Simulating the Tensile Properties of Highly Regular Polymer Networks

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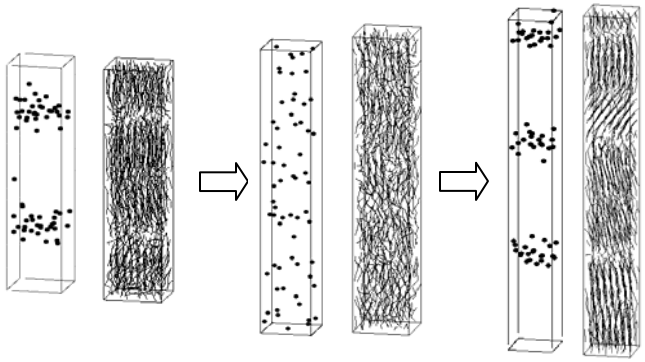
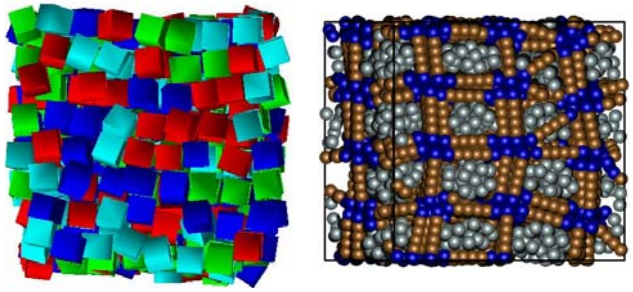
Molecular simulation is being used to explore novel approaches, based on the self-assembly properties of some polymers and particles into regular nano-structures, that could be used as templates to generate idealized polymer networks with regular topologies. It is hypothesized that by transplanting the regular order of block copolymer meso-structures and of nanoparticle-based liquid crystalline phases into polymer networks, one could obtain networks with such properties as built-in modularity in its elastic response, set bounds for extensibility or compressibility (as is often seen in some natural materials), tunable modulus, high elongation, and very large ultimate strength (due to the very uniform distribution of stresses throughout the sample).

Snapshots showing crosslinks (dots) & chains (lines) at different stages of straining of a "diamond" network. Segregation & mixing of crosslinks leads to "shock-absorbing" jumps in elastic response.

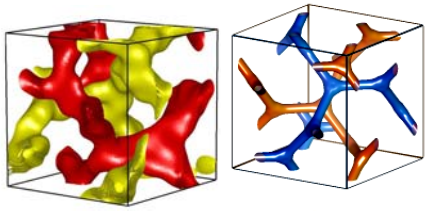


Self-assembled, liquid crystalline phases formed by nanoparticles of odd shapes (e.g., cubes) could be used as scaffolds to produce regular networks

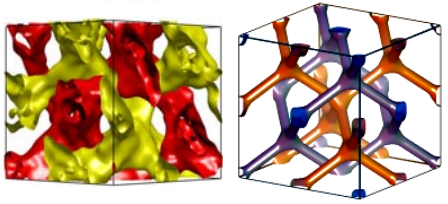


<u>Below</u>: Simulated (left) & ideal (right) bicontinuous phases of block copolymers are being explored as scaffolds to create regular networks (only domains of minority block shown)

Gyroid



Double diamond



Plumber's nightmare