591c Nucleation and Growth of Quasicrystals

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Quasicrystals are a remarkable class of solids that exhibit long-range aperiodic ordering. Due to their unique physical, chemical, optical and electromagnetic properties, quasicrystals have found novel applications in almost every realm of engineering. Many unanswered questions remain in the theory of quasicrystals, including one of the most fundamental and important questions: how do quasicrystals grow?

We investigate quasicrystal growth from the standpoint of nucleation from the supercooled liquid. Using a combination of Monte Carlo, molecular dynamics, transition path sampling, and umbrella sampling, we study the factors that lead to the liquid-to-quasicrystal phase transition. We determine the size, shape and structure of the quasicrystal critical nucleus that initiates the growth of the bulk solid phase. We show evidence that the growth of quasicrystals is fundamentally different than the growth of periodic crystals on an atomic level. Specifically, quasicrystal growth is derived from the combined effects of nucleation and glassy behavior in the supercooled liquid.