Glass structure – crystallization relationships through EPSR modelling of synchrotron X-ray total scattering data of Na, Li, Fe, and B, substituted aluminosilicate glasses

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Abstract

Advanced diffraction techniques have been applied towards the understanding of the structure of sodium aluminosilicate (NAS) glasses of varying Al/Si addition as far back as the late 1970's - early 1980's. It has been determined previously that despite the similarities among the average local structures of vitreous aluminosilicates, the crystallization behaviors vary significantly among these systems during cooling from the molten state. In the present work, we expand on these previous findings through the compositional substitution of NAS glasses with Li, B, and Fe. Substitution of Al with B and Fe have been found to increase crystallization at low B and Fe fractions and eventually frustrate crystallization. Substitution of Na with Li results in complex crystallization behavior which is likely influenced by the mixed alkali effect. The influence of Al/Si and Fe/Si ratio on crystallization has also been explored and is strongly dependent on the fraction of SiO2. The measurement techniques employed in this study include: synchrotron X-ray total scattering, nuclear magnetic resonance, Raman spectroscopy, and X-ray diffraction. Structure models were calculated through Empirical Potential Structure Refinement (EPSR) of the measured X-ray pair distribution functions (xPDFs). Our models of glass structure suggest an influence of alkali coordination number on crystallization propensity and that further crystallization may be promoted by chemical partitioning during crystal growth.

Keywords: Silicate glass structure, synchrotron total scattering, structure modelling

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