A Neutron and X-ray Diffraction Study of the Structure of Nd Phosphate Glasses

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Diffraction experiments were performed on two $(Nd_2O_3)_x(P_2O_5)_{1-x}$ glasses for studying the environmental order of the Nd^{3+} cations. In case of the metaphosphate glass (x = 0.25) a combination of X-ray and neutron diffraction data was used to separate the Nd-O and O-O first neighbor peaks. An Nd-O coordination number of 6.6±0.3 and a mean Nd-O distance of (0.239±0.001) nm were determined. In the ultraphosphate glass studied (x = 0.20) these values increase to 6.9±0.3 and (0.240±0.001) nm where the Nd-O coordination number is equal to the number of terminal oxygen atoms (O_T) which are available for coordination of each Nd^{3+} cation. This indicates the formation of NdO_n polyhedra not sharing any O atom where also all O_T's are in Nd-O_T-P positions. In the metaphosphate glass the NdO_n polyhedra have to share some O_T sites.

Key words: Neutron Scattering; X-ray Scattering; Short-range Order; Phosphate Glasses.