 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 relation between the structure and hydration activity of CaF₂ from the understanding of crystal structure and chemical bond.

PS-08.01.25 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. Waa, 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: 200–400 Torr; gas flow rates: 50–120cm³/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 finger-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 equilibrium.
Reference:

Fig.1 Fig.2

PS-08.01.50 MAGNESIODUOMORPHITE: A NEW MINERAL FROM DORA-MAIJA MASSIF (ITALY): ITS CRYSTAL STRUCTURE AND VERY-HIGH-PRESSURE METAMORPHISM. By G. Ferrarini¹, J. Ivery¹, O. Chopin², R. Compagnoni¹, G. Davidson¹ and A. Davis².
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Magnesioduromorphite is the magnesium analogue of duromorphite with an orthorhombic site of (100) independent ones which is Al-free and is occupied by Mg as the most abundant cation. It occurs as rare inclusion within pyramids of coarse-grained white micas (Dora-Maira Massif, western Alps, Italy). Pink to red; biaxial (+), α = 1.678, β = 1.000, γ = 1.015, 2V = 38.5°, D(calc) = 3.22 g/cm³. An anisotropic refinement of the structure with X-ray data collected from a very small (0.07 x 0.07 x 0.05 mm³) single-crystal diffractometer, MoKα radiation converged to R = 0.031 for 1807 independent reflections and 47 parameters, including occupancy factors for two tetrahedral (T) and four octahedral (X) sites.