The formation of liquids, glasses and the anti-glass phase in the system Bi2O3-Nb2O5-TeO2

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Abstract

Glasses formed in the technologically important system Bi2O3-Nb2O5-TeO2 show formation of spherulitic inclusions within a glassy matrix upon annealing resulting in textures that are reminiscent of those used to describe "polyamorphism" in the Y2O3-Al2O3 system. However, in the tellurite system the inclusions are crystalline and have been identified as an "anti-glass" phase, i.e., a solid with long-range cation order but with a disordered anion sublattice. The similarity of the textures have caused us to investigate the possibility of links between the formation of anti-glass inclusions in tellurites and polyamorphic behaviour in the aluminate system. In this part of our study we report high energy X-ray diffraction data for liquids and glasses formed in the Bi2O3-Nb2O5-TeO2 system at the compositions known to give rise to anti-glass formation. The data were collected for stable and deeply supercooled liquids to the point of vitrification in order to test for evidence of an underlying liquid-liquid phase transition (LLPT). There is however no evidence from the diffraction data to suggest the presence of an LLPT. The study is being continued using molecular dynamics (MD) simulations to explore the metastable region further and investigate the relative stability of different glassy configurations and clusters that form as the glassy state is approached. We suggest that the apparently contrasting behaviour in the two systems can be understood by considering the kinetics of ordering on the cation and anion sites and that initial glassy forms evolve towards more thermodynamically stable states during annealing. The large cations in the Bi2O3-Nb2O5-TeO2 glasses can readily adopt a positionally ordered

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arrangement giving rise to the anti-glass phase, mediated by the more mobile O2- anions that form a sublattice with disordered vacancies. In Y2O3-Al2O3, the system encounters a polyamorphic transition, revealed by the emergence of spontaneous and random density fluctuations in MD simulations. However, it is worth noting that the Y2O3-Al2O3 system also exhibits simultaneous crystallisation of a metastable garnet solid solution that competes with the low density (LDA) glassy form. This could represent the equivalent of the anti-glass formation in the Bi2O3-Nb2O5-TeO2 system.

Keywords: tellurites, polyamorphism, anti, glass, diffraction, molecular dynamics simulation, energy landscapes