There are minor differences between the chemical compositions of baratovite and berezanskite and their blocks in the crystal structure of faizievite. Baratovite, $KLi_3Ca_7Ti_2(Si_6O_{18})_2(OH)_2$, and the baratovite block in faizievite, $K_2(Ca_6Na)Li_6Ti_4(Si_6O_{18})_2F_2$, are related by the substitution: $^{VI}Ca^{2+} + (OH)^-_2 \leftrightarrow {}^{VI}Na^+ + F^-_2$. Berezanskite, $K^{IX}\square L_3Ti_2(Si_{12}O_{30})$, and the berezanskite block in faizievite, $KNaLi_3Ti_2(Si_{12}O_{30})$, are related by the substitution: $^{IX}\square \leftrightarrow {}^{IX}Na^+$. Therefore assembley of faizievite from baratovite and berezanskite components is accompanied by the following substitution:

$^{VI}Ca^{2+} + {}^{IX}\square + (OH)^-_2 \leftrightarrow {}^{VI}Na^+ + {}^{IX}Na^+ + F^-_2$.
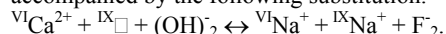
[1] Pautov, L.A. & Agakhanov, A.A. *Zap. Vser. Mineral. O-va*. 1997, 126(4), 75.
[2] Sandomirskii, P.A., Simonov, M.A., Belov, N.V. *Dokl. Akad. Nauk SSSR*, 1976, 231, 615.

MS41 P23

Crystal structures of new pyrovanadates $A_2MnV_2O_7$ (A = K, Rb) Hamdi Ben Yahia, Etienne Gaudin, Jacques Darriet, *Institut de Chimie de la Matière Condensée de Bordeaux, Université Bordeaux 1, 87 Avenue du Docteur Schweitzer, 33608 Pessac Cedex, France.*
E-mail: benyahia@icmcb-bordeaux.cnrs.fr

Keywords: Melilite layered structure, Crystal structure determination, Single crystal diffraction

The compounds $A_2MnV_2O_7$ (A = K, Rb) with structures related to the melilite-type [1] have been synthesised. The crystal structures of $K_2MnV_2O_7$, $KRbMnV_2O_7$ and $Rb_2MnV_2O_7$ were determined using single crystal samples. The compound $K_2MnV_2O_7$ has tetragonal unit cell parameters a = 8.6091 Å, c = 5.5375 Å and crystalize with $P\text{-}42_1m$ space group, Z = 2 whereas $Rb_2MnV_2O_7$ and $KRbMnV_2O_7$ crystalise in $P4_2/mnm$ space group, Z = 4 with unit cell parameters a = 8.5304 Å, c = 11.4659 Å and a = 8.5766 Å, c = 11.8094 Å respectively. The structures contain layers build up by MnO_4 tetrahedra and V_2O_7 pyrovanadate units. The linkage of tetrahedra forms five-membered rings which form sheets parallel to (001). The eight coordinated A alkali cations are positioned between the sheets and form distorted square antiprisms in $K_2MnV_2O_7$ and distorted square prisms in $Rb_2MnV_2O_7$ and $RbKMnV_2O_7$.

[1] Warren B.E., *Z. Kristallogr*. 1930, 74, 131.

MS41 P24

Analysis of structural ordering of mineral solids from microscopic images Yevgeny A. Golubev *Institute of Geology, Russian Academy of Sciences, Syktyvkar, Russia.*
E-mail: golubev@geo.komisc.ru

Keywords: AFM-STM studies of minerals and glasses, supramolecular structures, statistical distribution

We solved a problem of studying of supermolecular structures ordering of natural X-ray amorphous substances. We was shown earlier that the most part of these substances have nanodispersed structure [1]. The most effective method of studying of nanostructurized substances is direct observation of their structure by microscopy. In case of a nonregular arrangement of structural units there is a question on a degree of their ordering. The statistical methods are necessary for

studying ordering, allowing to determine local structural characteristics of system. In this work the modernized method *of n-symmetric points* [1, 2] was used. This method based on statistical approximation of dependences of spatial distribution of points (particles), enabled to determine a randomness of points arrangement. At their regularity distribution this method enables to receive the appropriate statistical appraisal, for example, to measure of scale of particles aggregation (on two, on three etc).
We carry out research of supermolecular structures ordering of natural X-ray amorphous substances by SEM and AFM. Among the investigated substances only two have revealed the disorder supermolecular constitution. In the others tendencies to aggregation from two to seven particles in aggregate were found [2].

