A Gaussian Slip-Link Model for Polymer Single and Double Networks

JAY D. SCHIEBER, Professor, MAHNAZ ESKANDARI, Ph.D. student, HAMID ARASTOPOUR, Professor — In this study, we developed Schieber’s slip-link model for lightly cross-linked polymers assuming the equilibration of deformed Gaussian chains. Our simulation consists of two steps: preparation and deformation. In the preparation step, cross-links and slip-links are assumed to be distributed randomly along the chain, but with independent statistical parameters: the average number of Kuhn steps between entanglements, $N_e$, and the average number of Kuhn steps between cross-links, $N_c$. In the second step, the cross-links and slip-links are deformed affinely, but since the chain can slide through the slip-links, its deformation is non-affine. The stress tensor can be determined as a function of deformation using Brownian dynamics as a sort of Monte Carlo algorithm. The Mooney plot of our simulation result has good agreement with most experimental data for uniaxial elongation deformation for cross-linked NR, PDMS, and PBd. The model is used to predict values for the Mooney plot parameters ($C_1$ and $C_2$) as a function of $N_e$ and the $N_c/N_e$ ratio. The $C_2/C_1$ ratio is found to be strongly dependent on $N_c/N_e$, but weakly dependent on $N_e$. This observation provides a new way of predicting the cross-link density and separating it from the entanglement density and for systems of known $N_e$ and $N_c$, the model requires no adjustable parameters. We are also developing our model for double network polymers in order to demonstrate different applications for the model.

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