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**DYNAMIC MECHANICAL PROPERTY
PREDICTION BY GROUP INTERACTION
MODELLING**

J.P. Szabo, W.M. Davis, and R. Petitpas

**Defence
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Establishment
Atlantic**



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Approved by: R.M. Morchat
Head / Dockyard Laboratory (Atlantic)

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Abstract

Group Interaction Modelling (GIM) is a new procedure that relates the chemical structure of polymers to real-world observables. In this work, the equations specific to calculating the complex moduli of polymers were presented and implemented in MATLAB. GIM was used to calculate the mechanical moduli of several polymers and some differences were found when the results were compared to values presented in earlier work. Two problems with the GIM modelling of dynamic mechanical moduli were identified and explored. The first problem deals with the GIM variable $\tan D_g$, which should be always a positive number, but in fact was found to be negative in some cases. The second problem identified was the behaviour of the modulus in the complex plane, which was not consistent with the behaviour of thermorheologically simple materials.

Résumé

La modélisation d'interaction de groupes (MIG) est une nouvelle méthode permettant de relier la structure chimique des polymères aux phénomènes observables dans le monde réel. Dans ces travaux, nous avons présenté et appliqué dans le MATLAB les équations spécifiques permettant de calculer les modules complexes des polymères. Les modules mécaniques de plusieurs polymères ont été calculés par modélisation MIG; nous avons constaté certaines différences lorsque nous avons comparé les résultats avec les valeurs obtenues au cours de travaux précédents. Nous avons décelé, dans la modélisation MIG des modules mécaniques dynamiques, deux problèmes que nous avons ensuite examinés. Le premier a trait à la variable $\tan d_g$; en effet, cette variable doit toujours être un nombre positif, mais nous avons constaté qu'elle était parfois définie par un nombre négatif. L'autre problème a trait au comportement du module dans le plan complexe, qui ne concordait pas toujours au comportement de matières thermorhéologiquement simples.

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Dynamic Mechanical Property Prediction by Group Interaction Modelling

J.P. Szabo, W.M. Davis, and R. Petitpas

EXECUTIVE SUMMARY

Introduction

The purpose of this work was to examine a relatively new theory known as Group Interaction Modelling (GIM) used to model the physical properties of polymers, and was part of a TTCP study of polymer modelling. This work consisted of the implementation of GIM equations into a computer program designed to predict several physical properties of the polymer including the glass transition temperature, the loss tangent and several mechanical moduli as a function of frequency and temperature.

Principal Results

The GIM equations describing dynamic mechanical behaviour of polymers were successfully implemented using MATLAB code. Example calculations carried out with this program identified some differences with previously reported results, and two significant areas where GIM requires clarification or re-work. One area is the behaviour of the Cole-Cole plot, which should be invariant of frequency and temperature. A second issue identified was the GIM variable $\tan D_g$, which had several definitions and was not always "well-behaved".

Significance of the Results

The results of this study are significant to those who wish to use GIM as a tool for predicting the complex moduli of polymers. It identifies several aspects of this theory that need to be addressed.

Future Plans

GIM will continue to be examined as a tool for modelling polymers, and work at DREA will emphasize support of TTCP collaborative research.

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1. Introduction

Polymers are used in a variety of ways to decrease the acoustic signature of naval vessels. In particular, vibration isolation materials, flexible couplings, structural damping materials, and external hull decoupling materials may be used to decrease the passive sonar signature of ships and submarines. Anechoic coatings are used to decrease the active sonar signature of submarines. The performance of these materials depends strongly on their dynamic mechanical moduli, which are both temperature and frequency dependent. The design and optimization of polymers for sound and vibration damping may be aided by models which link the chemical structure of a polymer to its dynamic mechanical properties.

The primary objective of polymer modelling is to predict engineering properties of a polymer quantitatively as a function of basic polymer parameters. A specific model used to allow the prediction of dynamic mechanical properties is the Group Interaction Modelling (GIM) method developed by David Porter [1]. GIM predicts bulk engineering properties of a polymer from its chemical and morphological structure. As the name suggests, GIM uses the intermolecular energy of interaction between groups of atoms in adjacent polymer chains as a basis for predicting these properties. With the exception of Reference 1, very little has been published on the application of GIM to the calculation of dynamic mechanical properties of polymers. The purpose of this work was to implement GIM equations for prediction of dynamic mechanical properties using MATLAB [2], and to test this software on several polymers. This report presents the relevant GIM equations and details the results of the GIM implementation.

2. DMTA Measurements

The tensile storage modulus and loss factor for a nitrile rubber were measured to give us some experimental comparisons for Cole-Cole plots. These experiments were carried out using a Dupont DMA 983 Dynamic Mechanical Thermal Analysis (DMTA) instrument in multi-fixed frequency mode. The sample was 20.10 x 11.80 x 3.31 mm in size, the oscillation amplitude was 0.3 mm, and measurements were made at 5°C intervals from -90°C to 15°C at 0.05, 0.1, 0.2, 0.5, 1, 3, 5, and 10 Hz.

