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Ternary diagrams of $\text{Li}_2\text{O}-\text{Nb}_2\text{O}_5$ with different oxides (MgO , TiO_2 , ZrO_2 , Fe_2O_3 , MnO , etc) were studied because of the interest in the electrical and optical properties of the phases obtained in those systems. In the ternary system $\text{Li}_2\text{O}-\text{Nb}_2\text{O}_5-\text{MgO}$ were founded several solid solutions regions, joint lines and new phases. $\text{Li}_6\text{MgNb}_2\text{O}_9$ is a new compound synthesized on the line $\text{Li}_3\text{NbO}_4-\text{MgO}$. It has a disordered polymorph prepared as metastable phase similar as the reported in the system $\text{Li}_3\text{NbO}_4-\text{Li}_2\text{TiO}_3$ (Aragón-Piña et al. *J. Mat. Sc. Lett.* (1984), 3, 893).

The ordered phase was prepared by reaction of the oxide starting materials at 1000°C within 120 hours. Cation disordering occurs at 1050°C within 1 hour. The disordered phase has cubic symmetry (isostructural with periclase), the precise cell parameter is $4.208(3)$ Å and statistical population of the crystallographic positions 1/3. The ordered phase has triclinic symmetry (space group P1) and cell parameters $a=7.852(3)$, $b=8.913(4)$, $c=6.050(5)$ Å, $\alpha=100.75(2)^\circ$, $\beta=97.63(3)^\circ$ and $\gamma=105.89(3)^\circ$, with crystallographic population of the positions equal one. Measurements were made in the Siemens D5000 diffractometer with $\text{Cu K}\alpha_1$ radiation. The ordered phase was indexed by TREOR 90 (P.E. Werner, University of Stockholm, private comm.) and the precise lattice parameters were refined with LSUCRI (R.G. Garvey, North Dakota State University, 1990) and PARAMETROS (R. Pomés et al, *Rev. Cub. de Física* (1981), 1, 95).

PS-08.01.25 CRYSTAL STRUCTURES OF $(\text{CH}_3)_2\text{NH}_2\text{Al}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ ($\text{CD}_3)_2\text{ND}_2\text{Al}(\text{SO}_4)_2 \cdot 6\text{D}_2\text{O}$, AND $(\text{CH}_3)_2\text{NH}_2\text{Ga}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$

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Crystals of $(\text{CH}_3)_2\text{NH}_2\text{Al}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ (DMAS) have been reported (Kirpichnikova, L.F., Shuvalov, L.A. and Ivanov, N.R., *Ferroelectrics*, 1989, 36, 313-317) to be ferroelectric ($T_c = 150\text{K}$) and ferroelastic. DMAS represents a family of isomorphous crystals investigated in our laboratories, with the following lattice parameters:

	a(Å)	b(Å)	c(Å)	β (deg)
$(\text{CH}_3)_2\text{NH}_2\text{Al}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ (T=295K)	6.403(2)	10.747(3)	11.128(2)	100.47(2)
$(\text{CD}_3)_2\text{ND}_2\text{Al}(\text{SO}_4)_2 \cdot 6\text{D}_2\text{O}$ (T=295K)	6.399(1)	10.741(2)	11.131(2)	100.44(3)
$(\text{CD}_3)_2\text{ND}_2\text{Al}(\text{SO}_4)_2 \cdot 6\text{D}_2\text{O}$ (T=130K)	6.437(1)	10.684(2)	11.116(2)	99.82(3)
$(\text{CH}_3)_2\text{NH}_2\text{Ga}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ (T=295K)	6.376(3)	10.731(6)	11.365(6)	100.86(5)

In the paraelectric phase (space group $\text{P}2_1/\text{n}$) the nitrogen atom of the methylammonium molecule occupies at random two positions related by the symmetry center. The vector connecting these positions is almost parallel to the polarization vector P_s in the low temperature ferroelectric phase (space group Pn). The paraelectric-

ferroelectric phase transition is therefore of the order-disorder type and goes on with the ordering of the methylammonium molecule. The polarization reversal is connected with the switching of the nitrogen atom in the methylammonium molecule.

