Krmer-Grestモデル(N=40)とRouseモデルの比較

Kremer-Grest model (NVT)

$T = 1.0 \qquad \Gamma = 0.5$

LJ cut-off $\quad r_c = 2^{1/6}$

$N = 40 \quad (< N_e \approx 70$ 程度??)

250 本

$\rho = 0.85$ (モノマー密度)

分子鎖密度

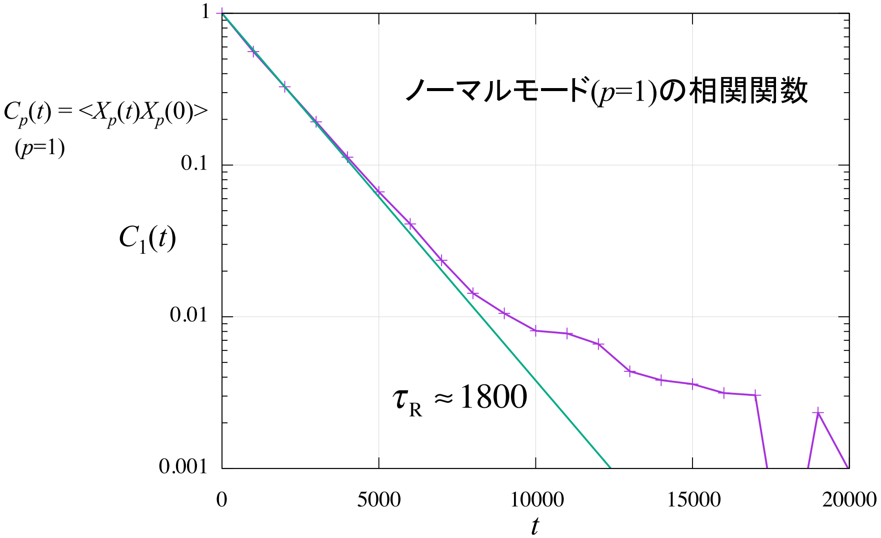
$$\nu \equiv \frac{\rho}{N}$$

mean-square end-to-end distance

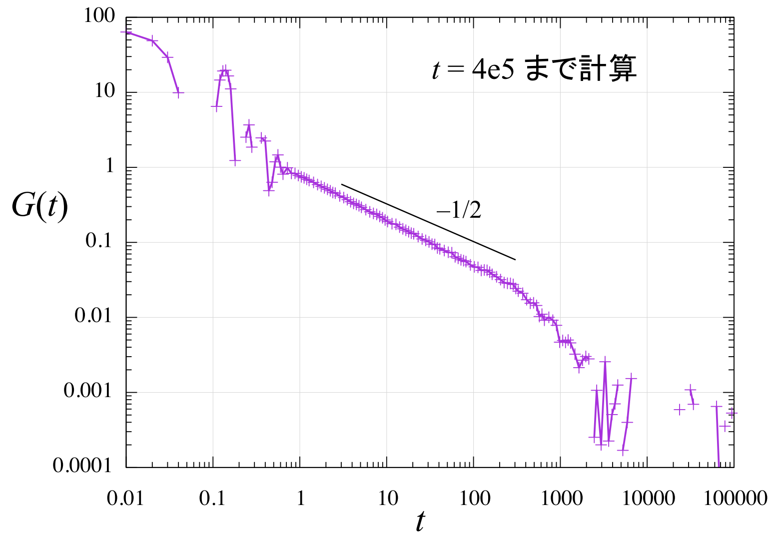
$$\langle \mathbf{R}^2 \rangle \approx 63.3 \qquad \sqrt{\langle \mathbf{R}^2 \rangle} \approx 7.96$$