3. Theoretical Background and Implementation

This section will briefly present the key equations necessary to model dynamic mechanical properties of polymers. The reader is referred to David Porter's book, *Group Interaction Modelling of Polymer Properties* [1], for a detailed discussion of GIM theory and derivation of equations. Note that the equation numbers used here are the same as in Porter's book, except for those labelled with a letter, which were derived from GIM equations. GIM uses five model parameters specific to each polymer:

GIM Parameter	Units	Description
M	g/mole	Molecular weight of the mer unit
V _w	cm ³ /mole	Volume of the mer unit
E _{coh}	J/mole	Cohesive energy
N	(mer unit) ⁻¹	Number of skeletal modes of vibration
θ ₁	K	Reference temperature of skeletal modes
L	M	Length of a mer unit in the chain axis

The derivations presented in Reference 1 do not consistently carry forward the units for numerical constants which appear in the equations. M, V_w, and L are calculated directly from the monomer structure. The cohesive energy can be found experimentally using solubility or, alternatively, calculated using several textbook methods [3]. The remaining parameters are calculated using the GIM selection rules outlined in Porter's book. MATLAB [2] was used to create programs incorporating the equations presented below.

We begin by first defining τ₀, the free relaxation time of skeletal mode oscillations.

$$\tau_0 = \frac{h}{2\pi k\theta_1} \quad (3.4.10)$$

where h is Plank's constant and k is Boltzmann's constant. τ₀ is used in calculation of the glass transition temperature (T_g) for the polymer at various frequencies.

A basic GIM expression is

$$T_{g1} = 0.224\theta_1 + 0.0513 \frac{E_{coh}}{N} \quad (3.2.9)$$

where T_{g1} is the glass transition temperature at ω = 1 rad/s.

The lower limiting value of the glass transition temperature, T_{g0}, may be approximated [1] by

$$T_{g0} = T_{g1} - 50$$

The frequency dependence of the glass transition temperature is given by equation 3.4.4

$$T_g = 0.224\theta_1 + 0.0513 \frac{E_{coh}}{N} \frac{1.25}{(1 + 0.5 \exp(-\omega\tau))} \quad (3.4.4)$$

where τ is the characteristic time of mer unit oscillations or relaxation events, and is given by equation 3.4.12

$$\tau = \tau_0 \exp\left(\frac{1280 + 50 \ln \theta_1}{T - T_{g0}}\right) \quad (3.4.12)$$

The glass transition temperature may be calculated by setting $T = T_g$ in 3.4.12, and simultaneously solving 3.4.4 and 3.4.12 for T_g . There is no analytical solution to this problem, but we have found several ways to solve for T_g numerically. For example, Figure 1 shows the glass transition temperature for poly(styrene) calculated using equation 3.4.4. and the GIM parameters in Table 1. In this calculation τ is calculated over a range of temperatures according to equation 3.4.12. The T_g for a particular frequency is determined by finding the point on the line at which $T = T_g$. The solid line in Figure 1 shows that for $\omega = 1$ rad/s, $T_g = 99^\circ\text{C}$ and at $\omega = 100$ rad/s, $T_g = 107.7^\circ\text{C}$. If this procedure is repeated over a range of frequencies, then a plot of T_g versus frequency may be constructed as in Figure 2. Since the low frequency region of these plots is not smooth, a 4th order polynomial was fit to this region in our procedure to determine $T_g(\omega)$. The shape of this plot is very similar to the plot illustrated on page 314 of Reference 1.

It should be noted that the procedure described in the paragraph above is not detailed in Reference 1, and was developed here in order to have a consistent and logical method of calculating $T_g(\omega)$. In Reference 1, the approximation

$$T_g = T_{g1} + 4\log(\omega)$$

is used frequently. As shown in Figure 2, this approximation is useful for frequencies close to $\omega = 1$.

Porter assumes that the profile of the loss peak is a Gaussian function, with a width s that is dependent on the glass transition temperature:

$$s = 6 \left[\frac{T_g - T_{go}}{50} \right]^2 \quad (4.2.21)$$

Then next two equations, 4.4.20 and 4.2.15, are necessary for the calculation of $\tan D_g$, the local value of volumetric loss tangent

$$\Delta T_g = 4.4 \frac{(T_g - T_{go})^2}{50^2} \quad (4.4.20)$$

$$B_{gam} = 5.68 \frac{E_{coh}}{V_w} \times 10^6 \quad (4.2.15)$$

B_{gam} is the bulk modulus of the polymer in the glassy state.

An equation for $\tan D_g$ is derived using

$$\tan D_g = \frac{1.5 \times 10^5 L \Delta B_g}{\theta_1 M \Delta T_g} \quad (4.2.12)$$

and

$$\Delta B_g = B_{gam} (0.1 + 0.9 \tan D_g) \quad (4.2.17)$$

From 4.2.12 and 4.2.17, it follows that

$$\tan D_g = \frac{0.1}{\frac{\theta_1 M \Delta T_g}{1.5 \times 10^5 L B_{gam}} - 0.9} \quad (a)$$

The real part of the bulk modulus can now be calculated in the following manner:

$$B(T) = B_{gam} - \Delta B_g \int_0^T 0.067 \exp \left[\frac{-(T - T_g)^2}{2s^2} \right] dT \quad (4.2.19)$$

