Visualizing Shuttleworth's relation: Is there a difference between surface free energy and surface stress?

Classically, the study on wetting has focused on the interaction of liquids with hard surfaces. There exist a lot of cases however, in which a surface is not hard and rigid, yet soft and deformable. Due to the low elastic modulus of these materials, the surface free energy and surface stress of an interface are not necessarily equal. The relation between the two is given by the Shuttleworth equation:

$$\Upsilon = \gamma + \frac{d\gamma}{d\varepsilon}$$

in which Υ is the surface stress, γ is the surface free energy, and ε is the elastic strain parallel to the surface.

In this research, we try to get more insight into the Shuttleworth equation. We simulate generic, coarse-grained gels with differing degrees of stiffness, using Molecular Dynamics. The elastic moduli of these gels are determined by stretching and pinning the gels in one direction.

Next, we determine the surface tension of these gels by creating a Lennard Jones (LJ) fluid and gel interface. By stretching the gel-fluid interface, we monitor the internal stress build-up of the gel, and the value for the surface tension.

Last, we perform measurements on the wetting behavior of a LJ droplet on top of a gel. By regarding the contact angle of the droplet for a gel in different degrees of stretch, we hope to confirm the Shuttleworth equation.

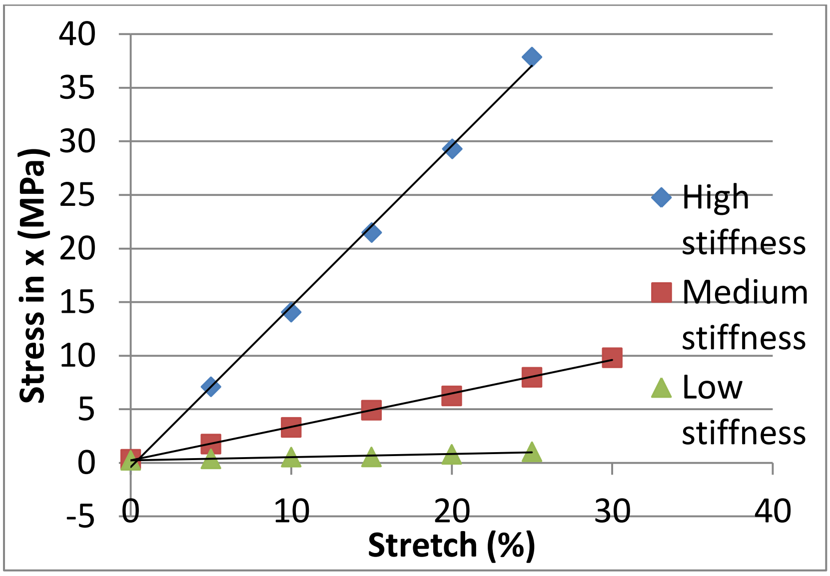

Figure 1.-Stress-strain diagram for gels crosslinked at: 4, 1.5 and 0.8 links/nm^3(high, medium and low stiffness, respectively). The slope of the linear fits gives the Young's modulus.

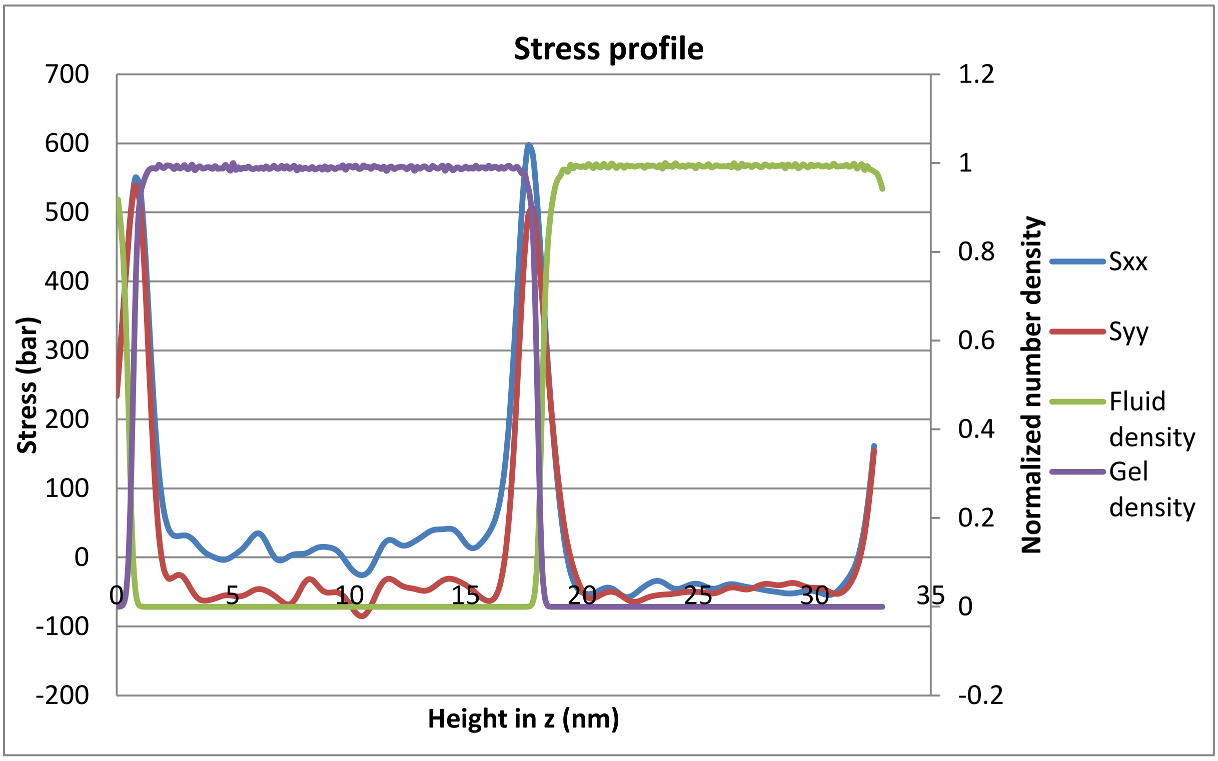

Figure 2.- The local stress profile for a gel-fluid system, stretched to 30% in direction xx. The stress is measured in lateral directions x (Sxx, blue), and y (Syy, red). The profile is pictured over the height in z. The local density profiles of the gel (purple) and fluid (green), are pictured for extra clarity. Due to periodic boundary conditions, two interfaces are present.