relaxation behaviour of the scattering phenomenon have been studied in detail.

α-lithium iodate is a quasi 1-dimensional ionic conductor whose carriers are interstitial Li ions and Li vacancies (Zhang An-dung et al., Acta Physica Sinica (1980) 29, 1158). The local deformation of the crystal takes place when the carriers are migrating under the action of a dc field. The fluctuations of the strain in the crystal cause fluctuations of the optical axis. The thermal average values of the dielectric tensor element ϵ_{xz} and ϵ_{yz} are non-zero and have spatially periodic distribution (caused by defects). Therefore, the abnormal scattering of light will be produced (P. G. de Gennes, The Physics of Liquid Crystals, sec. 3.4).

oxygen in the spinel-block and the occupation of the crystallographic site varies from 0.17 at low temperature to 0.10 at 620K.

Other hydrogens are strongly delocalized in the conduction region, forming long (O-H)-lengths (1.73 Å) ; no definite evidence of the existence of an H_3O^+ entity has been found during this structural study. At the higher temperature, there are less hydrogen atoms and their thermal vibration amplitudes are large, so that it becomes more difficult to locate them precisely. However, some of these hydrogens seem to be distributed around the oxygen which links the spinel-blocks together.

These results emphasize the possibility that the delocalized hydrogens participate in the conduction mechanism.

07.3-04   TEMPERATURE DEPENDENCE OF THE HYDRATED HYDROGEN β″-ALUMINA STRUCTURE BY NEUTRON DIFFRACTION STUDY. By M. Anne and D. Tranqui, Laboratoire de Cristallographie, C.N.R.S., 166X, 38042 Grenoble Cedex, France, and W. L. Roth, General Electric Research and Development Center, P.O. Box 8, Schenectady, NY 12301 U.S.A., and M. S. Lehmann, I.L.L., 156X, 38042 Grenoble Cedex,France.

Following previous conductivity measurements, quasielastic neutron scattering and thermal gravimetric analysis on hydrated hydrogen β″-alumina, a neutron diffraction study on a single crystal has been undertaken. The interesting physical properties of this compound called for a precise structure analysis. Hydrated hydrogen β″-Alumina exhibits a protonic conduction (10^{-5}ohm^{-1}cm^{-1} at room temperature) much higher than that of the β-phase (10^{-11}ohm^{-1}cm^{-1}) (G.C. Farrington and J.L. Briant, Fast Ion Transport in Solids, North Holland, New York, 1979), and the composition is relatively stable up to about 500K. Quasielastic neutron scattering has confirmed these results. To obtain further details of the location and number of the protons, neutron diffraction data for hydrated hydrogen β″-alumina were collected at three temperatures : 110K, 300K and 620K.

The compound is rhombohedral, space group R3̄m, and the lattice parameters in the hexagonal unit cell are :
T = 110K ; a = 5.625(4) Å ; c = 34.182(36) Å
T = 300K ; a = 5.626(8) Å ; c = 34.234(34) Å
T = 620K ; a = 5.630(13)Å ; c = 33.852(47) Å

Thermal gravimetric analysis shows that approximately 64% of H$_2$O is weakly bound and desorbed at 580K (W.L. Roth, M. Anne, D. Tranqui and A. Heidemann, Fast Ion Transport in Solids, North Holland, New York, 1979) ; this is consistent with the important decrease of the c-parameter between room and high temperature.

At low temperature, the composition found by neutron diffraction is 1.64H$_2$O-0.49MgO-5.18Al$_2$O$_3$ per spinel-block.

Essentially, one hydrogen atom is covalently bonded to an

07.3-05   NEUTRON AND X-RAY STUDIES FOR Na$^+$β″ ALUMINA STABILIZED WITH Mg^{2+} OR WITH Mg^{2+}-Li$^+$. By D. Tranqui and M. Anne, Laboratoire de Cristallographie, C.N.R.S., 166X, 38042 Grenoble Cedex, France, and W. L. Roth and B. Dunn, General Electric Research and Development Center, P.O. Box 8, Schenectady, NY 12301 U.S.A.

Measurements of conductivity versus temperature for Na$^+$β″ alumina stabilized with Mg^{2+} or with mixed Mg^{2+}-Li$^+$ have shown significant difference between the two compounds : The Ln(σT) plot for the mixed compound consists of two straight lines with activation energies of 0.16 eV below 135°C and 0.10 eV above this temperature whereas that of the Mg^{2+} stabilized is nearly constant (0.32 eV) below 135°C and decreases smoothly to reach ∿ 0.10 eV at 390°C. It has also been observed that the conductivity of the mixed phase is slightly higher than that of the Mg^{2+} phase, at least in the low temperature range.

Mg^{2+} and Mg^{2+}-Li$^+$ stabilized Na$^+$β″ alumina are rhombohedral, space group R3̄m with the following a and c hexagonal unit cell parameters :
a = 5.625 Å ; c = 33.601 Å for Mg^{2+}, Na$^+$β″ alumina
a = 5.616 Å ; c = 33.726 Å for Mg^{2+}-Li$^+$, Na$^+$β″ alumina.
Both X-Ray and neutron diffraction data at room temperature indicated that the average bond length Al-O of the tetrahedral site Al(2) in the spinel block is significantly longer (1.849 Å) than that in the Mg^{2+}-Li$^+$ stabilized phase (1.839 Å) suggesting that the Al(2) site occupancy (by Al^{3+}, Mg^{2+} and Li$^+$) has been modified by Li$^+$ insertion. However the lithium positions are still unkown. Further neutron data refinements are underway in order to determine their location.