線形粘弾性

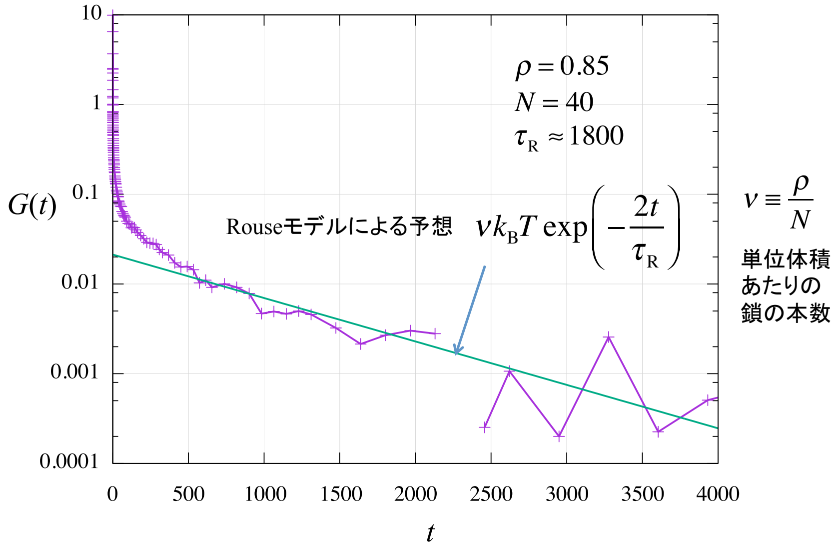
Rouse緩和時間の見積もり



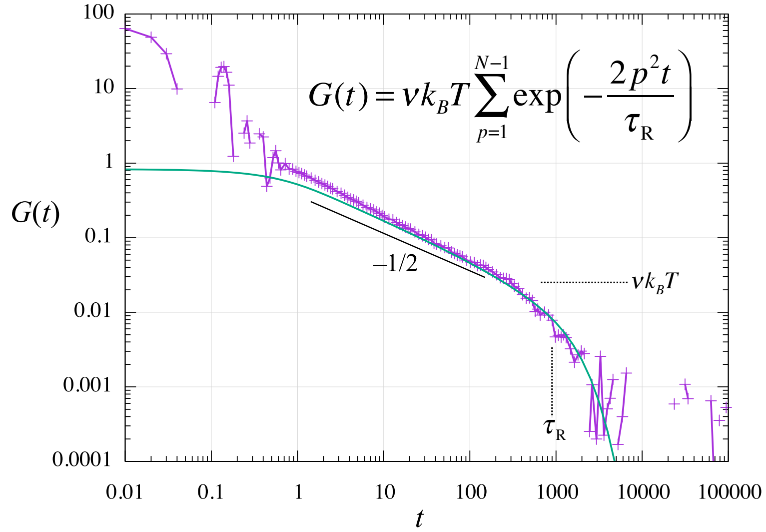
線形緩和弾性率 $G(t)$



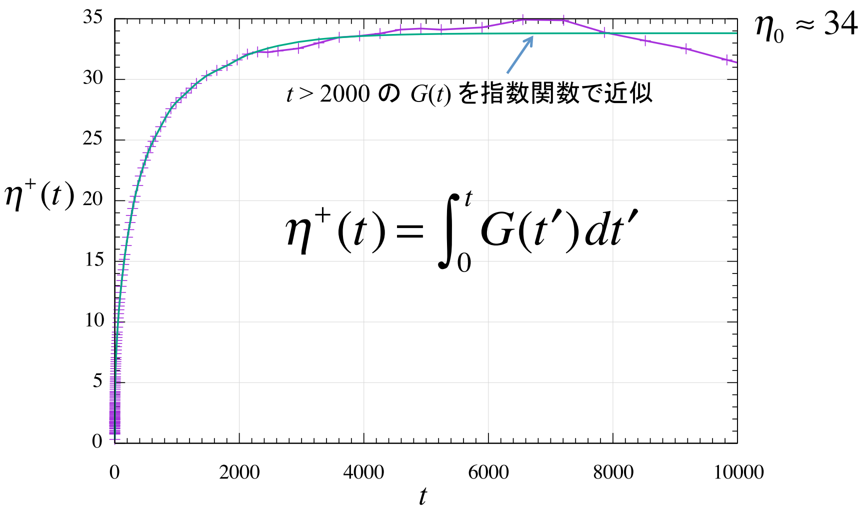
$G(t)$ の最長緩和成分



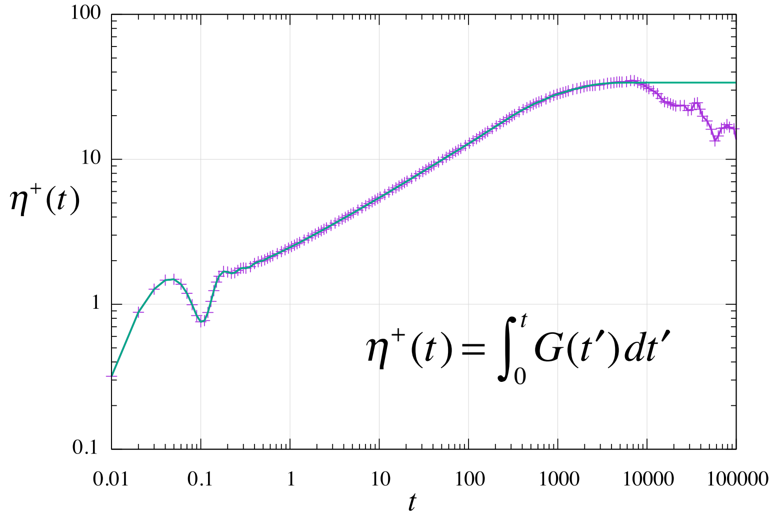
$G(t)$: Rouseモデルとの比較



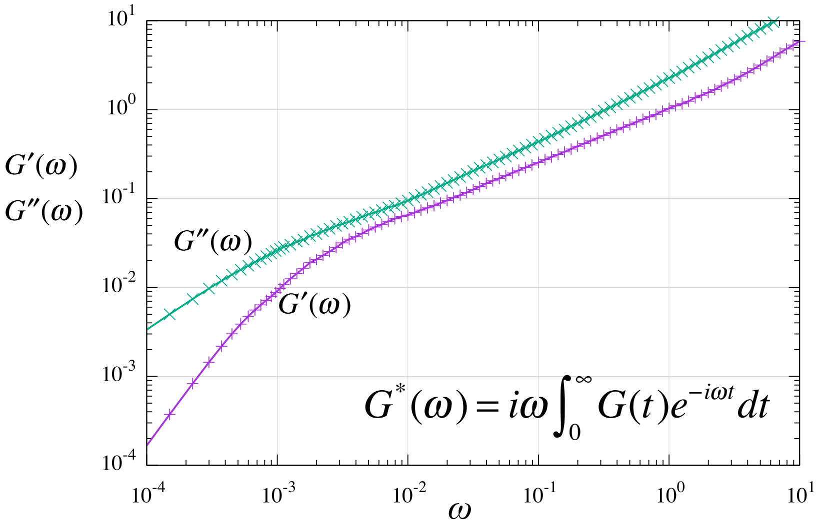
ゼロずり粘度の予測



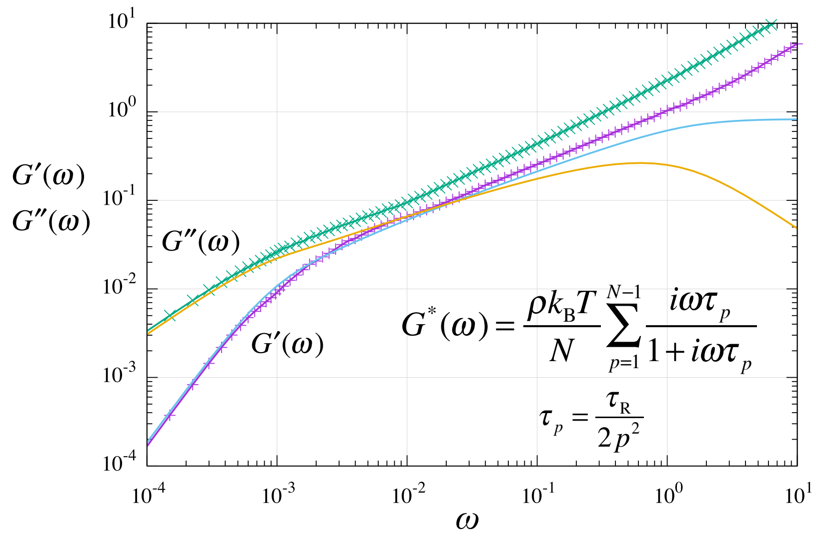
線形粘度成長関数



動的粘弾性



$G^*(\omega)$: Rouseモデルとの比較



法線応力差係数の予測

Steady state

