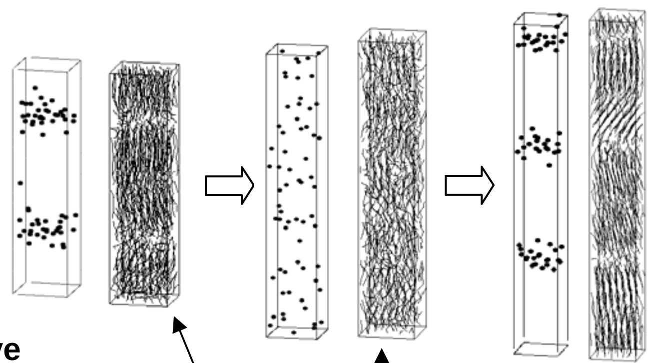
Simulating the Tensile Properties of Highly Regular Polymer Networks

Fernando A. Escobedo

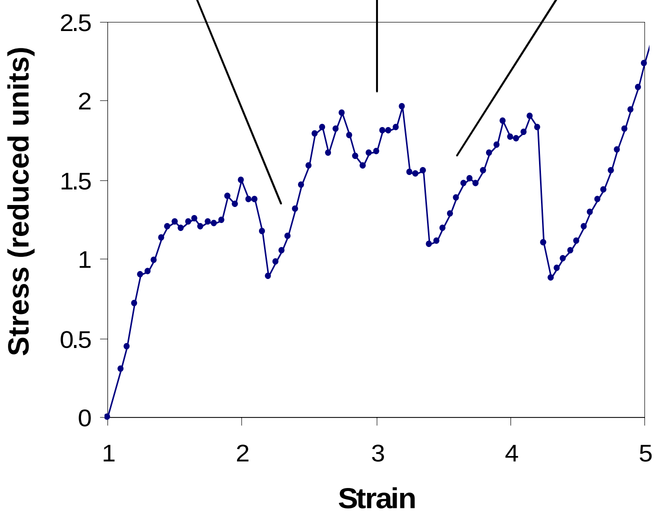
Cornell University
School of Chemical and Biomolecular Engineering

Idealized polymer networks are being studied wherein polymer chains are interconnected regularly and with minimal defects. Such systems can more readily exhibit order-disorder phase transitions and can impart reproducible modularily that sets extensibility or compressibility limits (as is often seen in natural materials). Such networks are expected to have tunable modulus, high elongation at break ("super-elasticity"), and very large ultimate strength (due to the very uniform distribution of stresses throughout the sample). By simulating the stretching of a regular (diamond) network via molecular dynamics, multiple order-disorder transitions are seen to occur sequentially, producing a "saw-tooth" stress-strain curve, akin to that of supertough natural materials like abalone shells' glue.

Sample snapshots showing crosslinks (dots) & chains (lines) at different stages of straining. The sequential segregation & mixing of crosslinks gives rise to the 'teeth' in the stress-strain curve that act as "shock absorbers"

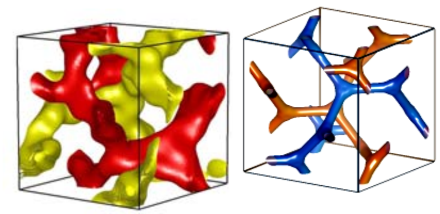


Saw-tooth stress-strain curve of model diamond network (with semiflexible chains) found from iso-strain molecular dynamics runs

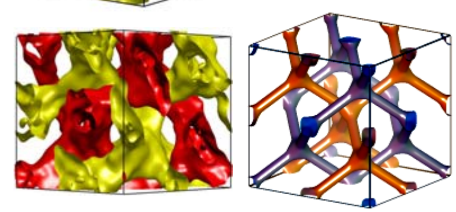


<u>Below</u>: Simulated (left) & ideal (right) bicontinuous phases of block copolymers are being explored as scaffolds to create regular networks (only domains of minority block shown)

Gyroid



Double diamond



Plumber's nightmare