The Art and Science of glass formation. Ideal glassformers as opposed to “ideal glass”es.

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There is a common belief in glass science that, if a liquid of known melting point supercools readily, its glass transition temperature, Tg, can be predicted from the “2/3 rule”, viz., Tg = 2/3Tm. We start by arguing that this “law” is a tautology. Accordingly, we look for extreme violations to the high end, seeking “ideal” glassformers defined by the condition $T_m << T_g$. Of course, T_m cannot be determined if $T_m << 1.5T_g$ so the search must be conducted indirectly, by extrapolation of systematic results, with no final guarantee that the “ideal” glassformer has been found. Our principal strategy is systematic study of melting properties of closely related systems of simple character, which we conduct using molecular dynamics simulations with “potential tuning”. We commence with known crystals of a system, perturb their interaction potentials systematically, and determine the temperatures at which they “melt” (or amorphize). Having found systems in which there appears to be no crystal with a positive heat of fusion, (hence no stable crystal phase), we then consider the effects of second components that mix non-ideally, on the liquidus relations. The conclusion is that “ideal” glassformers can, and do, exist.

The existence of liquids that cannot crystallize is important conceptually since the non-Arrhenius, non-exponential, non-linear character of viscous liquids can then be disconnected from their metastability with respect to crystals (and supposed pre-crystalline fluctuations). The fluctuations of importance then become more easily identified, and these will be discussed, in order to facilitate a current resolution of the venerable Kauzmann paradox.