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The glass-forming ability of patchy repulsive spheres[1] KAI ZHANG, YANHUI LIU, JAN SCHROERS, Yale University, MARK SHATTUCK, The City College of New York, COREY O'HERN, Yale University — In bulk metallic glasses (BMGs) involving nonmetallic elements, anisotropic interactions are essential to describe their structural relaxation, mechanical properties, and glass-forming ability (GFA). Here, we employ a repulsive sphere model that includes attractive interactions between patches on each sphere to study the glass-forming ability of alloys that include non-metallic components (e.g. metal-metalloid alloys). Using molecular dynamics simulations, we quantify the GFA by measuring the critical cooling rate below which crystallization occurs as a function of the size and spacing of the patches, as well as the symmetry of the crystalline state that competes with the glass. We find that the glasses can dissolve no more than 20-30% solute nonmetallic atoms (such as B, Si, and P), which explains why non-metallic elements occur at low number fractions in BMGs.

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