

The structure of phosphate glasses

Details of the P-O bonds and of the Me-O first-neighbour distances in different series of phosphate glasses (Me stands for the modifier metal atom) have been studied. Two different P-O bonds occur in the PO_4 units whose frequencies and lengths change with the specifics and fraction of modifier oxide. The Me-O distances of many Me form highly asymmetric

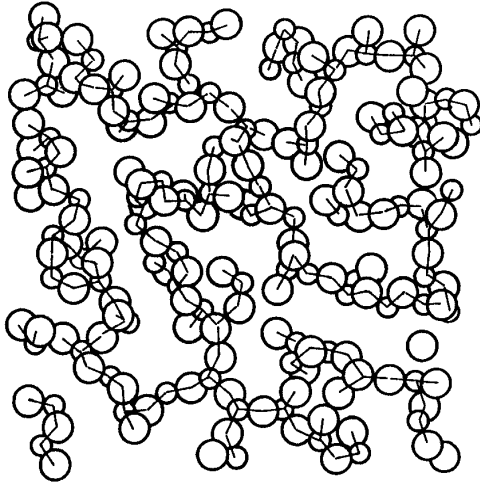


Fig. 1: A slice of the model of $v\text{-P}_2\text{O}_5$. The P atoms and the bridging oxygens are illustrated by the small and large circles, respectively. The terminal oxygens are not shown for clarity.

distributions. For strong scatterers such as Pb, La, Ba, Sr, the Me-Me and Me-P correlations can be extracted from the X-ray scattering data. The combination of the X-ray and neutron scattering data applying the reverse Monte-Carlo simulation yields a suitable approach to the intermediate range order in order to obtain Me-Me, Me-P and P-P pair correlations. The first features of the scattering functions (main maxima, prepeaks) are related with definite distances in these correlations, for example, the prepeak in the X-ray scattering data of the LaP_3O_9 glass is attributable to La-La distances of 0.64 nm.

Magnesium and zinc phosphate glasses with compositions covering the entire glass forming range have been examined by X-ray and neutron diffraction (WAXS, WANS) and ^{31}P magic

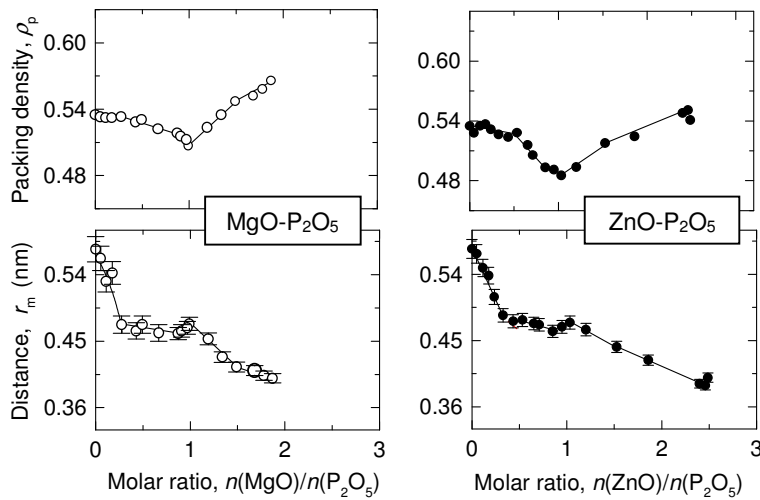


Fig. 2: The composition dependence of the packing density, ρ_p , and the real-space distance, $r_m=7.7/s_m$, determined from the position of the main peaks, s_m , of the total structure factors, $S(s)$.

obtained provide an explanation for the unusual changes in composition-property dependence. The depolymerization of the polyphosphate glasses with decreasing P₂O₅ mol% content is quantitatively described by the distribution of the phosphate structural groups determined by NMR. A small-angle scattering effect which is evidence for the presence of heterogeneities of electron density is observed in the glass systems studied. Information on the nature of the heterogeneities is gained from examinations of heat treated samples and by anomalous small-angle scattering (ASAXS) experiments on the ZnO-P₂O₅ glass samples.

angle spinning nuclear magnetic resonance (NMR) spectroscopy to extract information on their short-range, intermediate-range and submicroscopic structure. The packing densities, ρ_p , calculated for the glasses exhibit characteristic changes from ultra to orthophosphate composition (Fig. 2). To understand the structural background of the changes in ρ_p , compositionally-dependent variations of the real-space distances, r_m , (Fig. 2) and the metal-oxygen coordination numbers (Fig. 3) obtained from the diffraction experiments have been studied. The results

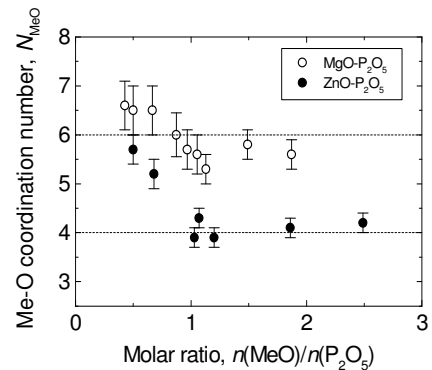


Fig. 3: The metal-oxygen coordination number in dependence on composition. Me stands for the metal ion.