

Fitting Linear-Viscoelastic Spectra to G' , G'' data

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Single-Mode Maxwell Model

$$\underline{\underline{\tau}} + \frac{\eta_0}{G} \frac{\partial \underline{\underline{\tau}}}{\partial t} = -\eta_0 \underline{\underline{\dot{\gamma}}}$$

$$\underline{\underline{\tau}}(t) = - \int_{-\infty}^t \left(\frac{\eta_0}{\lambda} \right) e^{-(t-t')/\lambda} \underline{\underline{\dot{\gamma}}}(t') dt'$$

λ relaxation time parameter

$$g = \frac{\eta_0}{\lambda} \quad \text{modulus parameter}$$

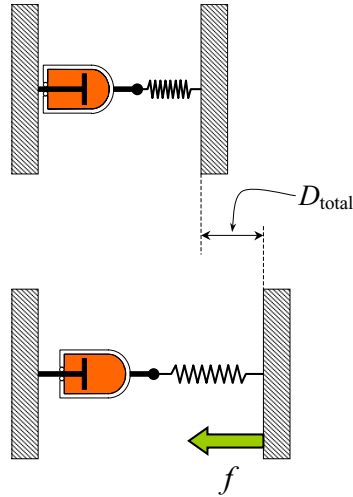
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Maxwell's model combines viscous and elastic responses

Spring (elastic) and dashpot (viscous) in series:

initial state
no force



final state
force, f , resists displacement

Displacements are additive:

$$D_{total} = D_{spring} + D_{dashpot}$$

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Predictions of the (single-mode) Maxwell Model

$$\underline{\underline{\tau}} + \frac{\eta_0}{G} \frac{\partial \underline{\underline{\tau}}}{\partial t} = -\eta_0 \underline{\underline{\dot{\gamma}}}$$

$$\underline{\underline{\tau}}(t) = - \int_{-\infty}^t \left(\frac{\eta_0}{\lambda} \right) e^{-(t-t')/\lambda} \underline{\underline{\dot{\gamma}}}(t') dt'$$

Step shear strain

$$G(t) = \frac{\eta_0}{\lambda} e^{-t/\lambda}$$

$$G_{\Psi_1} = G_{\Psi_2} = 0$$

Does predict a reasonable relaxation function in step strain (but no normal stresses again).

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Step Shear Strain Material Functions

Kinematics:

$$\underline{v} \equiv \begin{pmatrix} \dot{\zeta}(t)x_2 \\ 0 \\ 0 \end{pmatrix}_{123} \quad \dot{\zeta}(t) = \lim_{\varepsilon \rightarrow 0} \begin{cases} 0 & t < 0 \\ \dot{\gamma} & 0 \leq t < \varepsilon \\ 0 & t \geq \varepsilon \end{cases}$$

$$j\varepsilon = \text{constant} = \gamma_0$$

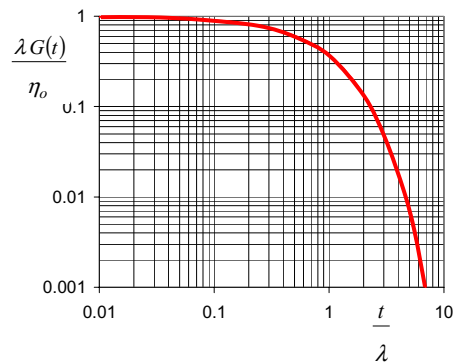
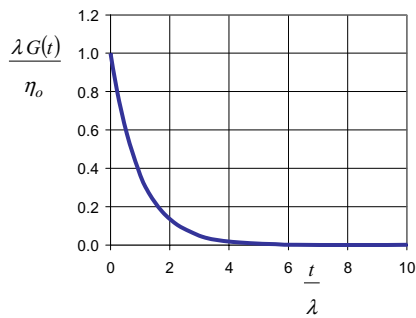
Material Functions:

$G(t, \gamma_0) \equiv \frac{-\tau_{21}(t, \gamma_0)}{\gamma_0}$	First normal-stress relaxation modulus	$G_{\Psi_1} \equiv \frac{-(\tau_{11} - \tau_{22})}{\gamma_0^2}$
Relaxation modulus	Second normal- stress relaxation modulus	$G_{\Psi_2} \equiv \frac{-(\tau_{22} - \tau_{33})}{\gamma_0^2}$

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Step-Shear-Strain Material Function $G(t)$ for Maxwell Model



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Comparison to experimental data

