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Grain boundaries and glasses: birds of a feather HAO ZHANG, University of Alberta, Canada, DAVID SROLOVITZ, Institute of High Performance Computing, Singapore, JACK DOUGLAS, Polymers Division, NIST, USA, JAMES WARREN, Metallurgy Division, NIST, USA — Polycrystalline materials can be viewed as composites of crystalline "grains" separated from one another by thin "amorphous" grain boundary (GB) regions. While GBs have been exhaustively investigated at low temperatures (T), where these regions are relatively ordered, much less is known about them at higher T where they exhibit structural disorder, and where characterization methods are limited. The time and spatial scales accessible to molecular dynamics (MD) simulation are appropriate for investigating the dynamical and structural properties of GB at elevated T and we exploit MD to explore basic aspects of GB dynamics as a function of T. It has long been hypothesized, based on the processing characteristics of polycrystalline materials, that GBs have features in common with glass-forming liquids. We find remarkable support for this suggestion, as evidenced by string-like collective motion, transient caging of atom motion, and non-Arrhenius T dependence of GB mobility. Evidently, the frustration caused by the inability of atoms in the GB region to simultaneously order with respect to competing grains is responsible for this similarity. The paradigm that grains are encapsulated by a "frustrated fluid" provides a powerful conceptual model of polycrystalline materials.

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