telluride. And then the metal atoms are packed between layers of Te atoms to form a sandwich, the adjacent sandwiches are held together by weak van der Waals interaction between Te atoms.

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PS-08.04.24 EXSOLUTION-DERIVED PHASEOUS INHOMOGENEITY OF POLYCOLORED TITANITE CRYSTALS FROM THE KHIBINA ALKALINE MASSIF, KOLA PENINSULA, RUSSIA.

by M.I.Lapina* and B.J.Boroutsky, *Institute of Geology of Ore Deposits, Petrography, Mineralogy and Geochemistry (IGEM), Russia Academy of Sciences, Moscow.*

Unusual crystals of titanite with the black heads have been found in a natrolite vein in rischorrite of the Khibina alkaline massif. The crystals are cuneiform ones with prismatic faces n{111} and t{$\bar{1}$11}, have been studied using detailed microscopic observation, chemical and electron microprobe analyses.

Very narrow range of +2V=26-27° is typical of the studied crystals which is quite different from all other Khibina titanites where 2V varies from 17° to 40°. Black colored spots are located at the sites of "a" axe exits. The crystals were found to have abnormal contents of Nb_2O_5 (5,2-6,7 wt%) as compared to average 1,21% for Khibina titanite. Black colored parts contain also elevated contents of Na_2O (1,6-1,9 wt%) and SrO (0,5-0,7%) but lowered of Fe_2O_3 (0,4-0,5%). Distribution of all elements throughout the black heads is fairly even which was confirmed by electron microscope studies and is suggestive of isomorphous entrance of these impurities into the crystal lattice of titanite perhaps according to the following pattern: $Ca^{2+}Ti^{4+} \rightarrow Na^{+}Nb^{5+}$. In more light colored basal parts of the crystals many alternating lighter and darker bands are seen. The lighter bands contain Nb_2O_5=3,2-3,5%, Na_2O=0,8-1,0%, Fe_2O_3=0,8-1,0% and SrO=0,5%, and the darker ones: Nb_2O_5=3,9-4,9%, Na_2O=1,06-1,2%, Fe_2O_3=0,9-1,2% and SrO=0,3%.

Rare xenomorphic micron-size inclusions of pyrochlore were found within light colored parts of the crystals near the hinter parts of the black heads. The number and size of such inclusions is evidently growing with the rising extent of secondary alterations of the host titanite and the size of pyrochlore grains or grain clusters sometimes is as large as 1 mm. The formation of the pyrochlore inclusions is assumed to be a result of Nb exsolution from Nb-titanite solid solution and subsequent recrystallization.

PS-08.04.25
ON THE STRUCTURE OF II III_2 □ VI_4
SEMICONDUCTING COMPOUNDS.

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There have been conflicting reports on the nature of the space group of a number of II III_2 □ VI_4 semiconductors. These materials have been described in space group $I\bar{4}2m$ as well as $I\bar{4}$:

$I\bar{4}2m$ [D_{2d}^{11}, N° 121]				$I\bar{4}$ [S_4^2, N° 82]			
II	in 2(a)	$\bar{4}2m$	0,0,0	II	in 2(a)	$\bar{4}$..	0,0,0
III	in 4(d)	$\bar{4}$..	0,½,¼	III(1)	in 2(b)	$\bar{4}$..	0,0,½
				III(2)	in 2(c)	$\bar{4}$..	0,½,¼
VI	in 8(i)	1	x,x,z	VI	in 8(g)	.m.	x,y,z

In the present study, a detailed structural analysis of the following materials: $CdAl_2S_4$, $HgAl_2S_4$, $HgGa_2S_4$, $HgAl_2Se_4$, $ZnIn_2Se_4$ and $MnIn_2Te_4$, has been performed. High-quality single crystal x-ray diffraction data published in the literature and collected in our laboratory were used. Particular attention was paid to the behavior of the different structural refinements in which only superstructures reflections were employed. An attempt to establish the possible cation ordering scheme due to order-disorder phenomena was tried in all cases. The intrinsic inability of x-ray diffractometry to distinguish subtle order-disorder details between neighboring elements of the periodic table have been considered throughout the analysis.

PS-08.04.26 THE POSSIBLE QUALITATIVE SFDP-FORMULAS OF THE CHEMICAL ELEMENTS (CE) by O.E.Gorchakova*, N.L.Smirnova, N.I.Kirillova, Department of Chemistry, All-Russian Institute for Scientific and Technical Information, Moscow, Russia

The most lengthly system of CE consists of 32 groups and 7 rows. After giving to every CE the number and group and row, we get the system of numerical binary designations of CE from 11 to Rn 32.6. In the most lengthy system there are four s,f,d,p blocks of CE, including 2,14,10,6 groups. CE within the limits of the block is marked by a 3-signs symbol: the letter of the block, the number of the group within the limits of the block, the number of the row. For example H si1, Ar p66. The third model of the system of CE is generaled by use of 8 numbers of A and B groups: in s-block 1,2, in f-block 3(1-14), in d-block 3,4,5,6,7,8(1-3),1 2, in p-block 3,4,5,6,7,8. In the three of rows are the same. While marking all of the group is omitted. The most general formulas of chemical compounds (CC) are being generaled with four letters sfdp. If the elements within the limits of the block are not distinguished, only 15 formulas of CC

are possible. There are 4 single (s,f,d,p), 6 binary (sf,sd,fd,sp,fp,dp), 4 ternary (sfd,sfp,sdp,fdp) and 1 quadruple (spdf) formulas of CC. There are 69 formulas at all. The sfdp–formulas have been distinguished in minerals and these formulas have been compared with 69 formulas. While correlating the formulas of ionic compounds they were divided into the cationic and anionic parts. The formulas of different ranges have been distinguished.

