Vitrification of Tetrahedral Liquids: from Water to Germanium and Beyond

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Many single component molecular liquids fail to crystallize on cooling, forming glasses at low temperatures. Pure atomic liquids, however, are very difficult to vitrify, both in experiments and molecular simulations. We report on the formation of monatomic glass formers for members of the family of tetrahedral substances by cooling the liquids in a region of the phase diagram where a metastable liquid-liquid transition lies close to a minimum temperature liquid-crystal-crystal triple point. The strategy is based on the realization that, for these substances, a liquid-liquid transformation is required to render a liquid with a structure that is closely related to the ground state crystal, thus providing for a way to halt the crystallization by preventing the liquid-liquid transformation.

The glassforming strategy was first derived and tested in simulations, producing an excellent monatomic glassformer model derived from a silicon potential[1], and then used in the lab to vitrify germanium under pressure, rendering the first successful vitrification of a pure metallic liquid.[2] We will discuss these two cases and the effect of the liquid-liquid transformation in the crystal nucleation of the most important molecular tetrahedral liquid, water.[3, 4]

References

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