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The relationship between efficient packing and glass-forming ability in hard-sphere systems[1]

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When supercooled liquids are rapidly quenched at rates R exceeding a critical value Rc, they avoid crystallization and form amorphous solids, such as bulk metallic glasses (BMGs). However, engineering applications of BMGs are often limited by the high cost of the constituent elements and their small casting thickness. Thus, we seek to design particular alloys with controllable stoichiometry and maximal critical cooling rate Rc. We perform numerical simulations to compress binary hard-sphere mixtures into glasses as a function of the particle size ratio and stoichiometry. We measure the packing fraction and local structural order for each glass to determine the critical compression rate. We find that large packing fraction differences between the crystalline and amorphous states implies poor glass forming ability, whereas small packing fraction differences yield better glass-formers. In addition, we show that an abundance of icosahedral order in amorphous packings enhances the glass forming ability of the mixtures.

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