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Liquid Metal Embrittlement: new understanding for an old problem

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When liquid metals are brought into contact with other polycrystalline metals, deep liquid-filled grooves often form at the intersections of grain boundaries and the solid-liquid interface. In some systems, e.g., Al-Ga, Cu-Bi and Ni-Bi, the liquid film quickly penetrates deep into the solid along the grain boundaries and leads to brittle, intergranular fracture under the influence of modest stresses. This is a form of liquid metal embrittlement (LME). This phenomenon is ubiquitous in material processing and is particularly important in nuclear reactor scenarios in which liquid metals are used as coolants and as spallation targets. The penetration of a liquid phase along the grain boundary is a complex phenomenon, involving several different types of simultaneous processes. The tendency for and rate of LME are also sensitive to externally controllable factors such as temperature and applied stress. Because of the interplay between the underlying phenomena that occur in LME, it has been difficult to perform experiments that can be interpreted to understand which processes control LME and which are simply parasitic. We study LME by performing molecular dynamics simulations of an Al bicrystal in contact with liquid Ga and investigate how Ga penetrates along the grain boundaries during the early stages of the wetting process. We use the simulation results to propose a new mechanism for LME and compare it with general trends gleaned from a series of LME experimental studies.