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**Are Metallic Glasses Stronger or Tougher than Their Crystalline Alloy Counterparts at the Nanoscale?** JINGUI YU, MINGCHAO WANG, SHANGCHAO LIN, Florida State University — Brittle failure in metallic glasses (MGs), which restricts their wide commercial applications, has been largely unexplored their inherently microstructural evolution at the atomistic level. Herein, we predict the influence of aspect ratios and compositions on the mechanical properties of nanoscale $Cu_xZr_{100-x}$ MGs and their crystalline counterparts using molecular dynamics (MD) simulations. We find that aspect ratio has a key role in the brittle-to-ductile transition (BDT) in MGs. From low to high aspect ratios, we attribute such BDT behavior primarily to the increasing number of small pieces of shear band and the slower reformation capability of icosahedra. In contrast, the $Cu_xZr_{100-x}$ crystal shows a composition-dependent BDT, that is, higher Cu content exhibits better ductility. Furthermore, unlike the failure mechanism of MGs, $Cu_{75}Zr_{25}$ and $Cu_{50}Zr_{50}$ crystals exhibit superplasticity and typical plasticity due to twinning and dislocation, respectively. As an outlier, $Cu_{25}Zr_{75}$ crystal exhibits a brittle behavior due to continuous voids ahead of the crack tip. More interestingly, the yield strength of single crystal is larger than that of MGs with the same aspect ratio due to the scarcity and low mobility of dislocations, coupled with constraint from tensile surface stresses. We observe weak size dependence in MGs, but very strong size dependence in single crystals, which leads to an exciting dimensional yield-stress crossover at ˜300 $\mu$m. This study provides fundamental guidance for the optimal design of MGs and single crystalline structural materials with high strength and ductility.

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