Projections on Structures and Material Strength in the Computational Context

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INTRODUCTION

This text summarizes the ideas associated with the subsequent viewgraphs. The primary motivation behind this presentation is to observe that certain macroscopic, microscopic and sub-microscopic phenomena are being understood that have basic influence on understanding the durability and high temperature sensitivity of polymers and polymer-based composites. This understanding covers important issues of long term stability with respect to residual stresses and deformations which can have very deleterious effects on structures used for long periods of time as a result of the heat-involving manufacturing process. Beyond this, important progress is being made in understanding the nonlinear material response of polymers in the fracture context, because the nonlinear mechanics of the material at the tip of a crack, either propagating or ready to do so, is being understood with increasing precision.

Projections on

STRUCTURES AND MATERIAL STRENGTH

in the computational context

Motivation:

MANUFACTURING PROCESSES INVOLVING

Effects of long term stability as in

Residual stresses (failure)

Residual deformations (space mirrors & antennas)

DEFORMATION PROCESSES

Non-linear mechanics

Non-linear material response (Rheology)

OUTLINE OF PRESENTATION

This understanding is necessarily coupled to extensive use of computers, but should not be separated from the physical understanding that must precede computer analysis if realistic advances are to be made in engineering. Three examples are to be presented that progress from the macroscopic to the increasingly microscopic domain, with attendant increase in computational need for adding understanding to the present state of affairs.

Needs:

Computer support

Experimental/physical phenomena
(not necessarily in that order)

1) **Structural size scale** (m)

2) **Macroscopic material size scale** (mm)

3) **Microscopic/molecular size scale** (mm,μ)

Examples:

