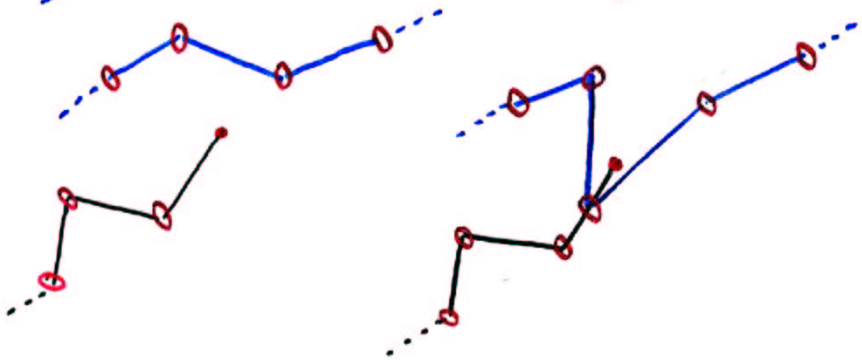
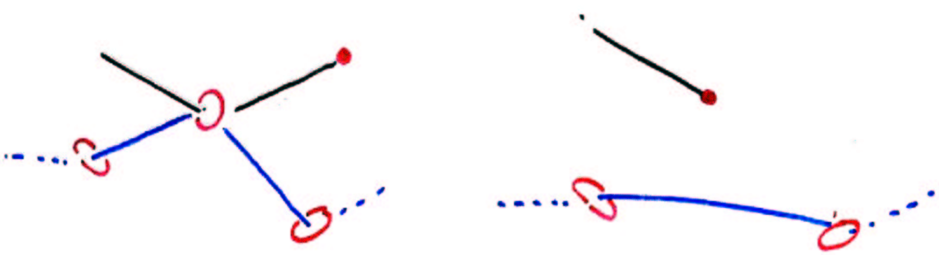
Topology renewal

Monitoring monomer number at chain ends every τ_e

a) slip-link creation if $n > 1.5\, n_0$



b) slip-link suppression if $n < 0.5\, n_0$



· Osmotic contribution in node equation

$$\frac{\text{osmotic force}}{\text{volume}} = -\underset{\sim}{\nabla} \Pi$$

$$\Pi(\underset{\sim}{R}) = kT\, \rho(\underset{\sim}{R})$$

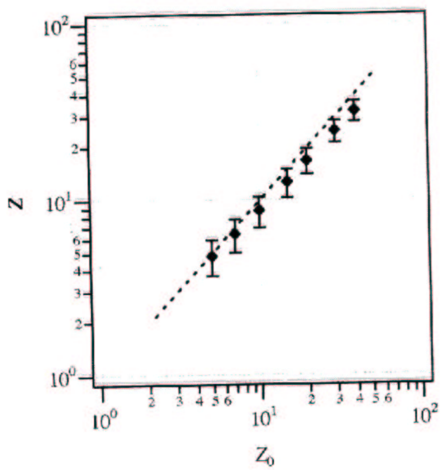
$$\rho(\underset{\sim}{R}) = \text{number density of nodes}$$

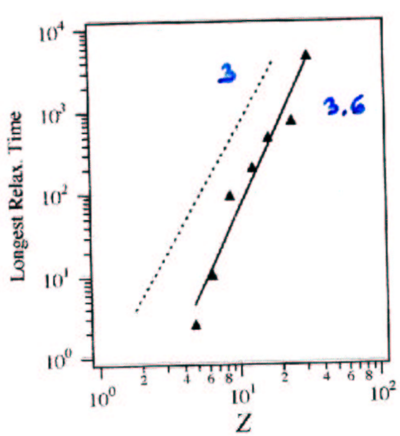
$$\frac{\text{osmotic force}}{\text{node}} = -\frac{1}{\rho} \underset{\sim}{\nabla} \Pi = -kT\, \underset{\sim}{\nabla} \ln \rho$$