The loss factor associated with the bulk modulus is related to the derivative dB/dT

$$\tan d_B = \frac{1.5 \cdot 10^5}{\theta_1 M} \left(\frac{dB}{dT} \right) \quad (4.2.22)$$

Combining 4.2.19 and 4.2.22, we get

$$\tan d_B = \frac{1.5 \cdot 10^5}{\theta_1 M} 0.067 \exp \left[\frac{-(T - T_g)^2}{2s^2} \right]$$

T_g and s are used to calculate $P(T_g)$, the fractional distribution of glass transition events.

$$P(T_g) = \frac{1}{s\sqrt{2\pi}} \exp - \left(\frac{(T - T_g)^2}{2s^2} \right) \quad (4.3.29)$$

$P(T_g)$ is used in the calculation of $\tan \Delta_g(T)$, the cumulative loss tangent.

$$\tan \Delta_g(T) = \int_0^T P(T_g) \cdot \tan \Delta_g dT \quad (4.3.30)$$

$$\tan \Delta_g = 0.0085 \frac{E_{\text{coh}}}{N_c} \quad (4.3.11)$$

The GIM expression for the tensile modulus is a function of $B(T)$ and $\tan \Delta_g(T)$, as presented below:

$$E(T) = \frac{B(T)}{(1 + \tan \Delta_g(T))^2} \quad (4.3.32)$$

The final function we are interested in being able to calculate is the loss tangent, $\tan d_E$, associated with the tensile modulus.

$$\tan d_E = \frac{\tan \Delta_g}{s\sqrt{2\pi}} \exp\left(-\frac{(T - T_g)^2}{2s^2}\right) \quad (4.3.29)$$

4. Results and Discussion

An area of difficulty encountered in this study with the implementation of GIM was in the calculation of $\tan D_g$. Equation (a) above did not always give positive results for $\tan D_g$ (see Table 2). A negative $\tan D_g$ can lead to negative values of ΔB_g (equation 4.2.17), and a bulk modulus B which increases with temperature. Because of this problem, we derived two additional methods for the calculation of $\tan D_g$ from equations in Reference 1.

The second "definition" of $\tan D_g$ arises from the implementation of the first and third terms of equation 4.2.18

$$\frac{\tan D_g}{0.1 + 0.9 \tan D_g} \approx 2 \tan D_g = 1.9 \cdot 10^{11} \frac{LE_{\text{coh}}}{\theta_1 M V_w} \quad (4.2.18)$$

$$\frac{0.1}{\tan D_g} + \frac{0.9 \tan D_g}{\tan D_g} = \frac{1}{1.9 \cdot 10^{11}} \frac{\theta_1 M V_w}{LE_{\text{coh}}}$$

$$\tan D_g = \frac{0.1}{\left[\frac{1}{1.9 \cdot 10^{11}} \frac{V_w \theta_1 M}{E_{\text{coh}} L} - 0.9 \right]} \quad (b)$$

A third "definition" of $\tan D_g$ uses the second and third terms in equation 4.2.18

$$\frac{\tan D_g}{0.1 + 0.9 \tan D_g} \approx 2 \tan D_g = 1.9 \cdot 10^{11} \frac{LE_{coh}}{\theta_1 M V_w} \quad (4.2.18)$$

$$\tan D_g = \frac{1.9 \cdot 10^{11}}{2} \frac{LE_{coh}}{\theta_1 M V_w} \quad (c)$$

It is unclear how the approximation in 4.2.18 was arrived at in Reference 1 and it may be a source of error in the calculation of $\tan D_g$.

The three "definitions", equations (a)-(c), give distinctly different values of $\tan D_g$ and are summarized in Table 2 for 4 polymers. As can be seen from Table 2, methods (a) and (b) give negative values for $\tan D_g$ for some of the polymers. A negative $\tan D_g$ can result in bulk and tensile moduli (equations 4.2.17 and 4.2.19) that increase with temperature, which is not consistent with the normal behaviour of polymers.

Method (a) will also give values dependent on the frequency as a result of ΔT_g appearing in the equation. ΔT_g is a function of the glass transition temperature (equation 4.2.21) which in turn is a function of frequency. Table 2 lists the values for method (a) at $\omega = 1$ rad/s. A change in the frequency has a large effect on the value of $\tan D_g$.

Method (c) always gives positive values of $\tan D_g$. However, the approximation used to get this equation in (4.2.18) is unclear and seems to have no sound theoretical background.

Because of the uncertainties outlined above, a value of $\tan D_g = 0.4$ was used for the calculations which follow, as this value has been suggested as representative of many polymers [4].

The values of T_{g1} , T_g , and s were calculated for poly(styrene), poly(carbonate), poly(styrene-acrylonitrile) and poly(vinyl-acetate) using the equations in Section 3 and compared to those listed in Porter's book [1]. The GIM parameters for these 4 polymers are listed in Table 1 and the results of our calculations are compared to the book values in Table 3. The calculated T_g and T_{g1} values agree to within 3 degrees of those in Reference 1, with the exception of the values for poly(styrene) which differ by about 14 degrees. The most important values to note are those for s which are significantly different for the two data sets.

Equation 4.2.21 implies that s should increase monotonically with the glass transition temperature, which in turn increases with frequency. As Table 3 shows, our calculated values for s increase monotonically with frequency, but those from Reference [1] do not.