$$\Psi_1(\dot\gamma) \equiv \frac{N_1(\dot\gamma)}{\dot\gamma^2}$$

$N_1(\dot\gamma) =$ 定常状態での第1法線応力差

$\dot\gamma \to 0$ での値は線形粘弾性から厳密に予測可能

$$\Psi_1(\dot\gamma = 0) = 2A_G$$

$$A_G \equiv \lim_{\omega\to 0} \frac{G'(\omega)}{\omega^2} = \int_0^\infty tG(t)\,dt$$

Start-up flow

$$\Psi_1^+(t, \dot\gamma) \equiv \frac{N_1(t, \dot\gamma)}{\dot\gamma^2}$$

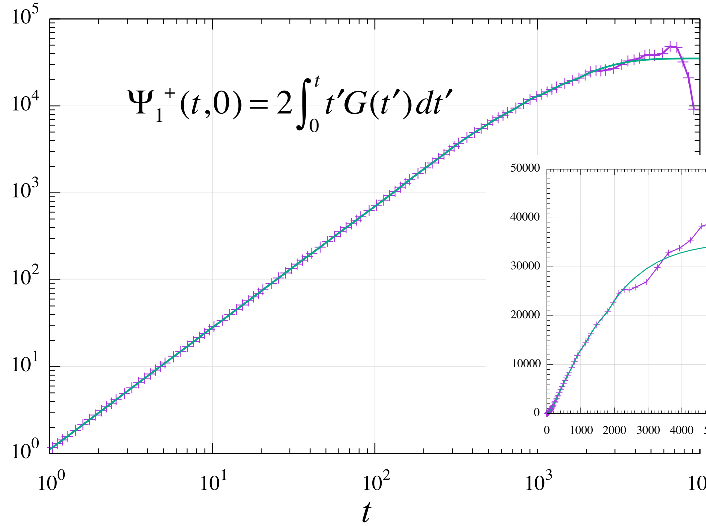
$N_1(t, \dot\gamma) =$ ずり速度 $\dot\gamma$ で流動開始後、時間 t 経過時の N_1