1) **Structural computational**

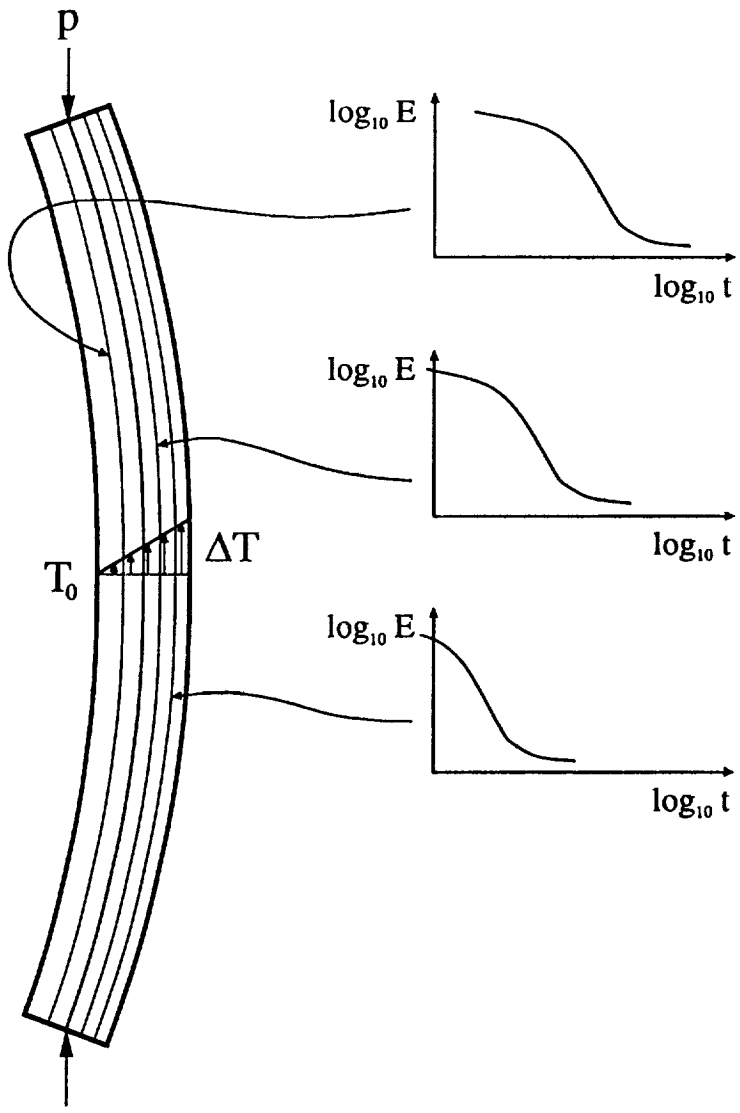
2) **Macroscopic/microscopic**

3) **Molecular aspects**

2) and 3) as examples of the Evolution of Computational Material Description

THERMOVISCOELASTIC BUCKLING PHENOMENA

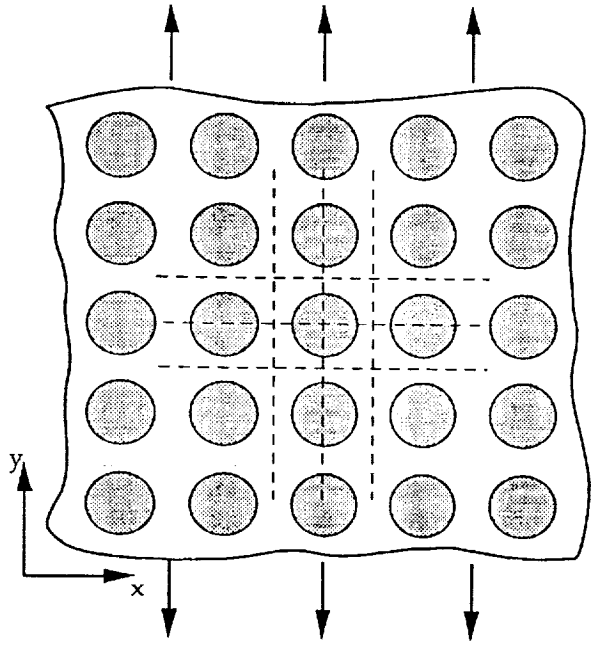
An example of a case for which the computational methods are fairly well understood but for which the analysis needs to be demonstrated as an incentive for design understanding relative to long term stability of structures is that of buckling under the influence of not only temperature, but thermal gradients. The effect of the thermal gradient is twofold: First, because of the different thermal expansion of the panel according to the local temperature the panel or column will bend, thus introducing an initial imperfection. In addition, it changes the time-dependent response of the polymer through the thickness of the panel and generates thus a time-dependent material structure that possesses inhomogeneous properties through the panel thickness. The solution to this problem is likely to be possible only in numerical rather than closed-form analytical terms.

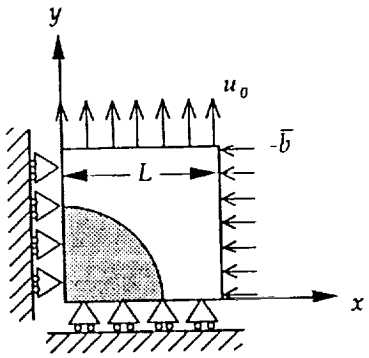


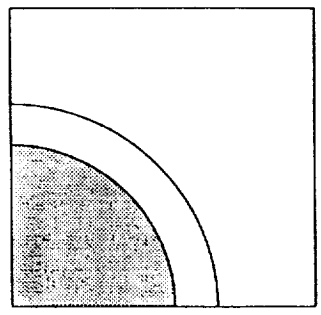
Compression of a Thermoviscoelastic Column/Plate under a Transverse Thermal Gradient

COMPUTATIONAL MATERIAL MECHANICS

There are many materials which at the microscale are composite solids. Examples are multiphase polymer blends with co-polymers for which different components are joined in order to render properties that are superior to the individual phases alone. Although the individual phases possess thermo-rheologically simple behavior, their combination does not, so that a simple test scheme for accelerated testing is questionable or not possible. It turns out that a relatively straightforward analysis procedure based on numerical modeling can provide a framework for accelerated determination for long-range properties which is only limited by the assumption of even phase distribution and by the precision of finite element analysis. The problem with more than two viscoelastic phases is treated with ease typical of numerical methods.