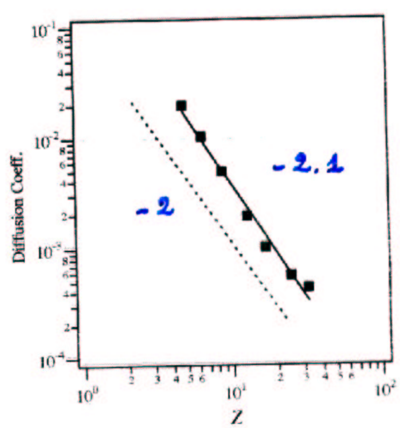
· Code name

New Algorithm for Polymeric Liquids Entangled and Strained

NAPLES







End-to-end statistics

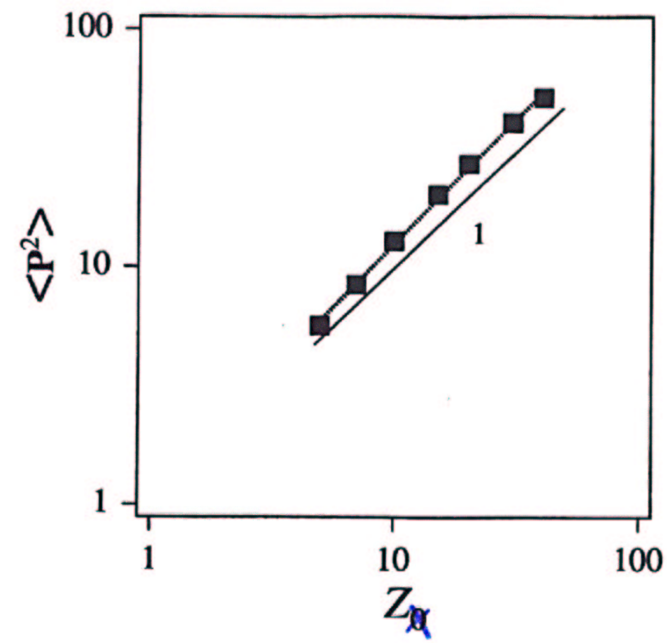


FIG. 6. Average square end-to-end distance $\langle \mathbf{P}^2 \rangle$ plotted against Z. The dotted line is the best fit of the data corresponding to $\langle \mathbf{P}^2 \rangle = Z^{1.08}$. Solid line corresponds to $\langle \mathbf{P}^2 \rangle = Z$.

We have also monitored relaxation of stress in terms of autocorrelation function $\mu(t)$, defined through the off-diagonal component σ_{xy} as

$$\mu(t)=\frac{\langle \sigma_{xy}(t+t')\sigma_{xy}(t')\rangle_{t'}}{\langle \sigma_{xy}^2\rangle_{t'}}. \qquad (18)$$

At any given time, the value of σ_{xy} is obtained through the following average over all chain segments in the simulation box:

$$\sigma_{xy} \propto \left\langle \frac{r_x r_y}{n} \right\rangle . \qquad (19)$$

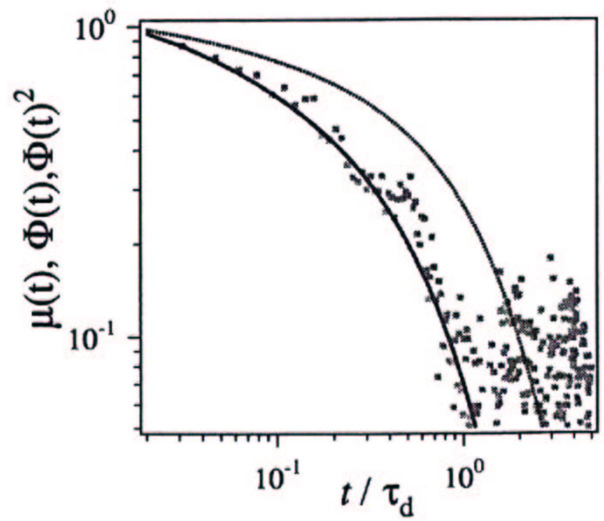
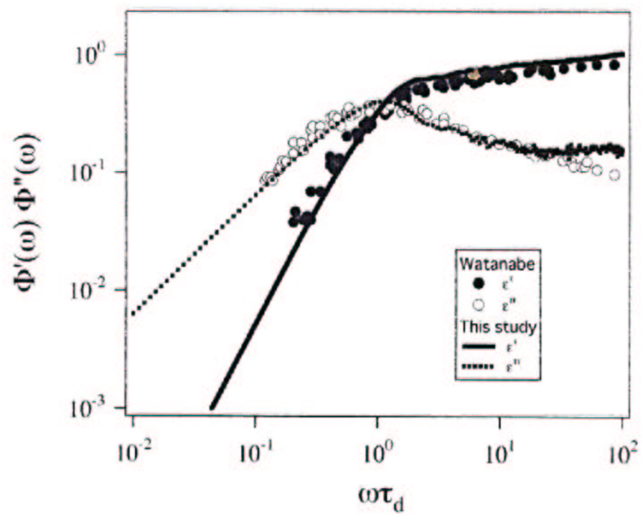
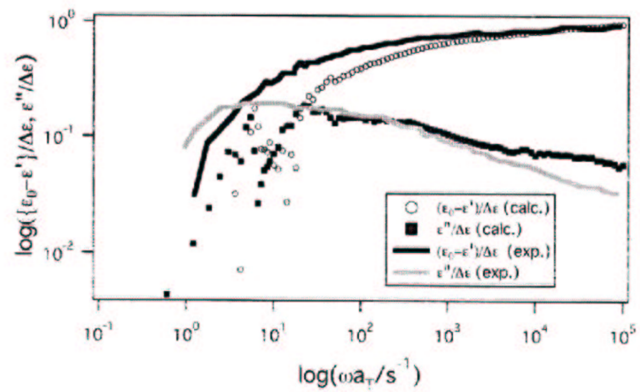


FIG. 9. End-to-end relaxation $\Phi(t)$ (dotted curve) and relaxation modulus $\mu(t)$ (scattered dots), both for $Z_0=10$. The solid curve is $\Phi^2(t)$.

Dielectric relaxation



· Star polymers



step strain

Z = 32