$$\Psi_1^+(t, 0) = 2\int_0^t t' G(t')\,dt'$$

Rouseモデルなどで成り立つ

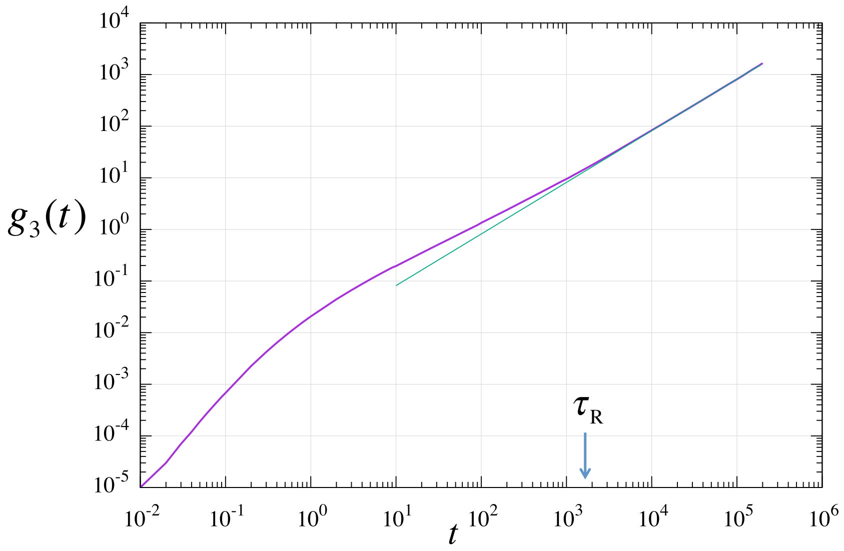
(Rouseモデルでは $N_2 = 0$)

法線応力差係数の予測(2)

