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A materials genomic approach to design of nucleating agents
ALEXANDER BOURQUE, MIT, REBECCA LOCKER, ExxonMobil Research and Engineering, GREGORY RUTLEDGE, MIT — Heterogeneous nucleation is frequently the first step in any system undergoing phase change. Nucleating agents are foreign materials introduced to modify and regulate this step. Control of nucleation kinetics permits modification of morphology in a broad range of crystallizable materials including those used for separators in batteries, fuel cells, etc. However, the mechanism(s) of action in heterogeneous nucleation are poorly understood, due in part to the small spatio-temporal scales over which nucleation occurs. Molecular simulation has been used to study the kinetics of homogeneous and, to a lesser extent, heterogeneous nucleation. We show that by systematically varying the intermolecular force field parameters that describe the nucleating agent, one can rapidly screen entire classes of materials to characterize both effectiveness and mechanism. The method is applied to the crystallization of n-pentacosane, a model surrogate for polyethylene, on the family of tetrahedrally coordinated crystals isomorphous with diamond and the family of 2D, hexagonally coordinated materials isomorphous with graphene. The induction time for heterogeneous nucleation is shown to depend strongly on crystallographic registry between the nucleating agent and the critical nucleus of the new phase, indicative of an epitaxial mechanism. Importantly, the severity of this registry requirement weakens with decreasing rigidity of the substrate and increasing strength of attraction to the nucleating agent. Employing this method, high throughput computational screening of nucleating agents becomes possible.

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