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\textsubscript{2}O\textsubscript{3})\textsubscript{x}(P\textsubscript{2}O\textsubscript{5})\textsubscript{1−x} glasses for studying the environmental order of the Nd\textsuperscript{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\textsubscript{T}) which are available for coordination of each Nd\textsuperscript{3+} cation. This indicates the formation of NdO\textsubscript{n} polyhedra not sharing any O atom where also all O\textsubscript{T}'s are in Nd-O\textsubscript{T}-P positions. In the metaphosphate glass the NdO\textsubscript{n} polyhedra have to share some O\textsubscript{T} sites.

\textbf{Key words:} Neutron Scattering; X-ray Scattering; Short-range Order; Phosphate Glasses.