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Atomic structure and energetics of amorphous–crystalline CuZr interfaces: A molecular dynamics study

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ABSTRACT

The local order of the binary alloy CuZr differs between the crystal (B2 phase) and the bulk metallic glass (BMG). In the B2 phase, both Cu and Zr reside in the center of polyhedra whose surfaces are composed of six tetragons and eight hexagons. In the glass, many different polyhedra occur with a large fraction of five-edged faces. However, little has been known hitherto about the local order in the interfacial region between glass and crystal. Using embedded-atom potential-based molecular-dynamics simulations, we find it differs markedly from that in the glass. For example, distinctly fewer pentagons occur on the surfaces of Voronoi polyhedra in the interface than on those in the BMG. Moreover, there is an increased variety of polyhedra allowing the interface to be more densely packed than the BMG. Details of the polyhedra distribution and consequently various interfacial properties depend on the orientation of the crystals. For the investigated surfaces, we find that the interfacial energy is the smallest and the crystallization activation energy the highest for the closest-packed crystalline surface. This result can be rationalized by the argument that the lattice spacing of the closest-packed surface is most commensurate with the wavelength associated with the density pair correlation function of the disordered system. In practice, our result implies that bulk-metallic glasses are best reinforced by nanocrystals with close-packed surfaces to reach maximum durability.

KEYWORDS: molecular dynamics simulation, interface, interfacial structure, interfacial energy, metallic glass