[1]. Golubev Ye. A. Journal of Crystal Growth, 2005, 275, e2357.
[2]. Golubev Ye. A. Supermolecular structures of natural X-ray amorphous substances Yekaterinburg: Nauka Press, 2006.

MS41 P25

Electron diffraction analysis of amorphous geological materials V.K.Kis[a], M. Pósfai[b], J.L. Lábár[a], I Dódony[c]
[a]*Research Institute for Technical Physics and Material Science, Budapest, Hungary* [b]*Department of Earth and Environmental Sciences, University of Pannonia, Veszprém, Hungary* [c]*Department of Mineralogy, Eötvös Loránd University, Budapest, Hungary*
E-mail: kis@mfa.kfki.hu

Keywords: disordered structures; electron diffraction; mineralogy

Poorly crystalline and amorphous materials occur in a wide range of geological environments. They include aluminosilicate glasses and opals in rocks, highly disordered Fe hydroxides and oxy-hydroxides in soils, and carbons such as soot in the atmosphere or shungite in the lithosphere.
A knowledge of the structure of poorly crystalline materials is useful for deducing formation/precipitation conditions and helps in understanding their physico-chemical behaviour such as adsorption properties, stability and reactivity.
Amorphous structures lack long-range order but can be described by the nearest neighbour interatomic distances. Since a Fourier transformation of diffraction data gives the frequency distribution of interatomic distances, information on the local structure can be inferred from diffraction data. Electron diffraction (ED) has some advantages over X-ray and neutron beam methods in structural studies. The high spatial selectivity of ED allows one to discriminate between the scattering contributions of the individual components of a heterogeneous material. The strong scattering power of electrons makes a short exposure time possible and results in good statistics in the signal. Light elements (such as carbon or oxygen) are also well measurable.
We used electron diffraction measurements to investigate the local structure of volcanic glasses (obsidian and pumice) and atmospheric soot. In the case of volcanic glasses amorphous, partly ordered, and nanocrystalline regions were distinguished and analysed separately. The deconvoluted atomic distances obtained from experimental diffraction patterns through total pair-distribution functions are consistent with distances for ideal SiO_4 tetrahedra. Partly ordered structures in pumices

are composed of plate-like fragments of tridymite/cristobalite layers, whereas obsidian contains quartz nanocrystals with abundant moganite-like planar faults.

Regarding atmospheric soot particles, a characteristic shift of the first nearest-neighbour interatomic distance was observed. Interatomic distances are proved to be as small as 0.134 nm, much shorter than in graphite (0.142 nm) or in amorphous carbon (0.141–143 nm), but larger than the typical value (0.131–0.132 nm) for a kerogen with significant hydrogen content (H/C=0.61). These results suggest that the first nearest neigbour interatomic distance measurable in soot is the superposition of first-neighbour C–C distances and C–H distances (around 0.143 and 0.11 nm, respectively). Hydrogen is related to the aromatic components in soot which can strongly influence the optical properties of soot particles.

Quantitative electron diffraction has proved to be an efficient method for studying the nanostructures of highly disordered geological materials.

MS41 P26

Compounds AMO_4 (A = Ca, Sr, Ba; M = W, Mo) with scheelite structure: growth, composition, structure peculiarities. Eremin A.[a], Kuz'micheva G.[a], Zharikov E[b]

a) Lomonosov State Academy of Fine Chemical Technology, Moscow, Russia b) Mendeleyev University of Chemical Technology, Moscow, Russia.
E-mail: Eremamitxt@yandex.ru

Keywords: sheelite, composition, structure

Single crystals with sheelite structure ($CaWO_4$), doped by rare earth ions meet very high interest of different scientific groups as active media for solid-state lasers. It is seen from numerous publications, appeared during the last years.

In this paper, we report a results of crystallochemical analysis of AMO_4 (A=Ca, Sr, Ba; M=W, Mo) compounds and a detailed structural study of $CaWO_4$ doped with Na^{1+} and Yb^{3+}.

In the scheelite structure (sp. gr. $I4_1/a$, z=4), Ca^{2+} is in a severely distorted dodecahedral oxygen coordination with two sets of bond distances (CN=4+4), W^{6+} is in a slightly distorted tetrahedral coordination, with identical W-O bond distances (CN=4) but different bond angles.