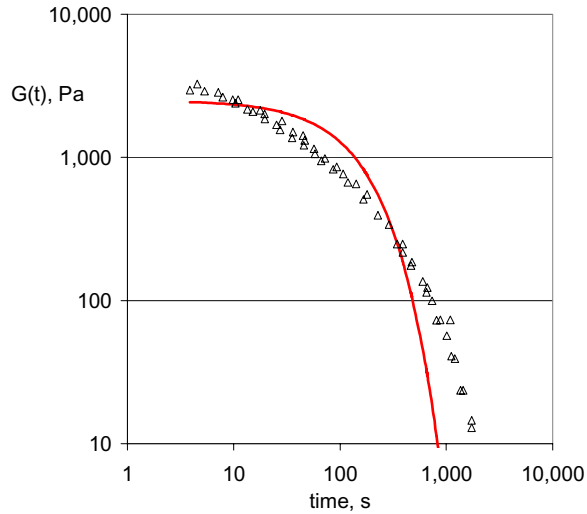


Figure 8.4, p. 274 data from Einaga et al., PS 20% soln in chlorinated diphenyl

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We can improve this fit by adjusting the Maxwell model to allow multiple relaxation modes

$$\underline{\tau}_{(k)} = - \int_{-\infty}^t \left(\frac{\eta_k}{\lambda_k} \right) e^{-(t-t')/\lambda_k} \underline{\dot{\gamma}}(t') dt'$$

$$\underline{\tau}(t) = \sum_{k=1}^N \underline{\tau}_{(k)}$$

**Generalized
Maxwell
Model**

$$\underline{\tau} = - \int_{-\infty}^t \left[\sum_{k=1}^N \frac{\eta_k}{\lambda_k} e^{-(t-t')/\lambda_k} \right] \underline{\dot{\gamma}}(t') dt'$$

2N parameters (can fit *anything*)

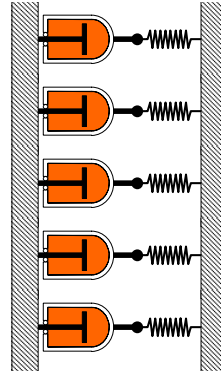
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Generalized Maxwell model combines Maxwell-elements in parallel

5 element Maxwell model is equivalent to this physical system:

$$\tau = - \int_{-\infty}^t \left[\sum_{k=1}^5 \frac{\eta_k}{\lambda_k} e^{-(t-t')/\lambda_k} \right] \dot{\gamma}(t') dt'$$



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Predictions of the Generalized Maxwell Model

$$\tau = - \int_{-\infty}^t \left[\sum_{k=1}^N \frac{\eta_k}{\lambda_k} e^{-(t-t')/\lambda_k} \right] \dot{\gamma}(t') dt'$$

Step shear strain

$$G(t) = \sum_{k=1}^N \frac{\eta_k}{\lambda_k} e^{-t/\lambda_k}$$

$$G_{\Psi_1} = G_{\Psi_2} = 0$$

This function can fit **any** observed data; note that the GMM does not predict shear normal stresses.

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Fitting G(t) to Generalized Maxwell Model

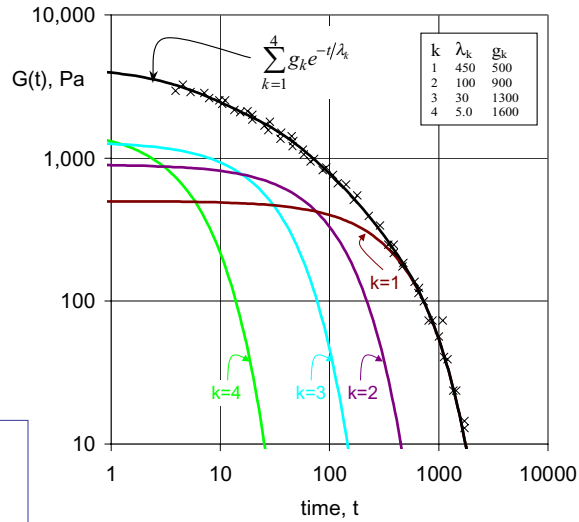


Figure 8.4, p. 274 data from Einaga et al., PS 20% soln in chlorinated diphenyl

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Small-Amplitude Oscillatory Shear Material Functions

Kinematics:

$$\underline{v} \equiv \begin{pmatrix} \dot{\zeta}(t)x_2 \\ 0 \\ 0 \end{pmatrix}_{123}$$

$$\begin{aligned} \dot{\zeta}(t) &= \dot{\gamma}_0 \cos \omega t \\ \gamma_0 &\equiv \frac{\dot{\gamma}_0}{\omega} \end{aligned}$$

Material Functions:

$$\frac{-\tau_{21}(t, \gamma_0)}{\gamma_0} = G' \sin \omega t + G'' \cos \omega t$$

$$G'(\omega) \equiv \frac{\tau_0}{\gamma_0} \cos \delta$$

Storage modulus

(δ is the phase difference between stress and strain)

$$G''(\omega) \equiv \frac{\tau_0}{\gamma_0} \sin \delta$$

Loss modulus

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Predictions of the Generalized Maxwell Model (GMM)

$$\underline{\tau} = - \int_{-\infty}^t \left[\sum_{k=1}^3 \frac{\eta_k}{\lambda_k} e^{-(t-t')/\lambda_k} \right] \underline{\gamma}(t') dt'$$

