C – 252 08. INORGANIC AND MINERALOGICAL CRYSTALLOGRAPHY

08.4-24 CRYSTAL CHEMISTRY OF SYLVANITE AND KRENNERITE. By F.Pertlik, Institut für Mineralogie und Kristallographie der Universität Wien, A-1010 Wien, Austria.

The crystal structures of the minerals sylvanite, AuAgTe₄, (TUNELL, G., Am.Min.<u>26</u>, 457, 1941) and krennerite (<u>Au</u>, Ag)Te₂, (TUNELL, G., MURATA, K.J., Am.Min.<u>35</u>, 959, 1950) were redetermined using single crystal X-ray data. Three dimensional data were collected on a Weissenberg type diffractometer (MoK \propto radiation, sin $2/\lambda = 0.7$ R⁻¹).

Sylvanite has a stoichiometric composition and an ordered crystal structure. The Au atom is surrounded by six Te atoms in a [4+2] coordination, around the Ag atom also six Te atoms are arranged, but in a [2+2+2] coordination. These polyhedra are combined via common Te-Te edges to planar sheets, which are connected by Te₂ dumbbells (Te-Te = 2,82 \Re) to a network.

Within the structure of krennerite, two of the three crystallographic different metal positions are occupied by (Au, Ag)atoms (ratio 75:25) in a [2+2+2] coordination by Te atoms. The third position is occupied by an Au atom in a typical [4+2] coordination. The three different polyhedra of the metal atoms are combined via common edges to wavelike sheets. These sheets are connected by Te₂ dumbbells (Te-Te = 2,86 Å) and Te₃ groups (Te-Te = 2,88 Å 2x). Krennerite is the first representative for a Te₃ group in crystal chemistry of minerals. The formula can be written as follows:

(Au_{2-x}Ag_x)Au₂[Te₃][Te₂]₂[Te]; x~0,75

 $08.4{-}25$ A SUBSTRUCTURAL STUDY ON HOKUTOLITE. By C. J. Chan and S. C. Yu, Department of Earth Sciences, National Cheng Kung University, Taiwan, Republic of China.

Single crystal X-ray diffraction study indicates that the hokutolite crystal has an orthorhombic symmetry with a space group of Pnma, identical to that of barite. Internal defect substructures were analyzed with X-ray and electron diffraction techniques. The results along with composition analysis suggest that the hokutolite crystal contains a large number of coherent single crystal domains. Each domain is approximately 1 µm in dimension. Mismatch in the crystallographic axes resulted from the variation in unit cell parameters, which orginated from the composition fluctuation, produces the diffused diffraction effect for both X-ray and electron diffraction measurements. Electron microprobe analyses show that the extent of the solid solution for hokutolite is limited between (Pb $_{.20}$ Ba $_{.80}$)SO₄ and (Pb $_{.35}$ Ba $_{.65}$)SO₄.

The accuracy in the determination for the range of the solid solution in hokutolite is confined by the small size of the coherent domain.

The present study indicates that the hokutolite crystals were crystallized in an unstable geological environment, which is consistent with the field observation. It is speculated that the zoning structure in hokutolite might be intimately correlated to the eruption cycles of the andesitic rocks in this area; which modify the bulk composition of the source material, flow rate of the hydrothermal solution, its pH value, temperature and etc. 08.4-26 NEUTRON AND X-RAY DIFFRACTION STUDIES OF NATURAL ZEOLITES. By S.A. Miller, T.W. Hambley and J.C. Taylor, Energy Chemistry Division, C.S.I.R.O., Lucas Heights Research Laboratories, P.M.B.7, Sutherland, N.S.W., 2232, Australia.

Single-crystal neutron diffraction studies have been carried out on an Australian stellerite, $Ca_{3-9}Na_{0-1}$ [Al_{8·3}Si_{27·7072}]24.9H₂O, (Fmmm, R=0.12, 1015 unique hkl), an Australian heulandite, Ba_{0·1}Ca_{2·2}Na_{1·4}Sr_{0·1} [Al_{7·9}Si_{28·5072}]24.5H₂O, (C₂/m, R=0.06, 1440 hkl), partially dehydrated heulandite (C₂/m, R=0.08, 1312 hkl) and a Scottish harmotome, Ba_{2-X}_X[(Si,Al)₁₆₀₃₂] 12H₂O (in B22₁2 R=0.13, 1483 hkl). The disordered water oxygen distribution in stellerite agrees with the X-ray study of Galli (Bull. Soc. Fr. Min. Crist., 98, 11(1975)), and the neutrons show disordered H with $\overline{O-H}$ pointing away from Ca⁺⁺ (at the center of a water cage), the H⁻⁻interacting weakly with framework and water O. In heulandite the cations bond to framework and water O, and the water shifts in heulandite. The harmotome shows a more ordered channel content. Three-dimensional X-ray data on Na, K and Ag - exchanged stellerite are being refined. Parallel neutron powder studies of stellerite at various stages of dehydration are in progress.

08.4-27 POSSIBLE USE OF BIOTITE MORPHOLOGY FOR A COMPARISON OF ANDESITES. By <u>M.Balan</u> and P.Andăr,Institute of Geology and Geophysics, 1 Caransebeş Street,Bucharest 78344,Romania.

Neogene volcanic rocks of the Săcărîmb region contain biotite phenocrysts. Ng=1.65-1.69 . Regular hexagon and polygons with four, five or six sides of all sizes are shapes of the biotite plates. The average of the six $|(a_1+a_2+a_3+a_4+a_5+a_6):6-a_1|$ deviations from the ideal hexagonal shape (an is the side of a hexagon) gives the medium deviation in millimeters. The ratio of this value to the length of the hexagon's medium side, multiplied by 100, is the medium deviation of a crystal per cent. Results: 19.2(Xa) or 15.6(Mo) for 885 crystals from Cetras quartz andesites and 19.4(Xa) or 17.3(Mo) for 2768 crystals from Săcărîmb quartz andesites. The sequence of some andesite-forming minerals may be this: apatite, zircon, ilmenite, magnetite, biotite, hornblende, diopside, allanite. In the biotite period the crystallization conditions were probably similar for the two andesite types.