Crystallochemical analysis of structural parameters of well- known AMO_4 (A=Ca, Sr, Ba; M=W, Mo) allowed to ascertain:

- the cell parameter a increases and the cell parameter c decreases in $CaMO_4$-$SrMO_4$-$BaMO_4$ and $AMoO_4$-AWO_4 series,

- the AO_8 dodecahedra are more regular in $AMoO_4$ structures than those in AWO_4 ones,

- the M-O interatomic distances in MO_4 tetrahedra do not depend on cation kind in dodecahedral sites,

-the increasing of A ionic radius leads to the formation of more regular tetrahedra (for AWO_4 appeared to be more than for $AMoO_4$),

-the change of A ionic radius affects only the change of tetrahedra angles (for $AMoO_4$ appeared to be more than for AWO_4),

We studied unannealed (I) and air-annealed (II) single crystals ($Ca_{1-2x}Na_xYb_x)WO_4$ (x=0.03, 0.10, 0.15) grown by the Czochralski technique. The crystals were ground into powder and examined by X-ray diffraction (XRD) on a HZG diffractometer (CuK_α radiation, 2θ = 10-100°, step

scan mode with a counting time of 10 s per data point and a scan step of 0.05°). Single-crystal structural analysis was carried out on a CAD-4 diffractometer at room temperature (MoK_α radiation, graphite monochromator, ω scan mode) for $(Ca_{0.8}Na_{0.1}Yb_{0.1})WO_4$ microcrystals.

With increasing x value, the lattice parameters of $(Ca_{1-2x}Na_xYb_x)WO_4$ crystals decrease, as would be expected (r_{Ca}=1.12Å, r_{Na}=1.18Å, r_{Yb}=0.99Å). The lattice parameters of the annealed crystal are smaller than those of unannealed for both powder samples and microcrystals, which correlates with the concentration of Na and Yb, as supported by single-crystal XRD data: $(Ca_{0.819}Na_{0.120}Yb_{0.061})WO_{3.970}$ (II) and $(Ca_{0.808}Na_{0.118}Yb_{0.074})WO_{3.978}$ (I)

In the case of unannealed $(Ca_{0.8}Na_{0.1}Yb_{0.1})WO_4$ (I) crystals it was observed that some XRD peaks are split (011, 012, 013, 004, 224 and so on) or their shape is distorted. This can be explained by one of two reasons: the formation of ordered phase (superstructure) or the separation of solid-solution with formation of two isostructural phases of different compositions. The same phenomenon we observed by X-ray study of $(Na_{0.5}Gd_{0.5})WO_4$ and $(Na_{0.5}Gd_{0.5})WO_4$:Yb crystals that has been explained by superstructure formation.

MS41 P27

Structure in layers or in tunnels to basis of uranyl - vanadate M. Saadi[a], S. Obbade[b], C. Dion[b], S.Yagoubi[b], C. Renard and F. Abraham[b] *[a]Laboratoire de Chimie du Solide Appliquée, Département de Chimie, Faculté des Sciences, Université Mohammed V Agdal, Rabat, Maroc [b]Laboratoire de Cristallochimie et Physicochimie du Solide, UMR CNRS 8012, ENSCL - USTL, Villeneuve d'Ascq Cedex, France.* E-mail : saadi@fsr.ac.ma

Keywords: Layerd structure -1, Uranyl -2, vanadate -3

The study of the association of uranyl ions and oxyanions presents an interest at the same time environmental, mineralogical, geological, structural and physical. From the physical property point of view these compounds are particularly interesting because they frequently generate original, two-dimensional structures (2D) by the formation of infinite layers, or the structures known as monodimensional by the formation of tunnels. These structures favours the mobility of the cations present in the tunnels or in spaces inter layers as well as the possibilities of intercalation and desintercalation of these cations. Within the framework of the search for new uranyl $(UO_2)^{2+}$ and oxyanions $X_mO_n^{p-}$ based materials , we began our study with uranyl vanadates of the type carnotite $M_2(UO_2)_2V_2O_8$, nH_2O (V/U = 1) of the monovalent cations (M = Na, K, Rb, Cs, Tl, Ag, NH_4). Their crystalline structure is formed by a stacking up of infinite layers $[(UO_2)_2V_2O_8]^{2-}$, resulting from the association of uranyl ions UO_2^{2+} and $V_2O_8^{6-}$ entities. The field of investigations then was widened to the compounds of report/ratio V/U = 3. This work allowed the focusing of the $CsUO_2(VO_3)_3$ phase whose the structure is formed by layers $[UO_2(VO_3)_3]^-$. The layers join per pairs without direct connection between them [1]. At the time of the tests of synthesis of the acid $(H_3O)_2(UO_2)_2V_2O_8$, nH_2O whose derives the carnotites family, a new compound of formula $(UO_2)_3(VO_3)_2$, $5H_2O$ was highlighted. Its structure is constituted by layers $[UO_2VO_4]^-$ interconnected by other uranyls ions UO_2^{2+} and the water molecules [2]. This