Small-amplitude
oscillatory shear

GMM

$$G'(\omega) = \sum_{k=1}^N \frac{\eta_k \lambda_k \omega^2}{1 + (\lambda_k \omega)^2}$$

$$G''(\omega) = \sum_{k=1}^N \frac{\eta_k \omega}{1 + (\lambda_k \omega)^2}$$

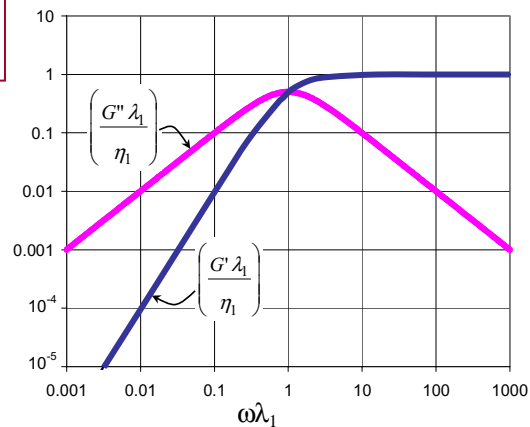
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Predictions of (single-mode) Maxwell Model in SAOS

$$G'(\omega) = \frac{g_1 \lambda_1^2 \omega^2}{1 + (\lambda_1 \omega)^2} = \frac{\eta_1 \lambda_1 \omega^2}{1 + (\lambda_1 \omega)^2}$$

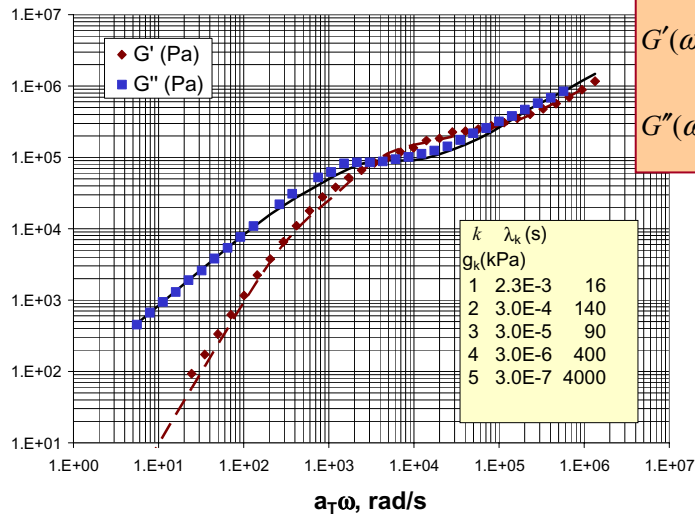
$$G''(\omega) = \frac{g_1 \lambda_1 \omega}{1 + (\lambda_1 \omega)^2} = \frac{\eta_1 \omega}{1 + (\lambda_1 \omega)^2}$$



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Predictions of (multi-mode) Maxwell Model in SAOS



$$G'(\omega) = \sum_{k=1}^N \frac{\eta_k \lambda_k \omega^2}{1 + (\lambda_k \omega)^2}$$

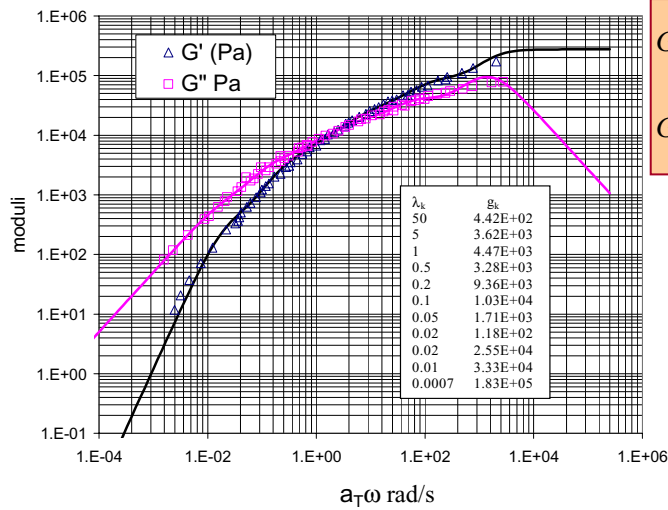
$$G''(\omega) = \sum_{k=1}^N \frac{\eta_k \omega}{1 + (\lambda_k \omega)^2}$$

Figure 8.8, p. 284
data from
Vinogradov, PS melt

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Predictions of (multi-mode) Maxwell Model in SAOS



$$G'(\omega) = \sum_{k=1}^N \frac{\eta_k \lambda_k \omega^2}{1 + (\lambda_k \omega)^2}$$

$$G''(\omega) = \sum_{k=1}^N \frac{\eta_k \omega}{1 + (\lambda_k \omega)^2}$$

Figure 8.10, p. 286
data from Laun, PE
melt

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**We can use Excel Solver to
solve for the parameters of the
GMM model.**

Demo file:

www.chem.mtu.edu/~fmorriso/cm4650/Demo_fitting_LVE_spectrum_new.xls

Reference: Faith A. Morrison, *Understanding Rheology*, Oxford, 2001, pp281-285

See also *Rheology Bulletin*, January 2007, volume 76(2), article by J. M. Dealy for discussion of significance of relaxation spectra.

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