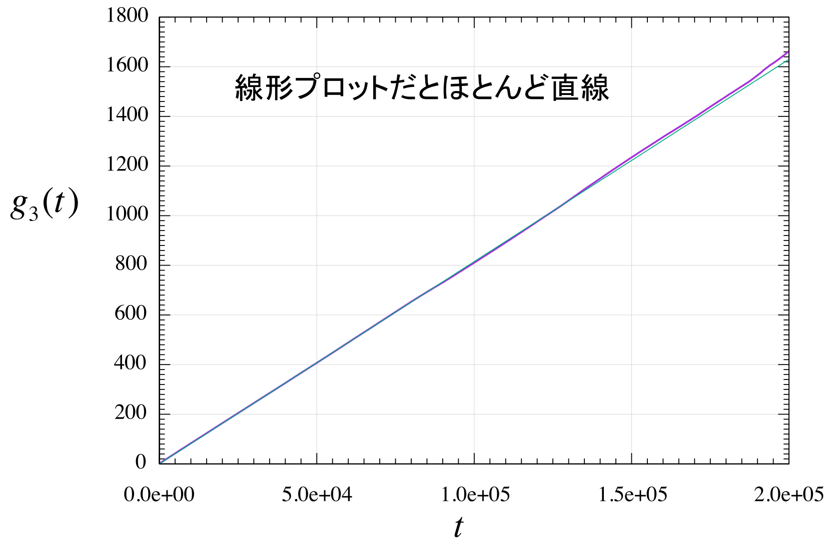


$$\Psi_1(0) = 2A_G$$
$$\approx 3.5 \times 10^4$$

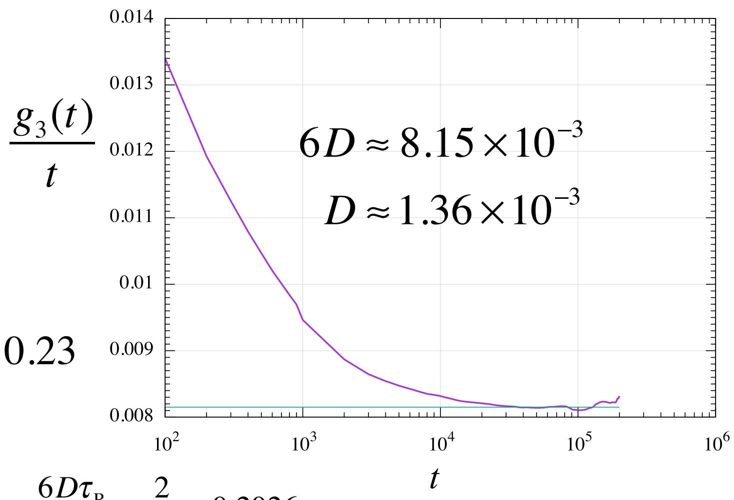
重心拡散: $g_3(t)$



重心拡散



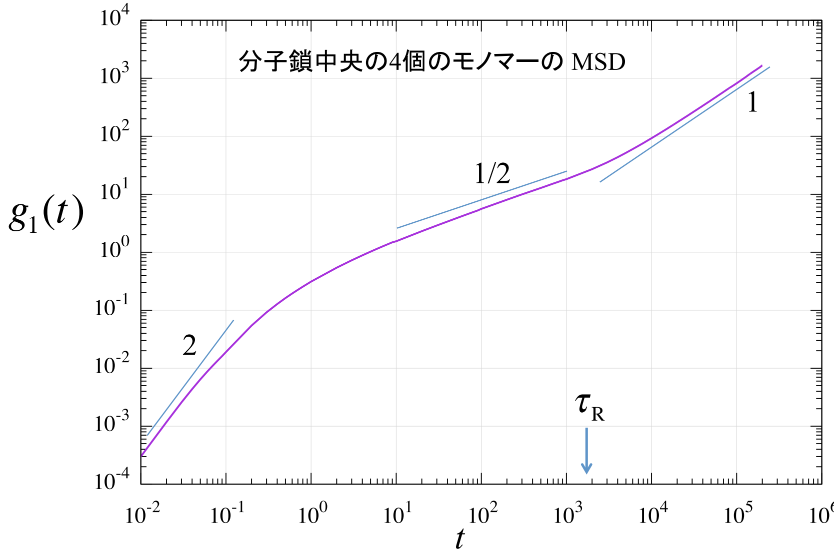
拡散係数の見積もり



$$\frac{6D\tau_R}{\langle \mathbf{R}^2 \rangle} \approx 0.23$$

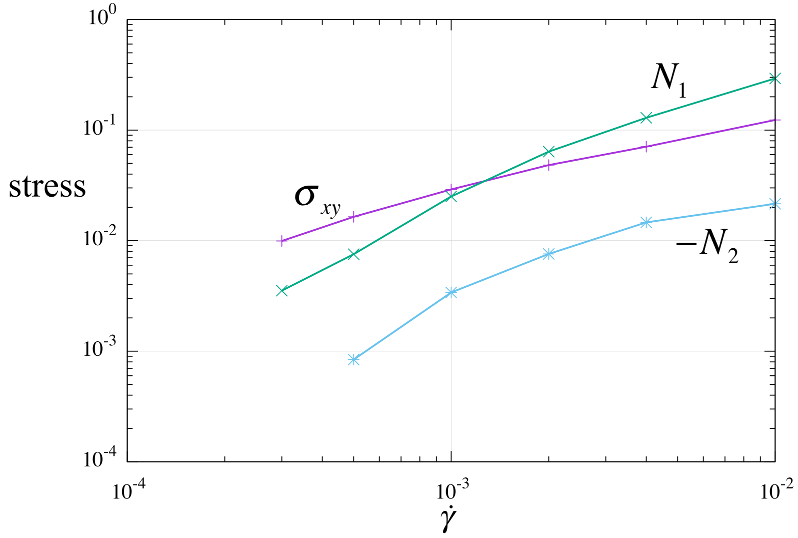
Rouseモデル $\dfrac{6D\tau_R}{\langle \mathbf{R}^2 \rangle} = \dfrac{2}{\pi^2} = 0.2026$

