

tures of $K_2Cd_2(SO_4)_3$ (Abrahams et al., J. Chem. Phys., (1978), 68, 1926) and $K_2Mn_2(SO_4)_3$ (Yamada et al., J. Phys. Soc. Japan, (1981), 50, 909) also exhibit the same tendency.

Diffuse scattering in all these compounds indicates the appearance of transversal elastic deformation waves parallel to the cubic axes. It has only a slight temperature dependence and reveals no abrupt changes near the structural phase transition $P2_13 - P2_12_12_1$ in $K_2Cd_2(SO_4)_3$.

08.4-31 COMPUTER SIMULATIONS OF THE STRUCTURAL AND PHYSICAL PROPERTIES OF THE POLYMORPHS OF Mg_2SiO_4 . By G.D.Price, Department of Geology, University College London, Great Britain, and S.C Parker, Department of Physical Chemistry, Cambridge University, Great Britain.

The aim of the work presented is to develop a computer simulation technique which will predict the structural and physical properties of forsterite, and ringwoodite, the major Earth-forming polymorphs of Mg_2SiO_4 . The technique is based upon energy minimization, in which all structural parameters are varied until the configuration with the lowest energy is achieved. The lattice energy and physical properties (e.g. elasticity and dielectric constants) are calculated from interatomic potentials, which include electrostatic and short-range terms. We investigate several types of traditional potential models, and present a new type of model which includes partial ionic charges and a Morse potential to describe the effect of covalency on the Si-O bond. This new form of potential model is highly successful, and not only reproduces the zero-pressure structural, elastic and dielectric properties of forsterite and ringwoodite, but also accurately describes their pressure dependence. In addition, the structure and energetics of the beta-phase polymorph, wadsleyite, and other spinelloid polytypic modifications of Mg_2SiO_4 have been investigated, and interpreted in terms of the relative magnitudes of the interaction energies between first, second and third neighbour structural modules. The results of this investigation shed light upon the possible mechanisms of deformation of ringwoodite and wadsleyite, and the rheology of the transition zone of the Earth's mantle.

08.4-32 CORRELATIONS BETWEEN Si-O BOND LENGTH, Si-O-Si ANGLE AND STATIC AND DYNAMIC DISORDER IN SILICA - AN EMPIRICAL METHOD TO CORRECT Si-O BOND LENGTHS. By F. Liebau, Mineralogisches Institut der Universität, 2300 Kiel, Germany.

Silicon-oxygen distances in silicates obtained from X-ray diffraction measurements, $d^x(\text{Si-O})$, have been correlated with the coordination number of oxygen, electrostatic bond strength and Si-O-Si angle (e.g. Baur & Ohta, Acta Cryst. (1982) B 38, 390). However, only 9 percent of the variation of $d^x(\text{Si-O})$ in SiO_2 polymorphs were explained by these authors indicating that one or more parameters have been ignored.

These $d^x(\text{Si-O})$ values are only apparent bond lengths. The real bond lengths, $d^{\text{real}}(\text{Si-O})$, are affected by various factors. The most important of these factors is the temperature factor obtained in the structure refinements, which accounts for both the influence of thermal motions and of static disorder.

Based on 25 structure determinations (performed at various temperatures) with 85 individual Si-O bonds of SiO_2 frameworks in clathrasils (Gies et al., Angew. Chem Int. Ed. Engl. (1982) 21, 206; Gies, Z. Krist. (1983) 164, 247) and in silica polymorphs the following regression equations have been derived:

$$\begin{aligned} [d^x(\text{Si-O})]_{\text{ind}} &= 1.6157 - 0.0070(6) [B(O)]_{\text{ind}} \text{ and} \\ [d^x(\text{Si-O})]_{\text{ave}} &= 1.6220 - 0.0075(11) [B(O)]_{\text{ave}} \text{ (Fig.)}, \end{aligned}$$

where ind and ave represent the individual and the average over all oxygen atoms of the structure respectively. These equations explain 63 and 67 percent of the total variation of the $d^x(\text{Si-O})$ values respectively.

With the aid of the equation $[d^{\text{real}}(\text{Si-O})]_{\text{ind}} = [d^x(\text{Si-O})]_{\text{ind}} + 0.007 [B(O)]_{\text{ind}}$ experimental Si-O distances can be corrected for dynamic and/or static disorder into real bond lengths.

For the present, the latter equation should be applied only to SiO_2 frameworks until it has been proved that the slope of 0.007 holds for bridging Si-O bonds in other silicates as well. It might be expected that a substantially different correction factor has to be used for terminal Si-O bonds. In any case, experimental Si-O distances should be corrected for disorder before reliable crystal chemical conclusions are drawn.

Corresponding correlations between the Si-O-Si angles and $B(O)$ have also been obtained.