Figures 3-5 show the GIM storage modulus, loss modulus, and loss factor for polystyrene, calculated using the equations presented above and the GIM parameters from Table 1.

The shapes of these curves are reasonable, and the direction of the shift of the loss tangent and loss modulus peaks with frequency is in accordance with experiment (Figures 4 and 5). There is also a large decrease in the peak heights and a broadening of the peak as the frequency is increased.

Jones [5,6,7] has shown that for thermorheologically simple polymers, the $\log(\tan \delta)$ versus $\log(\text{storage modulus})$ plot, also known as Wicket plot, forms an inverted U-shaped curve. Furthermore, if the complex modulus of a polymer is determined for various temperatures and frequencies, then all loss factor-modulus points associated with these temperatures and frequencies will lie on a unique curve. Jones has demonstrated this for several polymers, including polystyrene, an acrylic adhesive, a polyvinylchloride copolymer, and a plasticized polyvinylchloride [5,6].

It follows from the above that the Cole-Cole plot (loss modulus versus storage modulus) should also be invariant to changes in temperature and frequency, as illustrated in Figure 6 for nitrile rubber. In this study, we have tested the complex plane behaviour of the GIM modulus, and found that it does not follow the experimental trends discussed above. Figure 7 shows the Cole-Cole plot for polystyrene, generated using the GIM equations outlined in Section 3. Note that while the GIM Cole-Cole plot has the right shape, it depends on the frequency, which is not observed experimentally for polystyrene [6]. If the peak width s , as defined by equation 4.2.21, is set to $s = 6$, and kept constant with frequency, then the peak height, peak width, and Cole-Cole plot would also be invariant with frequency.

5. Conclusions

This document has illustrated recent attempts at implementing group interaction modelling for the prediction of the dynamic mechanical properties of polymers. MATLAB programs were developed to calculate the bulk modulus, the tensile modulus and the loss tangent of polymers. From the development of these programs, several problems with the implementation of GIM theory were identified. The definition and application of $\tan D_g$ requires clarification. The behaviour of the GIM calculated modulus in the complex plane varies with frequency, which suggests that some basic GIM equations need to be reworked.

Acknowledgements

The authors thank Dr. David Porter for useful discussions. WMD thanks the Natural Sciences and Engineering Research Council of Canada (NSERC) and the Department of National Defence (DND) for a Visiting Fellowship.

Table 1. GIM parameters for the polymers studied in this paper. The units of these quantities are listed in the Table on Page 2.

Polymer	Page*	M_w	V_w	L	E_{coh}	N	θ_1
Poly(styrene)	335	104	66	2.50E-10	36000	6	285
Poly(carbonate)	335	254	139	1.20E-09	83000	14	550
Poly(styrene-acrylonitrile)	367	81	49	2.52E-10	36000	6	323
Poly(vinyl acetate)	337	86	46.6	2.05E-08	36000	8	314

*from Reference 1.

Table 2. Results for tan D_g using the three different definitions.

Polymer	book results*	tan D _g (a)**	tan D _g (b)	tan D _g (c)
Polystyrene (pg.335)	0.43	0.46	0.45	0.44
Poly(vinyl acetate) (pg.337)	0.38	-0.61	-0.56	0.68
Polycarbonate (pg. 335)	0.43	0.97	0.93	0.48
Poly(styrene- acrylonitrile) (pg. 367)	----	-0.61	-0.61	0.67

*The results are taken from the pages listed in Reference 1.

**At $\omega = 1$ rad/s (see text for details).

Table 3. Comparison of results from Reference 1 and this study using the GIM parameters listed in Table 1.

Polymer	ω (rad/s)	Book value*			This work		
		T_{g1} (K)	T_g (K)	s	T_{g1} (K)	T_g (K)	s
Poly(styrene)	1	112	112	6	98.44	98.3	5.96
Poly(styrene-acrylonitrile)	10	108	112	5.2	106.95	110.98	7.00
Poly(carbonate)	100	154	164	3.7	154.14	162.58	8.20
Poly(vinyl acetate)	6000	31	46	10	27.99	47.29	11.53

*from Reference 1.