On the other hand the Na$^+$ concentration in the conduction plane is much higher (0.34) in the Mg^{2+}-Li$^+$ compound than in the Mg^{2+} compound (0.28).

Thermal expansion measurements of unit cell constants from room temperature to 450°C have shown a strikingly different behaviour between the two compounds : all para-

meters ($\underline{a}$ and $\underline{c}$) increase monotonically with increasing temperature but the $\underline{c}$ axis of the Mg^{2+}-Li^+ compound decreases rapidly between the temperature range $100°$-$220°C$ and starts to increase above $220°C$.

As yet there are not convincing proofs as to whether the anomaly in the thermal expansion should be attributed to phase transition as suggested by conductivity data or to a desorption of water from the interblock plane.

envisaged as associated in equal proportion in $H_5O_2^+$ and H_4O_2 dimers and this suggests a possible mechanism for proton conduction which can be probed by quasielastic neutron scattering.

For the single crystal neutron diffraction study of $Sr(Pr)Cl_{2.10}$ ($\lambda=0.53Å$) it is demonstrated that the anion interstitials are of two types: ($\frac{1}{2}vv$) $v\approx0.38$ and (xxx) x=0.285. The ratio of ($\frac{1}{2}vv$) interstitials to dopant cations is about 2.5. In contrast to the alkaline-earth fluorides, (www) $w\approx0.42$ or 0.38 interstitials are not important in this system. Defect energy calculations on anion-excess strontium chloride suggests that the clusters proposed for the alkaline-earth fluorides are less important for $SrCl_2/MCl_3$. Clusters based on the aggregation of <111> cation substitutional/anion interstitial pairs provide a more favourable mode of defect cluster formation. A cluster model based on this type of aggregation provides a good model for our observed ratio of anion interstitals to dopant cations but does not explain the observed proportion of anion vacancies.

07.3-06   NEUTRON DIFFRACTION STUDIES ON FAST ION CONDUCTORS (I) DUO_2ASO_4 $4D_2O$ and (II) $Sr(Pr)Cl_{2.10}$. By P.J. Bendall[i], C.R.A. Catlow[ii], B. E. F. Fender[iii] and A. F. Wright[iii].

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Neutron diffraction studies are reported on two different types of fast ion conductor. In one, high resolution powder diffraction techniques are employed to detect hydrogen ordering effects and occupancies in the good proton conductor $DUO_2ASO_4 4D_2O$; in the other, a high resolution single crystal investigation has been used to accurately locate the chloride ion positions in the anion excess fluorite system $Sr(Pr)Cl_{2+x}$.

The isostructural layered hydrates $HUO_2PO_4 4H_2O$(HUP) and $HUO_2ASO_4.4H_2O$ (HUAS) display high proton conductivities near room temperature (A. T. Howe and M. G. Shilton, J. Solid State Chem. (1980), 34, 149). Profile analysis of $DUO_2ASO_4 4D_2O$ above the transition temperature of $290 \pm 3°K$ was carried out in the space group $P4/ncc$ with a = 7.160 and c = 17.634. The structure of DUAs is very similar to HUP, with planar networks of water molecules alternating with layers of $\{UO_2PO_4\}_n^{n-}$. The neutron diffraction study shows (i) only one of two crystallographically distinct sites in a square of water molecules is occupied by hydrogen atoms and the occupancy is $3/4$; (ii) the hydrogen atoms directed towards the oxygen of an ASO_4^{3-} group are linked to the oxygen of a water molecule; (iii) the remaining hydrogen atoms (8 out of 36) are associated with a single maximum in scattering density midway between two oxygen atoms of water molecules in neighbouring water layers. The water molecules can thus be

07.3-07   STRUCTURE INVESTIGATIONS IN FAST IONIC CONDUCTORS. By H. Schulz, MPI Festkörperforschung, 7 Stuttgart 80, Germany.

In fast ionic conductors one sort of ions may move rapidly through the crystal lattice. The densities of these ions are often distributed over large parts of the elementary cell. The smeared out densities are caused by shallow atomic potentials. These potentials are (at least in distinct directions) so flat, that already thermally activated ions may show large thermal vibrations or jump from their site into a neighbouring site.

The thermal vibrations of these ions may be analysed by so-called anharmonic temperature factors. The corresponding probability density maps can be calculated by the Fouriertransform of the anharmonic temperature factors. These pdf maps can then be used to determine the atomic potentials of the ions under consideration.

We have used these formalisms for the first time up to the sixth order. Furthermore, we could show that temperature factors based on the Gram-Charlier expansion work much more effective than those based on the Edgeworth expansion, which has been used earlier for this type of structure investigation of fast ionic conductors. These calculations were carried out with the program system Prometheus, which allows the refinements of anharmonic temperature factors based on the above mentioned formalisms.   (Zucker, Perenthaler, Kuhs, Bachmann, Schulz, J. Appl. Crystal., submitted)