

Predicting mechanical constitutive laws of elastomers with mesoscale simulations

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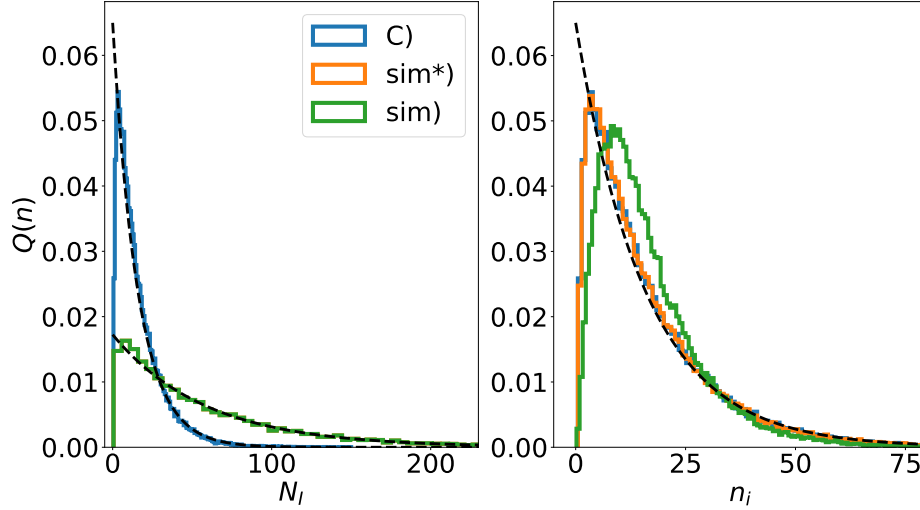


Figure 1: The effect of particle crossing on the shape of the chain/segment length probability density function $Q(n)$. Dashed lines represent target distributions, C) not entangled network, sim*) entangled network before mechanical relaxation, sim) entangled network after mechanical equilibration. Low n values are less likely to occur, because having over-extended chains is forbidden.

Table 1: Detailed simulation parameters

$a \times b \times c$ (nm)	Number of crosslinks	Number of entanglements
$60 \times 60 \times 60$	7776	20304
Connectivity	Number of segments	$\frac{a(t)-a(t_0)}{t-t_0}$ (cm s ⁻¹)
4	15552	0.04

Mooney-Rivlin representation of the stress

It is possible to find a simple expression for $(\lambda - 1/\lambda^2)$, resulting in the reduced stress found in the Mooney-Rivlin equation.^{1,2} This derivation is well known, but since we make explicit use of it in Fig.3, it is included here for completeness.

Suppose we have a strain energy function W that is expressed as a function of the three strain tensor invariants I_1, I_2, I_3 . These invariants are defined as:

$$\begin{aligned} I_1 &= \lambda_1^2 + \lambda_2^2 + \lambda_3^2 \quad , \\ I_2 &= \lambda_1^2 \lambda_2^2 + \lambda_2^2 \lambda_3^2 + \lambda_1^2 \lambda_3^2 \quad , \\ I_3 &= \lambda_1^2 \lambda_2^2 \lambda_3^2 \quad , \end{aligned} \tag{1}$$

with λ_i the deformation ratio of the i axis. These three expressions are independent of the choice of reference frame. The case of an incompressible material corresponds to $I_3 = 1$.

If we choose to stretch our material along the i axis, we can express the stress as the partial derivative of energy with respect to the deformation along this axis:

$$\sigma_{ii} = \frac{\partial W}{\partial \lambda_i} \lambda_i \tag{2}$$

To calculate the nominal stress σ_0 in the case of a uni-axial traction along axis 1, we have to evaluate $(\sigma_{11} - \sigma_{22})/\lambda$. This results in:

$$\sigma_{11} - \sigma_{22} = \frac{\partial W}{\partial \lambda_1} \lambda_1 - \frac{\partial W}{\partial \lambda_2} \lambda_2 \tag{3}$$

In order to change variables from λ_i to I_i , we need

$$\begin{aligned}\frac{\partial I_1}{\partial \lambda_1} &= 2 \lambda_1 \quad , \\ \frac{\partial I_2}{\partial \lambda_1} &= 2 \lambda_1 \lambda_2^2 + 2 \lambda_1 \lambda_3^2\end{aligned}\tag{4}$$

and by using the chain rule, we find

$$\sigma_{11} - \sigma_{22} = 2 (\lambda_1^2 - \lambda_2^2) \frac{\partial W}{\partial I_1} + 2 (\lambda_1^2 - \lambda_2^2) \lambda_3^2 \frac{\partial W}{\partial I_2}\tag{5}$$

$$\sigma_{11} - \sigma_{22} = 2 (\lambda_1^2 - \lambda_2^2) \left(\frac{\partial W}{\partial I_1} + \lambda_3^2 \frac{\partial W}{\partial I_2} \right)\tag{6}$$

In the case of uniaxial stress along axis 1 and by using the incompressibility approximation, we can write:

$$\begin{aligned}\lambda_1 &= \lambda \quad , \\ \lambda_1 \lambda_2 \lambda_3 &= 1 \quad , \\ \lambda_2 &= \lambda_3 = \frac{1}{\sqrt{\lambda}}\end{aligned}\tag{7}$$

and we find for the nominal stress:

$$\begin{aligned}\sigma_0 &= \frac{\sigma_{11} - \sigma_{22}}{\lambda} = 2 \left(\lambda - \frac{1}{\lambda^2} \right) \left[\frac{\partial W}{\partial I_1} + \frac{1}{\lambda} \frac{\partial W}{\partial I_2} \right] \quad , \\ \frac{\sigma_0}{\lambda - 1/\lambda^2} &= 2 \left[\frac{\partial W}{\partial I_1} + \frac{1}{\lambda} \frac{\partial W}{\partial I_2} \right]\end{aligned}\tag{8}$$

which is the expression of the reduced stress as defined by Mooney and Rivlin. If we assume a simple expression for W , such as $\frac{\partial W}{\partial I_1}$ and $\frac{\partial W}{\partial I_2}$ being constants, we obtain

$$\frac{\sigma_0}{\lambda - 1/\lambda^2} = 2 C_1 + 2 C_2 \frac{1}{\lambda}\tag{9}$$

which is the reason for plotting $\frac{\sigma_0}{\lambda - 1/\lambda^2}$ as a function of $\frac{1}{\lambda}$.

References

- (1) Mooney, M. A theory of large elastic deformation. *Journal of applied physics* **1940**, *11*, 582–592.
- (2) Rivlin, R. Large elastic deformations of isotropic materials IV. Further developments of the general theory. *Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences* **1948**, *241*, 379–397.