Developing Structure-Property Relationships in Optical Glasses to Optimise Functional Designs

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Abstract

An investigation of the structural motifs present in alkaline earth modified Tellurite glasses has been undertaken in order to further elucidate the effects of network connectivity across atomic structural units on higher level material functionality. With desirable optical properties including high refractive indices, third-order non-linear optical coefficients and near infra-red transmittance these glasses are of industrial value across a range of optical devices. Variations in polarizability between [TeO4] and [TeO3] units mediates these optical responses, with property changes driven by their relative ratio in the glass network. Classical structural techniques including neutron diffraction, X-ray diffraction and Raman scattering have been performed to show the occurrence of decreasing tellurium coordination number with increasing modifier concentration. Further to this, changes to the structural polyhedra as a result of modifier atoms have been observed using empirical potential structural refinement. Consideration has been given to the occurrence of a lone-pair environment for Tellurium through the use of dummy atoms; in this way robust models have been generated providing good agreement with the experimental structure factors. From this further understanding into the mechanisms behind structure-property relationships has been shown, helping to optimise future glass design.

Keywords: Tellurite, Structure, Property, Optical, Glass, EPSR, Neutron, Raman, X, ray

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