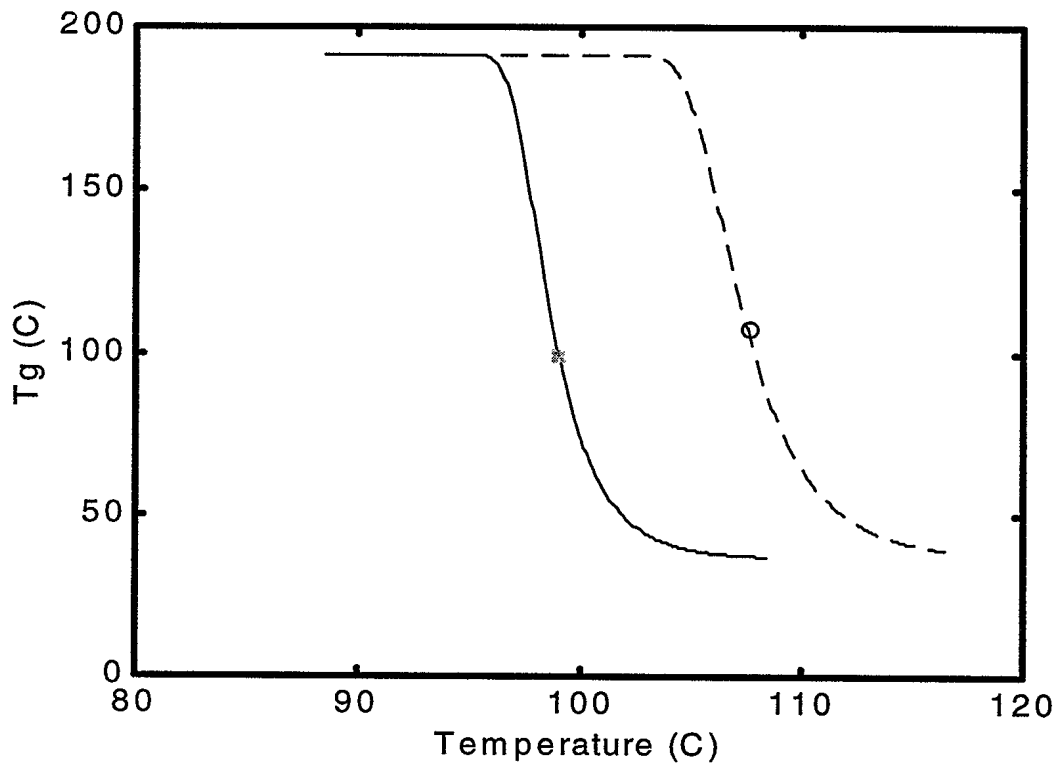


Figure1. Calculated T_g for polystyrene using equations 3.4.4 and 3.4.12 and the GIM values listed in Table 1 over a range of temperatures at $\omega = 1$ (solid line) and $\omega = 100$ rad/s (dashed line). The points represent solutions at $T = T_g = 99.0^\circ\text{C}$ and $T = T_g = 107.7^\circ\text{C}$ for $\omega = 1$ and $\omega = 100$ rad/s, respectively.

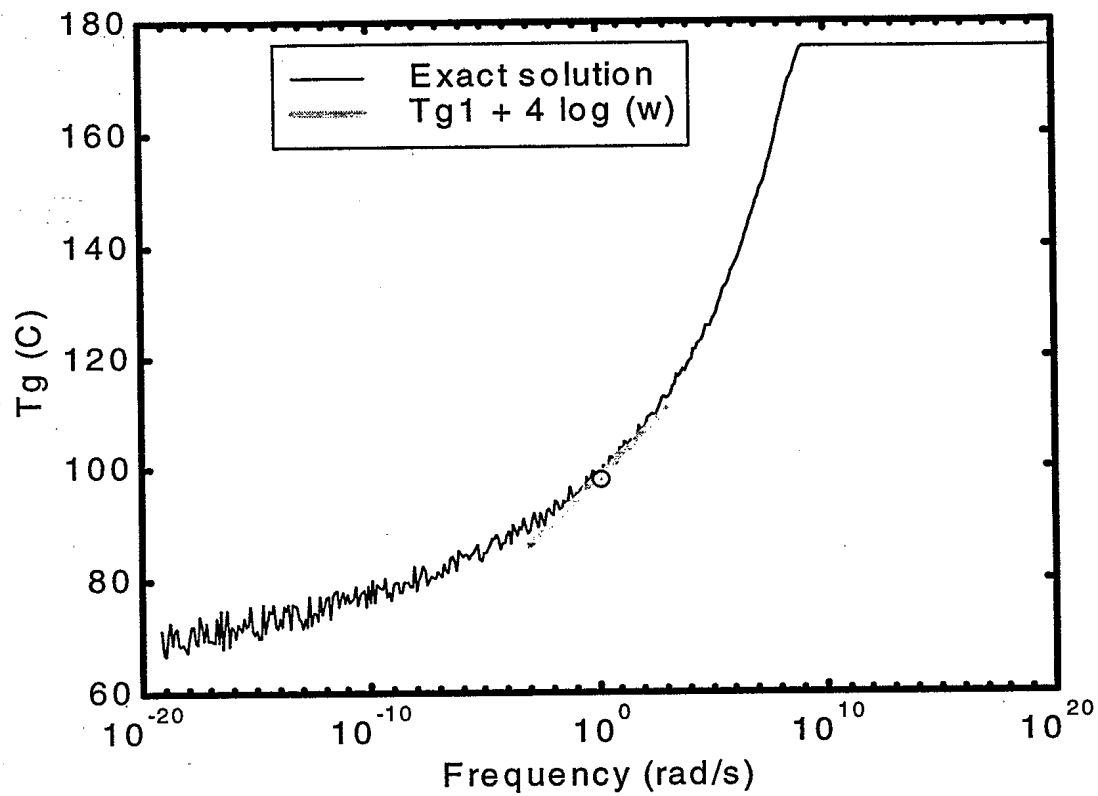


Figure 2. A plot of T_g versus frequency for poly(styrene). The point indicated is the value of T_g at $\omega = 1$ rad/s. The straight line is an approximate solution near $\omega = 1$ rad/s.

