

vertices and through the edges,  $[\text{OCu}_{2.5}]_{\infty}^{3+}$  ( $\text{Cu}_5\text{O}_2(\text{PO}_4)_2$ ); layers of six-fold rings formed by tetrahedra connected through the vertices with variable up and down orientation of free vertices,  $[\text{OCu}_{1.5}\text{Pb}]_{\infty}^{2+}$  ( $\text{Pb}_2\text{Cu}_3\text{O}_2(\text{NO}_3)_2(\text{SeO}_3)_2$ ); layers of fedotovite couples connected through the common vertices,  $[\text{OCu}_2]_{\infty}^{2+}$  (dolerophanite  $\text{Cu}_2\text{O}(\text{SO}_4)$ ); frameworks  $[\text{OCu}]_{\infty}^{\infty}$  (tenorite  $\text{CuO}$ ),  $[\text{OCu}_2]_{\infty}^{\infty}$  (cuprite  $\text{Cu}_2\text{O}$ ) and frameworks of cuprite type in  $\text{Cu}_2\text{O}$  ( $\text{SeO}_3$ ).

The average length of the bond O-Cu in the tetrahedron  $[\text{OCu}_4]$  increases from 1.916 Å for free vertices to 1.940 Å for vertices common to two tetrahedra, and 1.96 for vertices common to four tetrahedra (tenorite). Angles of bonds Cu-O-Cu take values mainly in the interval of 95-125°.

Tetrahedra  $[\text{OCu}_4]$ , polyions and compounds containing these tetrahedra may be formed from volcanous gases, self-igniting dumps of coal basins, blast furnaces and oxygen converters, and from the liquid phase in hydrothermal and other processes. Such complexes can preserve information on the structure of crystallization environment.

## PS-08.04.34

## LATTICE MISFIT IN MICAS AND THE GROWTH BENDING PROBLEM.

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The origin of micas with sphere bending of basal plane is part of the general problem of growth curvature of crystals. Complex investigation of phengite-muscovite from Urals amazonstone pegmatites has been performed to find out the connection between mica bending and chemical deformation of crystal lattice.

Goniometer research has shown sharp oscillations of crookedness in growth direction of crystals, with a trend diverging from the law of inheritance of crookedness. Geometry of bending and degree of deformation are different in various growth sectors for faces of various simple forms. This is the evidence of growth origin of bending and also of changeability of bending factor with time.

Variations of cell dimensions within the volume of the crystal have been determined by the X-ray powder diffraction method. They have been compared with local changes of chemical composition obtained by microprobe analysis. Linear correlation of lattice parameters (a and b) with iron content and of  $d_{001}$  with rubidium content has been found. Some increase of the parameter and  $d_{001}$  in growth sector (110) in comparison with those (001) sector has been revealed. Cation composition and lattice parameters of investigated crystals vary strongly within the crystal. The most significant variations have been observed for b parameter and estimated to be 1% of the mean value.

Data received prove the existing hypotheses to be insufficient. High polytype homogeneity ( $2M_1$ ) of crystals excludes bending because of coherence syntactic coalescence of polytypes. Random character of cell dimensions variations excludes the existence of constant moment on growth front. However existing differences in lattice parameters are sufficient for formation of mosaic structure. Mosaic structure of (110) growth sector confirms this proposal. A new mechanism of the bending of crystals is being sug-

gested. The bending of crystals is the consequence of geometrical selection of systematically misorientated blocks, derived by lattice misfit strains.

## PS-08.04.35 ESTIMATION OF HYDROTALCITE IN SERPENTINITES BY X-RAY DIFFRACTION AND IR SPECTROSCOPY.

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The amount of hydrotalcite  $\text{Mg}_3\text{Al}_2(\text{OH})_{16}\text{CO}_3\cdot 4\text{H}_2\text{O}$  (HT) in serpentinite is of importance since it is responsible for many properties of this material, as well as being acid absorbent and catalyst carrier of practical use in cement and metal corrosion technology, for studies of different geological processes. The determination of HT in natural mixtures by XRD is beset with problems of X-ray amorphous serpentinite, of preferred orientation and disorder in minerals. These reasons prevent to use the X-ray method alone to estimate HT content in mixtures, because often more than one crystal type—usually several serpentinite and other minerals—is present (Moroz T., Arkhipenko D., Geol. Geophys., 1991, 2, 58). The development of a simple and convenient IR spectroscopic method for quantitative determination of HT in serpentinite is based on measurements of the relationship between intensities of  $\nu_3$  vibrations of  $\text{CO}_3$  ions (at  $1375\text{ cm}^{-1}$ ) and  $\nu$  Si-O(Si), Si-O(Mg) vibrations (at  $980\text{-}1060\text{ cm}^{-1}$ ), the former being absent in serpentinite, the latter in HT. Calibration is required by another established method (DTA, microchemistry) and the accuracy of the calibration is  $\pm 10\%$ . The intensity and position of carbonate-related absorption defines the amount of interlayer carbonate and the local environments of the anions, and gives information about the cation order-disorder in octahedral sheets. The method appears to be applicable to crystallochemical estimation of natural HT from different deposits in mixture with chlorite and talc, for checking on the separation of fine fraction and determination of structural regularities of hydrotalcite after T, P-treatment.

## PS-08.04.36 STRUCTURAL PECULIARITIES OF PHASE TRANSITION ANATASE - RUTILE.

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In nature there are 3 polymorphic modifications of  $\text{TiO}_2$ : anatase -  $D_{2h}^8$ ,  $z=4$ , brookite -  $D_{2h}^8$ ,  $z=8$ , rutile  $D_{2h}^8$ ,  $z=2$ . It is known that anatase and brookite on heating transform to rutile. Methods of X-ray diffraction and vibration spectroscopy have been used. X-ray anomalous intensities ("AnI") of different hkl - reflections depending on temperature and heating conditions have been observed. The differences have been registered in IR and Raman-laser spectra as well. Lab IR - study of sorption of oleic acid on anatase, brookite and rutile structures showed essential differences. On the other hand X-ray analyses of samples of anatase and rutile from agold deposit registered "AnI" also; "markings" of phase transition: bipyramidal anatase forms were substituted by rutile. Samples of rutile with "AnI" from differ-