PS–08.04.27 CRYSTAL STRUCTURES OF BORON NITRIDES DETERMINED FROM X-RAY POWDER DATA. By H. Hiraguchi, N. Sudo*, H. Hashizume, S. Nakano (1) and O. Fukunaga (1), Res. Lab. of Engineering Materials, Tokyo Institute of Technology, Nagatsuta, Midori, Yokohama 227, Japan. (1) Dept. of Inorganic Materials, TIT.

The crystal structures of magnesium boron nitride Mg_3BN_3 in the low- and high-pressure forms have been determined *ab initio* from X-ray powder data. The powder patterns were decomposed to estimate individual reflection intensities, which were used to calculate Patterson functions and build try-and-error structure models. The obtained structure parameters were refined by the Rietveld method. 54 and 21 reflections were used to solve the structures of $Mg_3BN_3(L)$ and $Mg_3BN_3(H)$ respectively. Low-pressure $Mg_3BN_3(L)$ has a hexagonal cell (space group $P6_3/mmc$, $Z = 2$) with $a = 3.54453(4)$ and $c = 16.0353(3)$ Å while the high-pressure $Mg_3BN_3(H)$ cell is orthorhombic ($Pmmm$, $Z = 1$) with $a = 3.0933(2)$, $b = 3.1336(2)$ and $c = 7.7005(5)$ Å. The two structures commonly include linear N–B–N molecular anions, considered to play a role in the catalytic property of the material in the reaction converting hexagonal boron nitride into a cubic form at high pressure-temperatures. A 2 % shorter B–N interatomic distance was observed for $Mg_3BN_3(H)$.
Applications of standard direct methods to the $Mg_3BN_3(L)$ intensity data resulted in a very similar structure. High-quality electron density maps have been calculated for this form using the maximum-entropy method with phased structure factors. A separate application of maximum-entropy multisolution program (C. Gilmore *et al.: Acta Cryst.* A47, 830 (1991)) to the unphased structure factors yielded quite a similar map in support of the determined structure of $Mg_3BN_3(L)$.

A structure solution from $Sr_3B_2N_4$ X-ray powder data will also be reported.

PS–08.04.28 S_8 : A NEW LOOK AT AN OLD STRUCTURE. By Robin B. English, Department of Chemistry, Rhodes University, South Africa.

The crystalline structures of monoclinic and orthorhombic S_8 are explored using the Dirichlet domain construction.

PS–08.04.29   TWO-PHASE K-NA FELDSPAR STRUCTURE FROM SICHOTE-ALIN.   By N. I. Organova*, I. M. Marcille, I. V. Roshdestvenskaja, N. D. Zacharov, Y. A. Nistratov, Institute of Ore Deposits, Petrology, Mineralogy and Geochemistry of RAN, IKRAN Moscow, LNPO "Burevestnik" St. Petersbourg, Russia.

$Or_{62}Ab_{36}An$ is a result of exsolution and consists from K and Na components. For monoclinic K-phase there are a = 8.542(1), b = 13.0123(19) c = 7.182(10), β=116.054(8).
Refinement with massiv from 1091 reflections has been carried out to R = 2.7%. The values of some interatomic distances are: Si-O_1 1.648(1), Si_1-O_3 1.642(1), Si_1-O_4 1.649(1), Si_1-O_5;
   Si_2-O_2 1.638(1), Si_2-O_3 1.626(2), Si_2-O_4 1.637(1), Si_2-O_5 1.633(1).
Refinement of alkaline occupancy lead to 0.81K+0.19Na for 159 reflections with $\sin\theta/\lambda < 0.5$. Triclinic Na-phase is a periodic polysynthetic periclinic twin with $A = 14a_{Ab}$, what corresponds the TEM observations.

PS–08.04.30
DETERMINATION OF IRON VALENCE IN NATURAL MAGNETITES AND GARNETS BY EPMA.   A. By I. P. Laputina*, O. V. Polozova, Institute of Geology of Ore Deposits, Petrography, Mineralogy and Geochemistry {IGEM} Russian Academy of Sciences, Moscow, Russia.

The influence of various valence states of transition elements in chemical compounds on the L-emission spectra is well known. We have shown in earlier papers that the structural-chemical state of iron atoms in natural oxides, silicates and sulphides is exhibited in x-ray emission spectra of $FeK\alpha_{1,2}$ by distinct shifts of the wavelengths and of the band profiles as well as in changes of peak/integral intensity ratio [1].

In this study we attempted to determine the Fe valencies in natural Fe-spinels and garnets by EPMA. Crystal-chemical feature of Fe-O system, possibility of wide exchange between octahedral and tetrahedral sites for Fe^{2+} and Fe^{3+} and Fe^{3+} in different physico-chemical environments make this system very important in the investigations of natural processes, because magnetite and Fe-spinels are often throughgoing minerals formed during several stages of mineralization.

Optimum conditions of investigations have been defined. The measurements were performed at high voltage E=10 kV, i= 100 nA, t=50℃, using crystal-monochromator KAP and anti-contamination.

By measuring x-ray intensity FeL_β/L_α in standard natural ferrous oxides with known Fe^{2+}/Fe^{3+} ratios, three characteristic trends with corresponding crystal-chemistry feature were established : 1. for haematite-magnetite-wustite, 2. for haematite-ilmenite, 3. for magnetite- Ti-magnetite- ulvospinel-ilmenite and 4. for natural garnets of the series almandine-andradite. Based on these results, the equations for a quantitative determination of Fe^{2+} and Fe^{3+} were found. Having determined the intensities of FeL_α and FeL_β and total concentration of iron by EPMA, we designate :