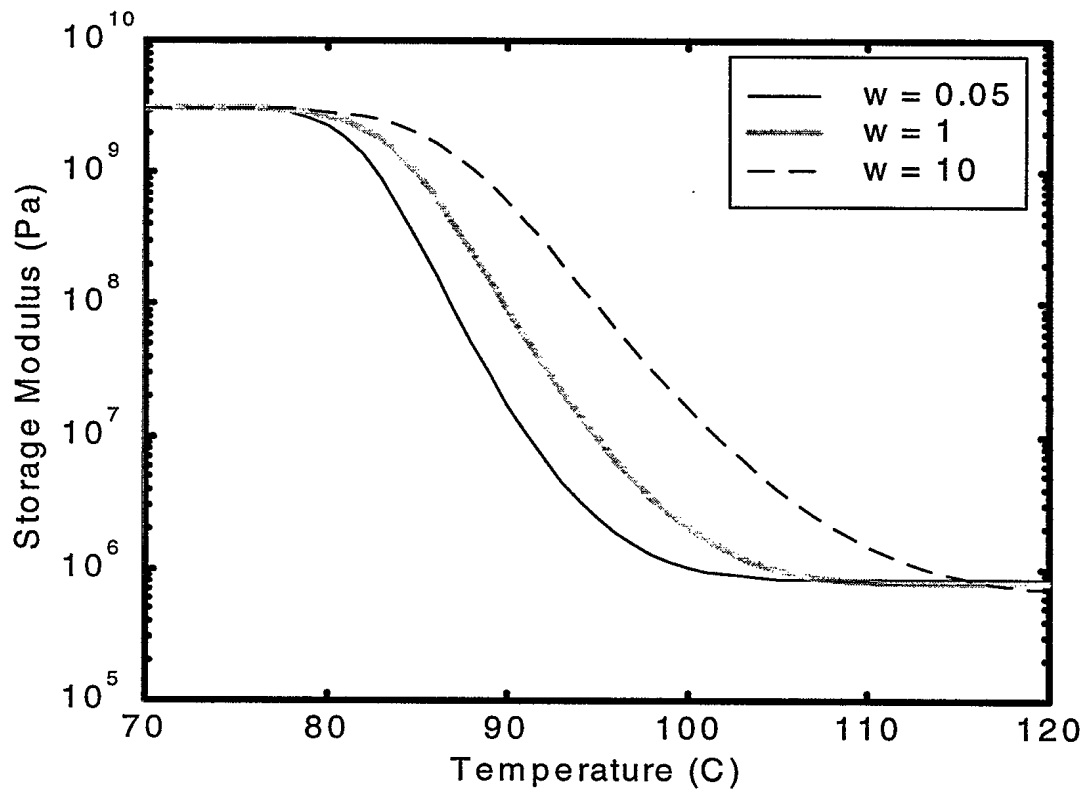


Figure 3. Plot of storage modulus versus temperature for poly(styrene) using GIM at three frequencies (in rad/s).

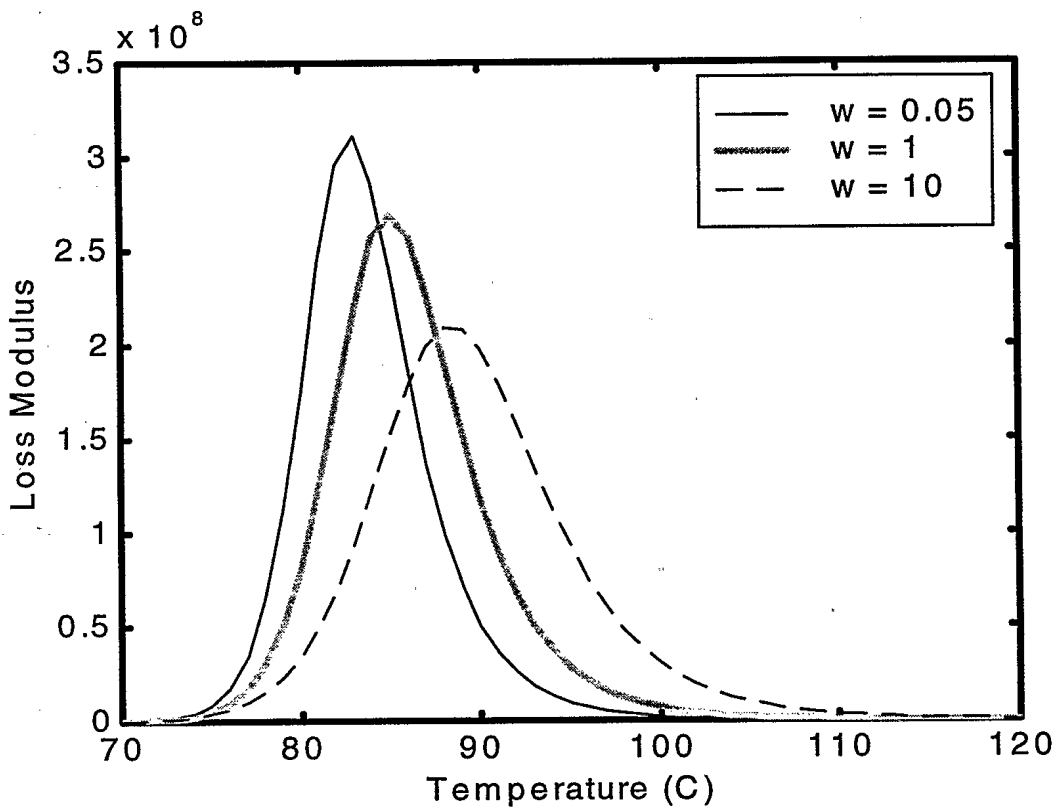


Figure 4. Plot of loss modulus versus temperature for poly(styrene) using GIM at three frequencies (in rad/s).

