Structure of Zinc Phosphate Glasses of 75 and 80 mole% ZnO Content Studied by X-Ray Diffraction and Reverse Monte Carlo Simulations

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X-Ray diffraction, using high-energy photons from a synchrotron, was used to extend the investigation of $(ZnO)_x(P_2O_5)_{1-x}$ glasses to samples of ZnO content close to $x = 0.8$ which were obtained by roller-quenching. The isolated PO_4 tetrahedra are surrounded by ZnO_n polyhedra, where Zn−O coordination numbers of ~ 4.5 are determined. The small increase of N_{ZnO} from ~ 4 at metaphosphate composition ($x = 0.5$) to ~ 4.5 is not sufficient to explain the strong increase of the packing density beyond the minimum at $x = 0.5$. The medium-range order was analyzed on the basis of partial $S_{PP}(Q)$ and $S_{ZnZn}(Q)$ factors obtained from Reverse Monte Carlo simulations of glasses with $0 \leq x \leq 0.8$. The positions of the first peaks in these factors, the number densities of P and Zn atoms and knowledge of definite P-P and Zn-Zn distances were used to check the applicability of simple models such as the dense packing of uniform P- and Zn-centered spherical environments for glasses with $x = 0.8$ and 0.5, the packing of corrugated sheets for vitreous P_2O_5 and the packing of phosphate chains for Zn metaphosphate glass.

Key words: X-Ray Diffraction; Glass Structure; Reverse Monte Carlo.