

## 08.4-15 THE X-RAY CHARACTERISTICS OF TAUSONITE, A NEW MINERAL OF THE PEROVSKITE GROUP

G.G.Afonina, A.N.Sapozhnikov, E.I.Vorobiev,  
A.A.Konev, I.U.V.Maishonok.

A.P.Vinogradov Institute of Geochemistry, USSR

Tausonite,  $\text{SrTiO}_3$ , is of a perovskite type, its unit cell is primitive, cubic, space group  $\text{Pm}\bar{3}\text{m}$ . The single-crystal study does not reveal supplement reflection, which could indicate a pseudo-cubic symmetry of this mineral. The powder data from a diffractometer (DRON-3,  $\text{CuK}\alpha$  - radiation) are identical to those of a synthetic  $\text{SrTiO}_3$ . The double-line  $\alpha_1$ - $\alpha_2$  is solving well, the halfwidth of reflections is comparable to that of quartz in close regions  $2\theta$ . The lattice parameters were obtained from a least-square refinement -  $3.9048(1)\text{\AA}$ . Taking into account the "ideal" cubic structure of tausonite, unit cell parameters help calculate the distance between atoms. The atom Sr is coordinated with 12 atoms O, and the Sr-O distance is  $2.761\text{\AA}$ . The atom Ti is coordinated with 6 atoms O, and the Ti-O distance is  $1.952\text{\AA}$ . Evidently tausonite is the first natural mineral in which the Ti-octahedra have the highest symmetry  $\text{m}\bar{3}\text{m}$ .

08.4-16 ON THE SIGNIFICANCE OF THE PHASE SIZE EFFECT FOR UNDERSTANDING THE PHENOMENA OF POLYMORPHISM AND POLYTYPOISM IN MINERAL CRYSTALS. By V.L.Tauson and M.G.Abramovich, A.P.Vinogradov Institute of Geochemistry, Irkutsk, USSR.

Considering the phase equilibria and thermodynamic properties of the small crystalline particles seems to be of great interest for mineralogy and crystallography since many of the minerals may occur in a dispersed state or indeed have passed through a microcrystal stage during their growth history. From the surface chemistry-state point equations are derived which describe the relationship between the shift of polymorphic equilibrium temperature and characteristics of size, habits and surface properties of crystals. These show a possibility for the phase size effect (PSE) in mineral crystals, that is to say the dependence of a phase transition point upon the crystal size. Experimental evidence for PSE in dispersed phases of ZnS and HgS is obtained. It is shown that the influence of crystal size on the  $3\text{C} \rightarrow 2\text{H}$  tran-

sition in ZnS, at temperatures much lower than  $1293\text{ K}$  (transition point in the bulk) is caused by the difference in specific surface free energies between  $3\text{C}$  and  $2\text{H}$ , being about  $0.2\text{ J/m}^2$ . The variations of the  $\alpha$ - $\beta$  transition point in HgS under annealing is presumed to be connected with the different particle size as well. The crystal polytypism could also be connected with the peculiarities of phase equilibria of small crystalline particles. From this an original mechanism for ZnS polytypes and microtwins formations in natural environments is proposed. It is based on the conception of PSE and presupposes the spontaneous accommodation of structure to the crystal size, constantly enlarging during the growth stage. The physicochemical consideration of the ZnS polytypism allowed to suggest the preference of structures having a higher percentage of cubic packing especially at elevated temperatures of the ore formation. The pure  $2\text{H}$ -form could preferably occur under low temperature conditions.

08.4-17 ON THE STRUCTURAL RELATIONSHIP BETWEEN TWO POLYMORPHS OF  $\text{Pb}_4\text{SO}_4(\text{CO}_3)_2(\text{OH})_2$ . By R.M. Highcock, G.W. Smith and M.E. Vickers, BP Research Centre, Sunbury-on-Thames, Middx.

Two minerals with the above formula have been found at Leadhills, Scotland. They have been named leadhillite, which is monoclinic, space group  $\text{P}2_1/\text{c}$ ,  $a = 11.582(2)\text{\AA}$ ,  $b = 20.809(3)\text{\AA}$ ,  $c = 9.111(3)\text{\AA}$ ,  $\beta = 90.48^\circ$ ,  $Z = 8$  and macphersonite, orthorhombic, space group  $\text{Pbca}$ ,  $a = 9.227(2)\text{\AA}$ ,  $b = 23.048(5)\text{\AA}$ ,  $c = 10.368(4)\text{\AA}$ ,  $Z = 8$ . Both structures have been solved by direct methods from single-crystal diffractometer data. The severe effects of strong absorption ( $\mu = 618\text{ cm}^{-1}$ ) have been investigated by applying semi-empirical, numerical and DIFABS correction procedures but the limitations inherent in all three methods have restricted refinement of the structures.

There are structural similarities between the two polymorphs. Both have alternating layers of carbonate and sulphate groups sandwiching the lead ions which are bridged by the hydroxyl groups. The difference between the structures lies in the relative positions of the cation and anion groups. A third polymorph, susannite also exists but so far good crystals are not available.