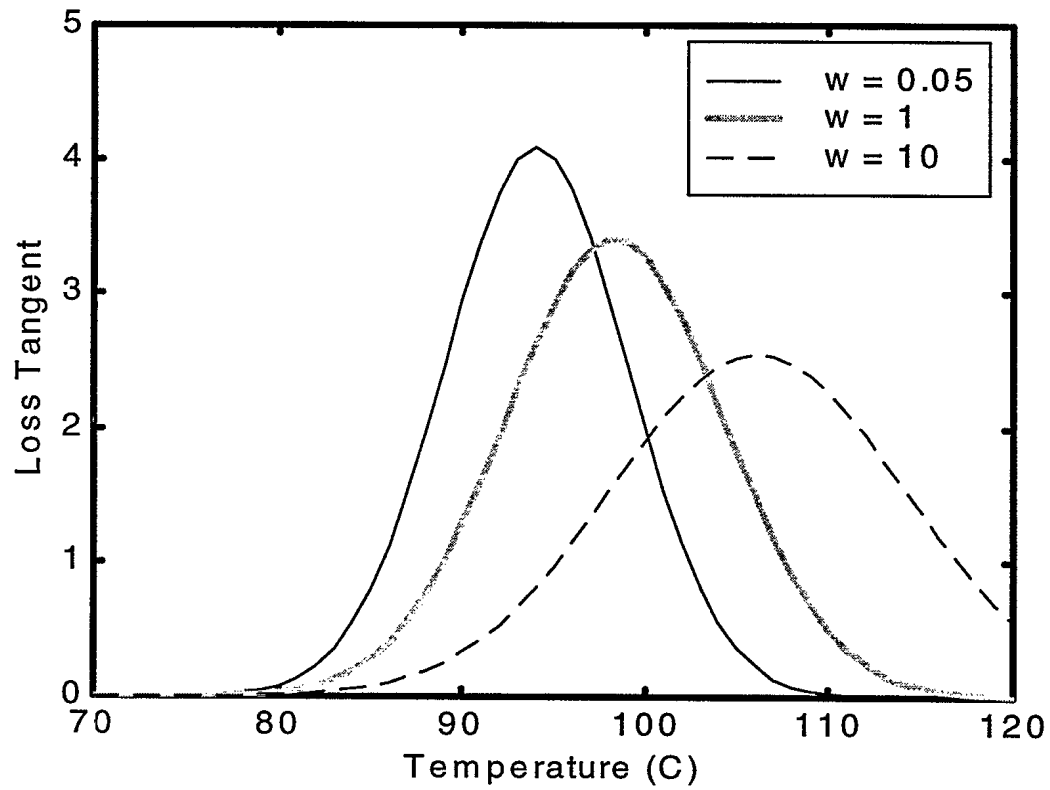


Figure 5: Plot of loss tangent versus temperature for poly(styrene) using GIM at three frequencies (in rad/s).

