Self-Assembly of an Icosahedral Quasicrystal Network

MICHAEL ENGEL, PABLO F. DAMASCENO, University of Michigan, CAROLYN L. PHILLIPS, Argonne National Laboratory, SHARON C. GLOTZER, University of Michigan — Icosahedral quasicrystals (IQC)s are a form of matter that is ordered but not periodic in any direction. IQCs have the highest symmetry of all crystals and therefore exhibit orientationally highly uniform properties. This makes them candidates for materials with a complete photonic bandgap or as specialized alloys. Unlike axially-symmetric quasicrystals, which have been reported experimentally in micellar or nanoparticle systems and suggested in bi-layer water, silicon, and mesoporous silica, IQCs have not been observed in the context of non-intermetallic systems. Here, we demonstrate the self-assembly of an IQC by means of molecular dynamics simulations. The IQC is a predominantly tetrahedral, body-centered-icosahedral network and is structurally related to clathrates and other tetrahedrally coordinated crystalline networks. The IQC self-assembles rapidly and reproducibly from a fluid phase in a one-component system of particles. We provide a crystallographic structure model and show the presence of a diffusion mechanism not available in periodically ordered solids. [1] M. Engel, P.F. Damasceno, P.L. Phillips, S.C. Glotzer, Nature Materials, in press (2014).