PS-08.01.26 SYNTHESIS AND CRYSTAL STRUCTURE OF $\text{F-Er}_2\text{S}_3$

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$\text{F-Er}_2\text{S}_3$ crystals were obtained by vapor transport in the presence of foreign atoms (Nb and Cl). The structure of $\text{F-Er}_2\text{S}_3$ was determined by single crystal X-ray diffraction. $\text{F-Er}_2\text{S}_3$ is monoclinic, space group $\text{P}2_1/\text{m}$, $Z = 4$,

$a = 10.901(1)$ Å, $b = 3.896(1)$ Å, $c = 11.167(1)$ Å, $\beta = 108.804(5)^\circ$, $R_F = 0.046$ for 2838 observed reflections with $I > 2.5\sigma(I)$. All atoms are located at the mirror planes. There are four crystallographically independent erbium atoms in $\text{F-Er}_2\text{S}_3$, half of them in six coordination, one quarter in seven and one quarter in eight coordination by sulfur. Half of the six types of sulfur atoms are coordinated in four, the other half in five by erbium atoms. From the bond valence calculation of $\text{F-Er}_2\text{S}_3$ and the $\text{D-Er}_2\text{S}_3$ (the stable phase at ambient conditions), it was found that the Er-S distances and bonding valences of the six- and seven-coordinated erbium atoms in $\text{F-Er}_2\text{S}_3$ are close to those in $\text{D-Er}_2\text{S}_3$. The eight-coordinated Er atom in $\text{F-Er}_2\text{S}_3$ is much weaker bonded to sulfur than expected and has a rather low valence ($V = 2.5$).

Three different stoichiometric Er_2S_3 phases are found to occur: D-, U- and $\text{F-Er}_2\text{S}_3$. $\text{D-Er}_2\text{S}_3$ is isostructural with $\text{D-Ho}_2\text{S}_3$, half of the Er atoms in six, the other half in seven coordination by sulfur. The molar volume of $\text{D-Er}_2\text{S}_3$ amounts to $69.71 \text{ cm}^3/\text{mol}$ (to compare with $V_m = 67.90 \text{ cm}^3/\text{mol}$ for $\text{F-Er}_2\text{S}_3$). $\text{U-Er}_2\text{S}_3$ was obtained under high pressure conditions (10.9 Kbar, 900°C). The molar volume is $62.87 \text{ cm}^3/\text{mol}$. It might be concluded that $\text{D-Er}_2\text{S}_3$ is the normal temperature and pressure phase, $\text{U-Er}_2\text{S}_3$ the high-pressure form. $\text{F-Er}_2\text{S}_3$ is a medium-pressure modification.

PS-08.01.27 Potassium deficient phases of rhombohedral KSbO_3
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A series of single crystals of rhombohedral KSbO_3 have been investigated with X-ray diffraction. The structure is of the ilmenite type with approximate hexagonal close packing of oxygen atoms (Spiegelberg, *Arkiv Kemi Mineral. Geol.*, 1940, No. 5), with space group $R\bar{3}$ and cell dimensions $a = 5.3762(2)$, $c = 18.2505(8)$ Å in the hexagonal description. Each of the cations occupies two thirds of the octahedral interstices in every second layer along c . However, some of the $R\bar{3}$ samples showed disorder in the oxygen arrangement, which could be interpreted as disorder in the stacking sequence of oxygen layers along c . In this way the coordination around potassium is modified from distorted octahedral to distorted trigonal prismatic in some of the layers.

Several crystals with an ordered ABBAABB... sequence were also studied. They have space group $R\bar{3}c$ with c twice that of the $R\bar{3}$ phase. The cell dimensions of this phase vary, but for all the crystals studied a is shorter and c longer than the corresponding $R\bar{3}$ values, eg. $a = 5.3254(4)$, $c = 37.338(3)$ Å. There is an approximately linear relationship between the c and a dimensions, as well as between the refined occupancy of one of the potassium sites and a or c . The lowest K:Sb ratio observed in four different crystals was 0.88.

One of the $R\bar{3}$ crystals used for structure determination showed additionally a small number of diffuse spots in the Weissenberg photographs, that could be indexed on a trigonal cell with $a = 5.37$ Å but with a c that is incommensurable with the c of the $R\bar{3}$ phase.

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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 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 $\bar{1}A3d$ 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 SiH_4 and H_2 . Only under certain conditions (cell pressure, 200-400Torr; gas flow rates, 80-120 cm^3/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. Ferraris¹, G. Ivaldi¹, C. Chopin², R. Compagnoni¹, C. Davidson³ and A. Davis⁴.

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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 (-), $\alpha = 1.678$, $\beta = 1.700$, $\gamma = 1.701$, $2V = 38.5^\circ$, $D_{\text{calc}} = 3.22 \text{ g/cm}^3$. 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 α 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.