モノマーの拡散: $g_1(t)$

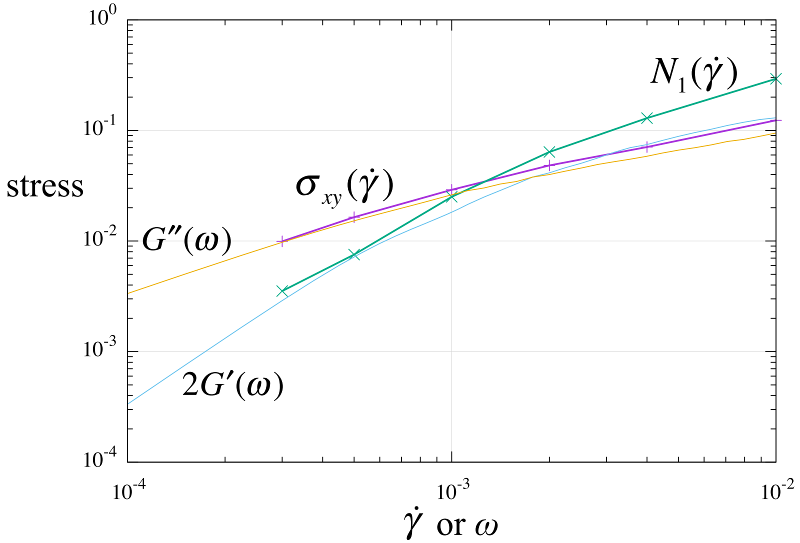


定常ずり流動

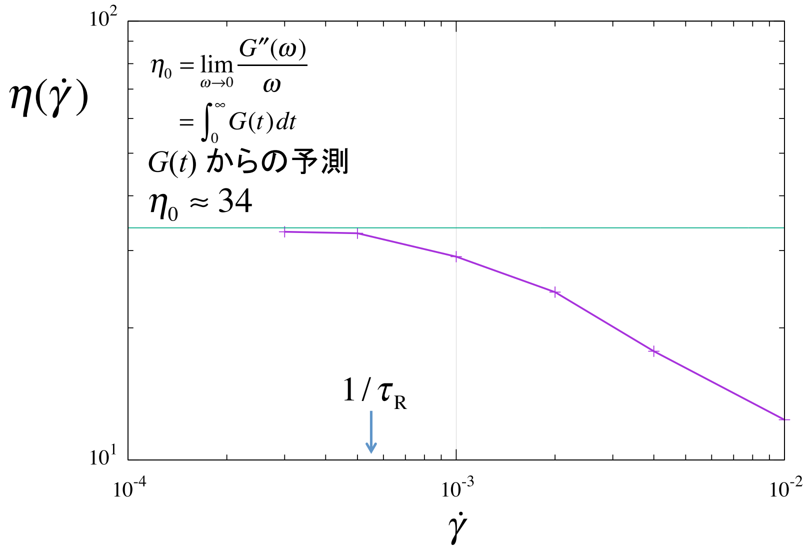
flow curve



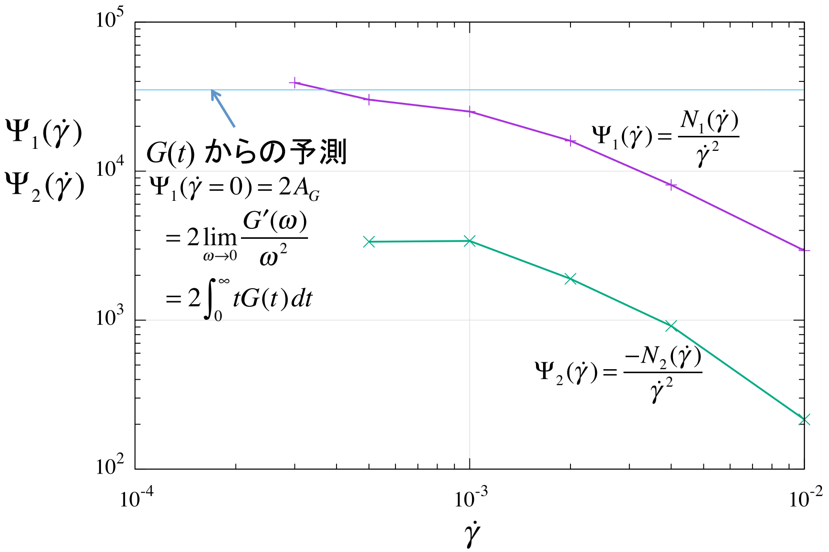
動的粘弾性との比較



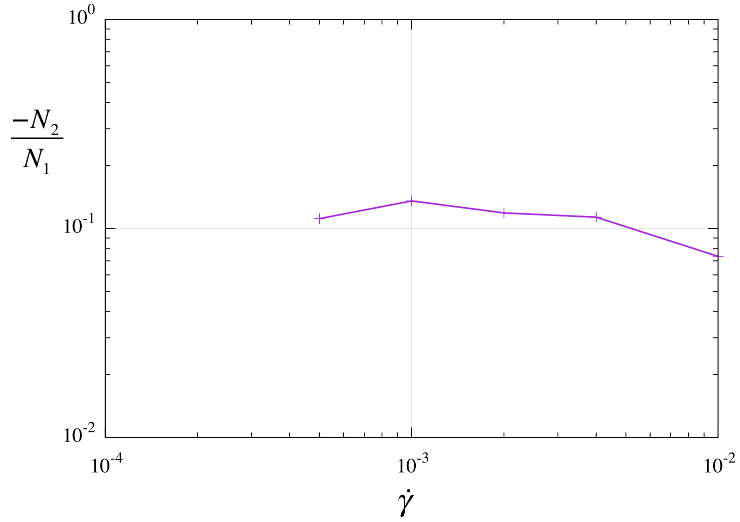
steady shear viscosity



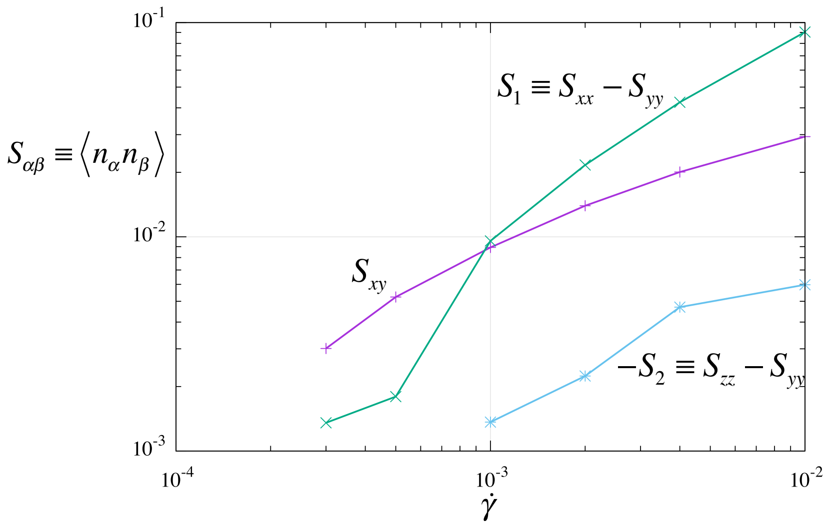
