Supporting Information for

Crosslinker energy landscape effects on dynamic mechanical properties of ideal polymer hydrogels

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Topology Measurements

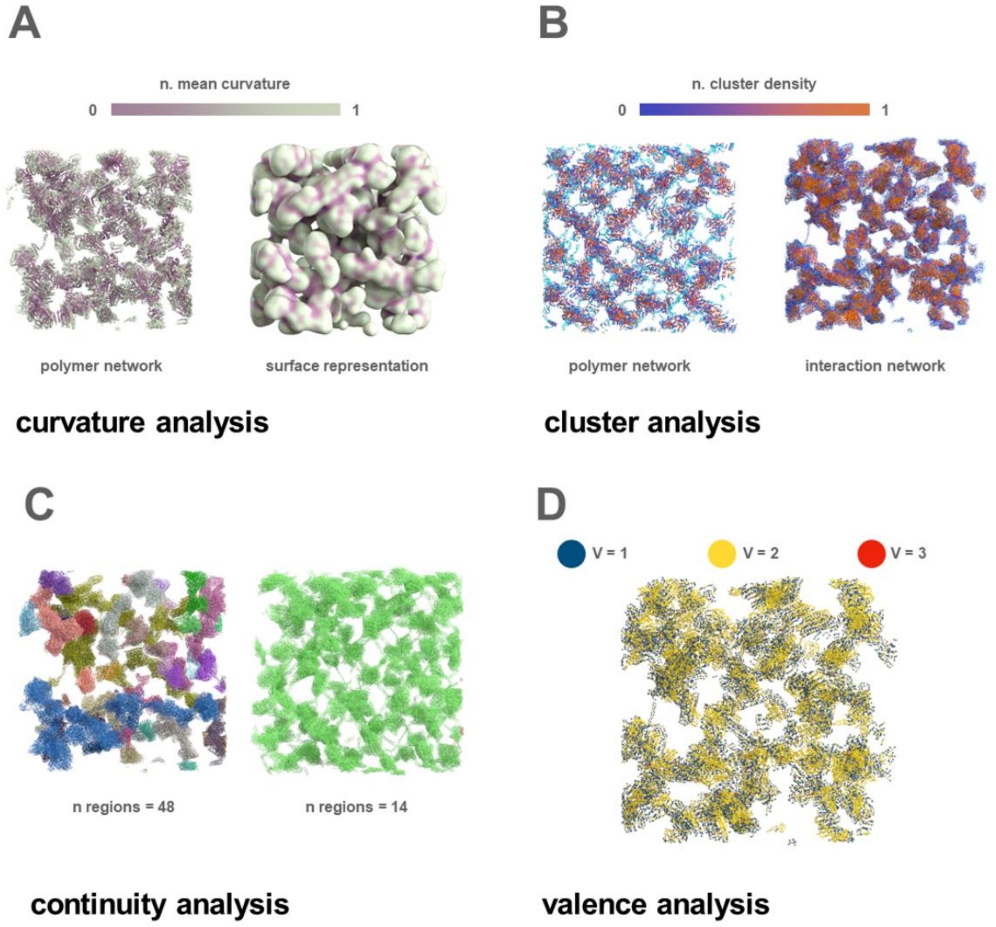

Figure S1. Additional methods of topology analysis were applied to the network. (A) The mean curvature of a surface representation of the network was computed to indicate regions of concave and convex curvature. (B) The density of atoms in the network was measured by the number of possible interactions within a 5 A radius. (C) Continuity was assessed based on the number of regions formed when all atoms within 5 A were connected with one another. (D) Valence was measured according to the number of atom-to-atom interactions within the network.

Curvature

Mean curvature was measured for the polymer network by creating a mesh surface representation of the network and sampling curvature at each vertex. First, a signed distance field (SDF) [1] was created from the point cloud of atom positions in the polymer network. Voxels in the SDF were assigned a radius of 1 A. This preliminary voxel field was expanded by increasing the radius engaged by each voxel by a factor of ten before applying a gaussian smoothing function for ten iterations [2]. The SDF was then converted to a quadrilateral mesh using the marching cubes algorithm, which resulted in the creation of a coarse-surface representation of the polymer network.

Mean curvature is a signed value that measures curvature in two principal directions perpendicular to the surface normal. While Gaussian curvature $K=\kappa 1\kappa 2$ is the square of the geometric mean of the principal curvatures $\kappa 1$ and $\kappa 2$, mean curvature $H=(\kappa 1+\kappa 2)/2$ is the arithmetic mean of $\kappa 1$ and $\kappa 2$. Principal curvatures describe the maximum $\kappa 1$ and minimum $\kappa 2$ curvature at every point on the surface. Low mean curvature in the mesh representation of the network occurs in regions where the network narrows into thin connections, while high mean curvature occurs in convex regions where atoms are clustered.

Valence
Valence is the number of direct connections for each atom in the polymer network according to the imported model. The vast majority of atoms in the network have a valence of 2, while a small number have either 1 or 3 connections.

Density
Density indicates the number of atoms within a region of the network. High density indicates a large number of atoms in a relatively small area, referred to as a cluster. A measurement of atom density was created by adding additional connections to all adjacent atoms within 5 A of one another and measuring the connections at each atom. The highest observed density in the network is 30 while the lowest is 1.

Continuity
Continuity indicates the number of connected regions in the network after connections are added to every atom within 5 A of another. A higher number of regions may indicate a more discontinuous network, or may simply indicate additional breakages in already isolated regions.

Supplementary Citations

1.Oleynikova, H., Millane, A., Taylor, Z., Galceran, E., Nieto, J., & Siegwart, R. (2016). Signed distance fields: A natural representation for both mapping and planning. In RSS 2016 workshop: geometry and beyond-representations, physics, and scene understanding for robotics. University of Michigan.
2.Getreuer, P. (2013). A survey of Gaussian convolution algorithms. Image Processing On Line, 2013, 286-310.