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Mechanism of quasicrystal nucleation and growth SHARON GLOTZER, AARON KEYS, Department of Chemical Engineering, University of Michigan — On cooling, liquids ordinarily solidify into glasses or into crystalline phases with long- range periodic ordering. However, it is also possible to form quasicrystals, ordered solids with long-range aperiodicity. Although quasicrystals have been observed in many materials, their formation is poorly understood. We present the results of a molecular simulation study to elucidate the process by which quasicrystals form from supercooled liquids. We show that, as has been speculated in previous theoretical and experimental works, icosahedral clusters play a significant role in quasicrystal formation. Specifically, icosahedral clusters facilitate the formation of the so-called quasicrystal “critical” nucleus, and, together with phasons, facilitate the complicated mechanism that allows quasicrystals to grow aperiodic structures via local interactions. Our findings suggest that direct correlations between liquid ordering and solid structure may be a requisite property for quasicrystal-forming systems, and is consistent with the class of systems that are known to form quasicrystals experimentally.

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