Normal stress coefficients



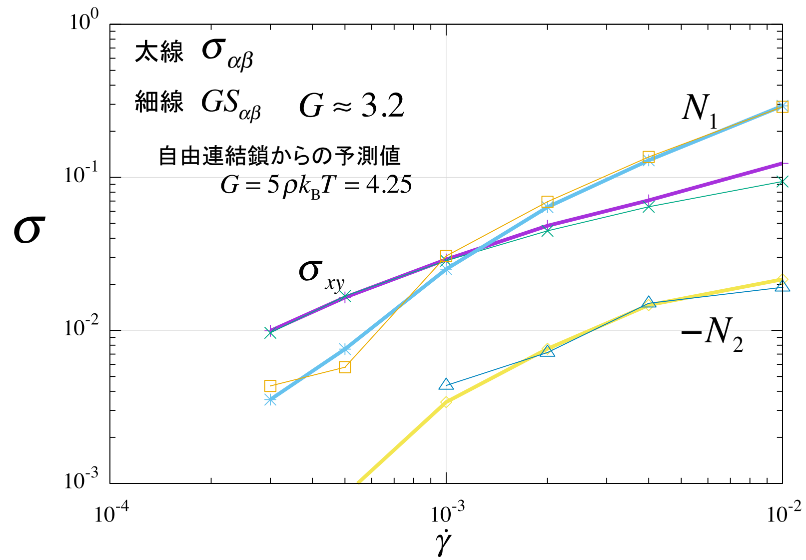
法線応力差比



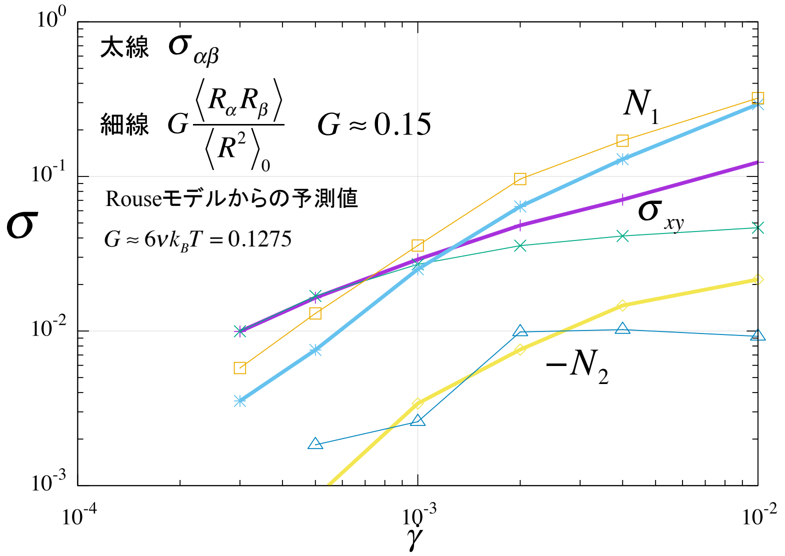
Bond orientation



Stress-optical rule



応力と $<R_\alpha R_\beta>$ の比較

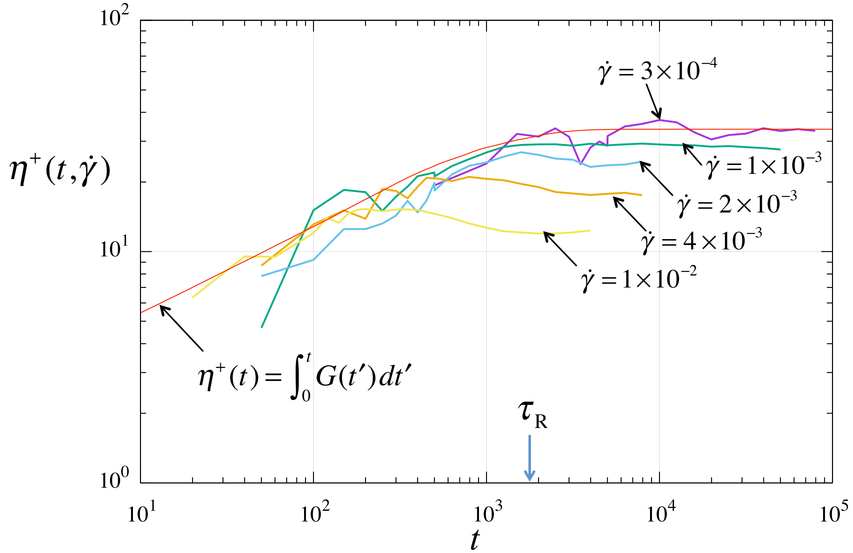


start-up flow