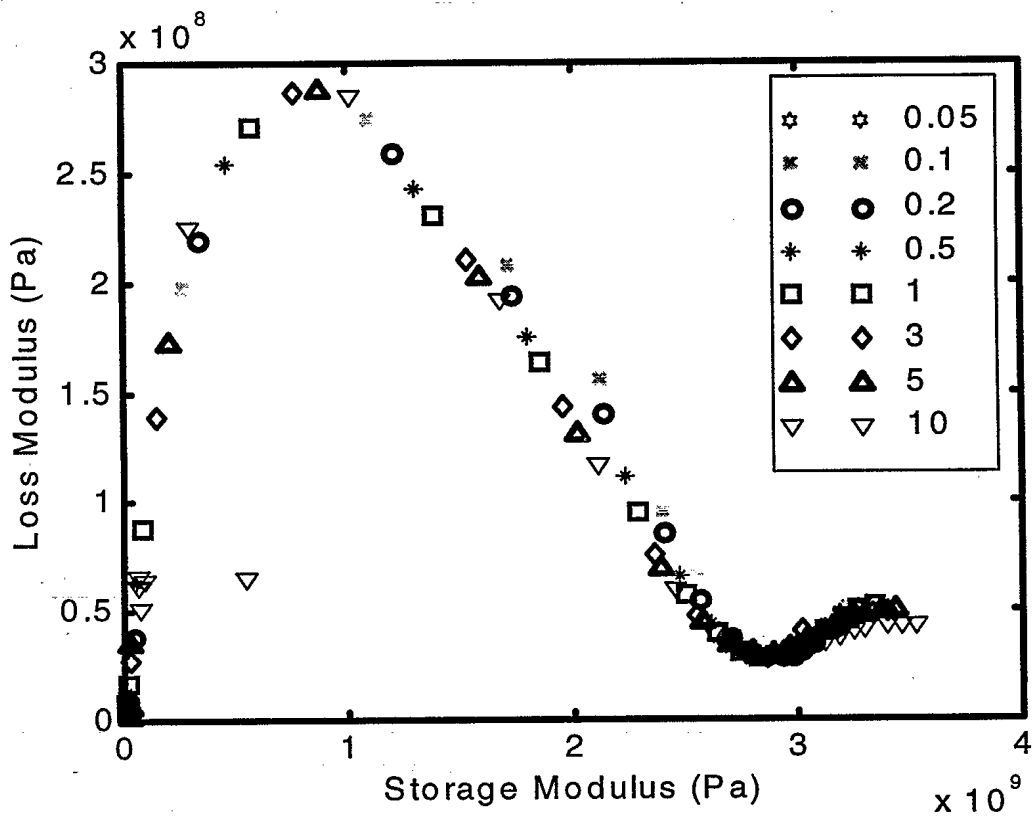


Figure 6. Effect of frequency and temperature on the Cole-Cole plot of the modulus for nitrile rubber as determined from DMTA measurements. Frequency as indicated in the legend is in Hz, and the temperature ranged from -90°C to 15°C .

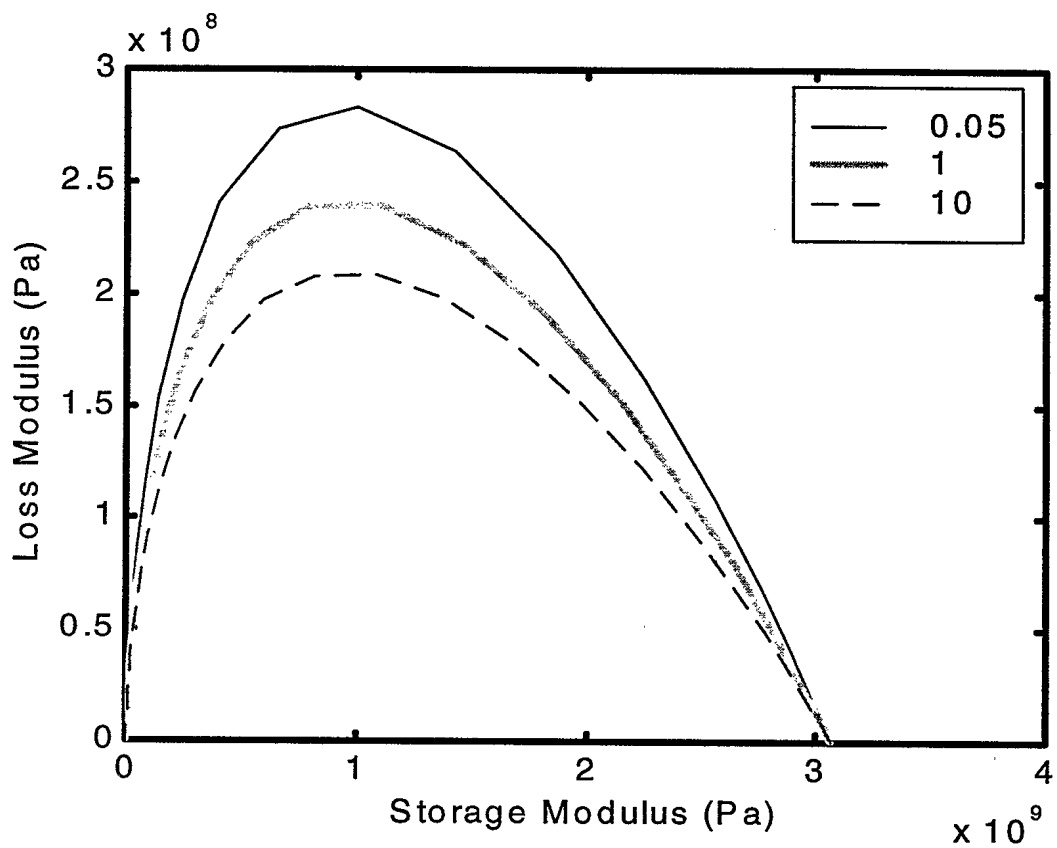


Figure 7. Effect of frequency on the Cole-Cole plot for polystyrene as calculated by GIM. Frequency is in Hz and the temperature range is 70-120°C.

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Group Interaction Modelling (GIM) is a new procedure that relates the chemical structure of polymers to real-world observables. In this work, the equations specific to calculating the complex moduli of polymers were presented and implemented in MATLAB. GIM was used to calculate the mechanical moduli of several polymers and some differences were found when the results were compared to values presented in earlier work. Two problems with the GIM modelling of dynamic mechanical moduli were identified and explored. The first problem deals with the GIM variable $\tan D_g$, which should be always a positive number, but in fact was found to be negative in some cases. The second problem identified was the behaviour of the modulus in the complex plane, which was not consistent with the behaviour of thermorheologically simple materials.

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Group Interaction Modelling
Polymer
Dynamic Mechanical Properties
Glass Transition Temperature

UNCLASSIFIED
SECURITY CLASSIFICATION OF FORM

**D
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A**



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