Interplay between crystallization and glass transition

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Abstract:

In this talk I will discuss the interplay between crystallization and glass transition in different binary mixtures by changing their inter-species interaction length and also the composition. We find that only those systems which form bcc crystal in the equimolar mixture and whose global structure for larger xA (xA = 0.6, where xA is the mole fraction of the bigger particles) is a mixed fcc + bcc phase, do not crystallize at this higher composition. However, the systems whose equimolar structure is a variant of fcc (NaCl type crystal) and whose global structure at larger xA is a mixed NaCl + fcc phase, crystallize easily to this mixed structure. We find that the stability against crystallization of this "bcc zone" is due to the frustration between the locally preferred structure (LPS) and the mixed bcc + fcc crystal. Our study suggests that when the global structure is a mixed crystal where a single species contributes to both the crystal forms and where the two crystal forms have large difference in some order parameter related to that species then this induces frustration between the LPS and the global structure. This frustration makes the systems good glass former. When xA is further increased (0.70! xA < 0.90) the systems show a tendency towards mixed fcc crystal formation. However, the "bcc zone" even for this higher composition is found to be sitting at the bottom of a V shaped phase diagram formed by two different variants of the fcc crystal structure, leading to its stability against crystallization.