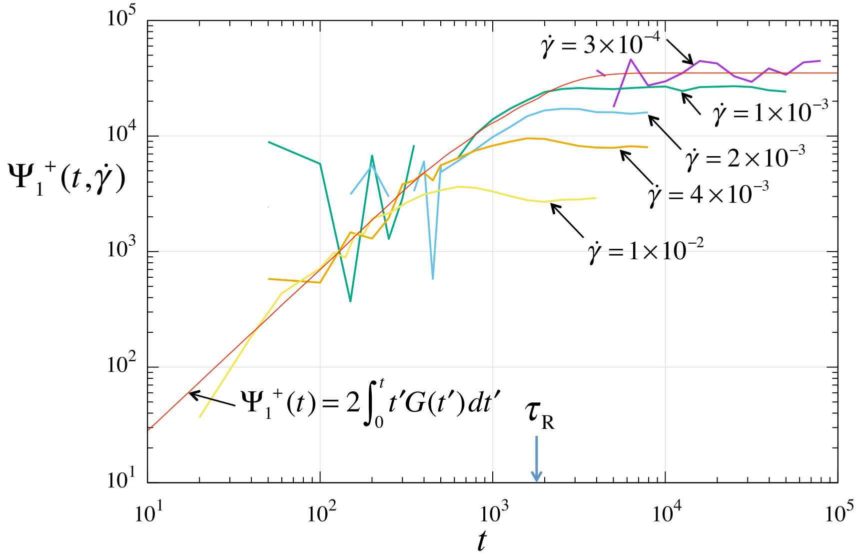
shear

uniaxial

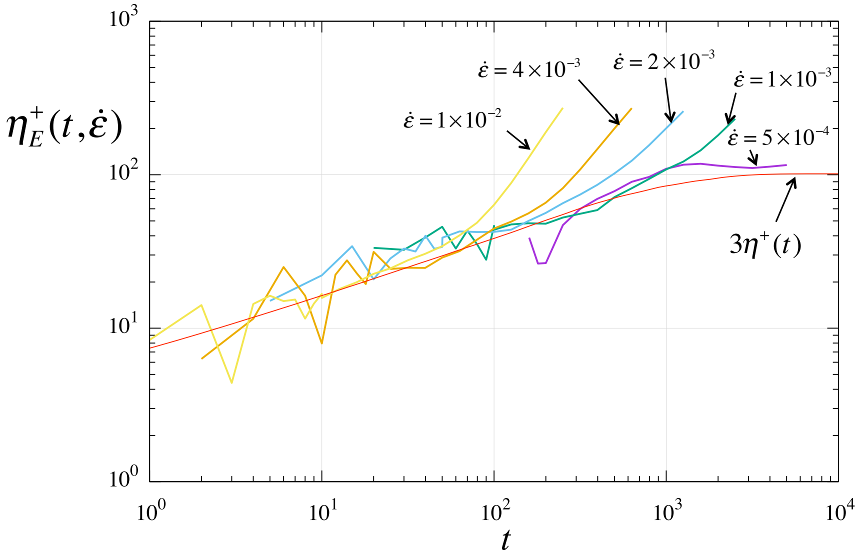
粘度成長曲線



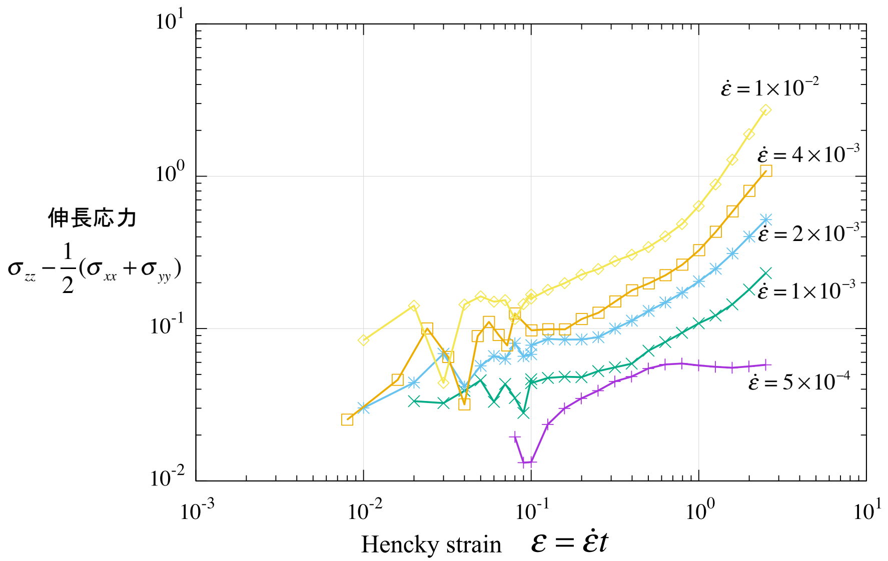
N_1 の成長曲線



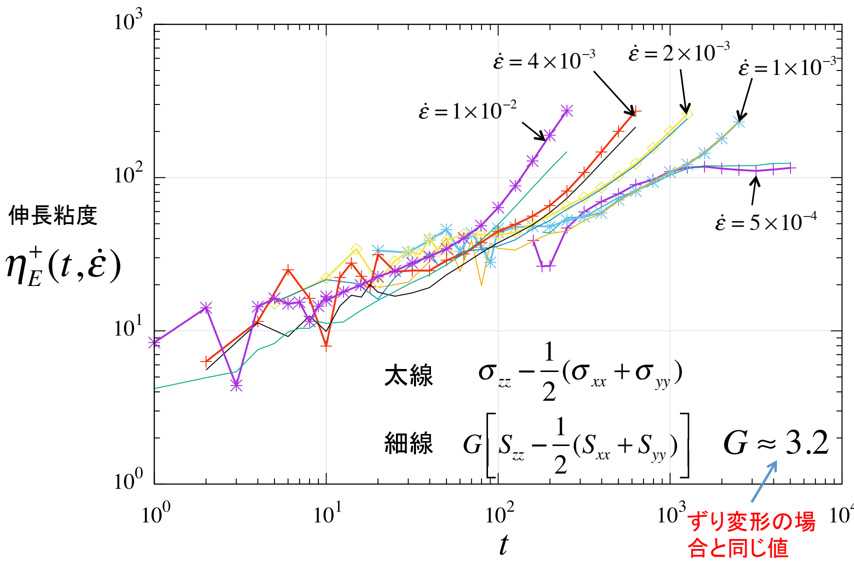
伸長粘度



stress-strain curve



Stress-optical rule



Stress-optical rule