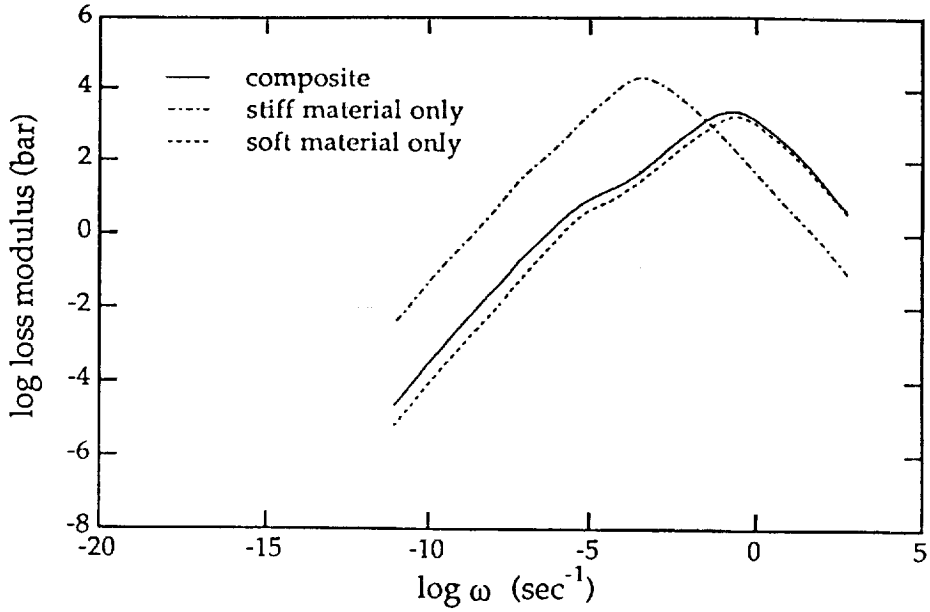


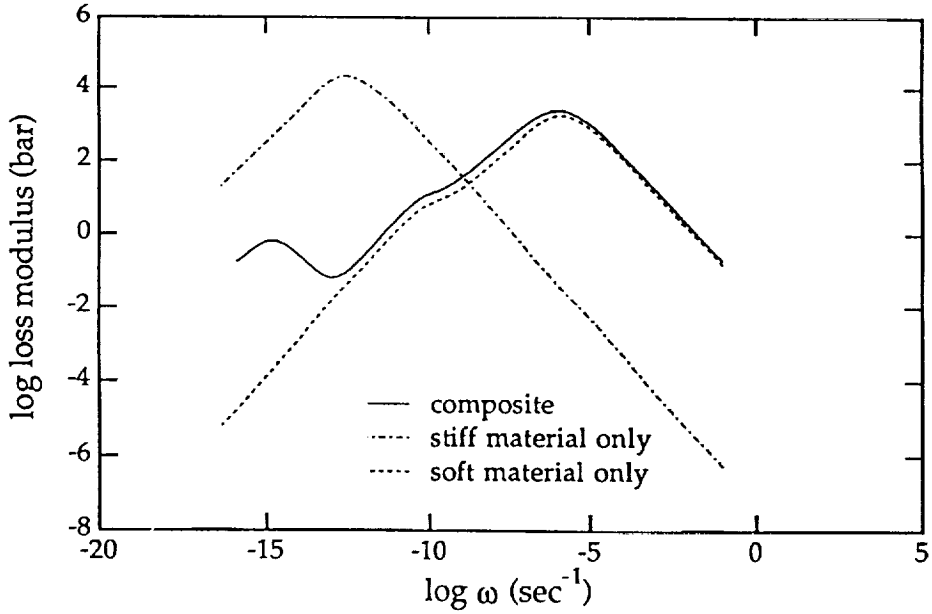




ANALYTICALLY DERIVED COMPLEX NATURAL BEHAVIOR

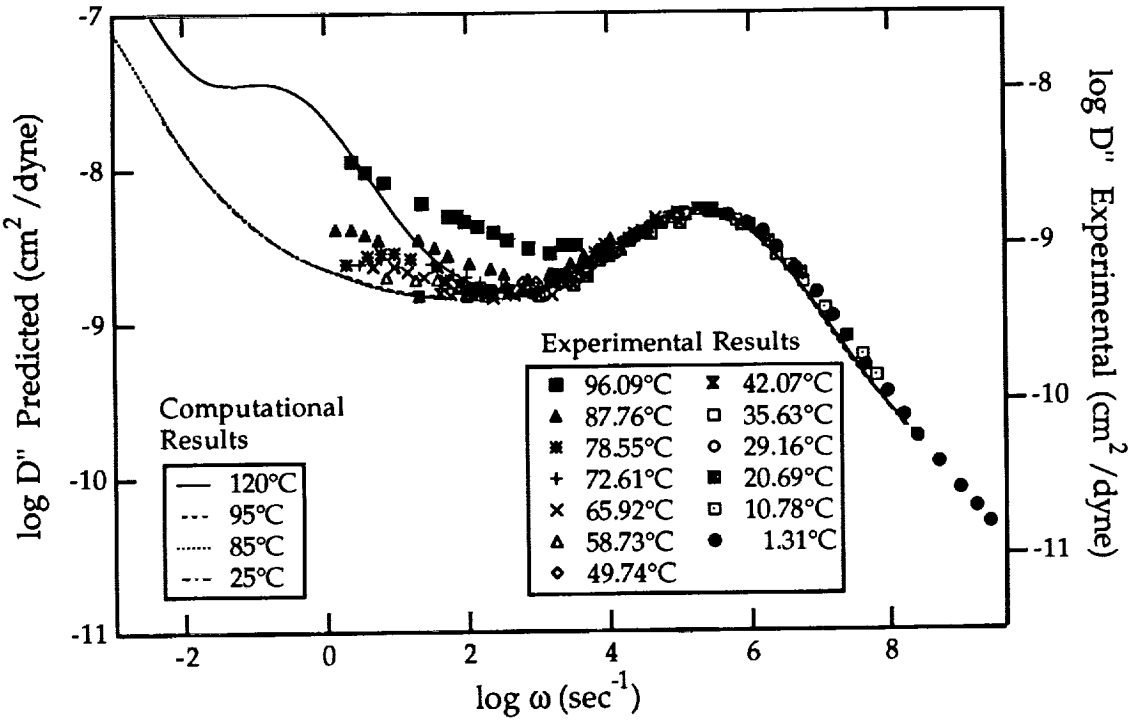
An example is shown of the complex modulus data assuming that only two discrete phases of the two basic building blocks exist. Note that the viscoelastic composite exhibits properties that are closer to those of the matrix material rather than following a rule of mixtures.





LOSS MODULUS FOR A TWO-PHASE MATERIAL MODEL

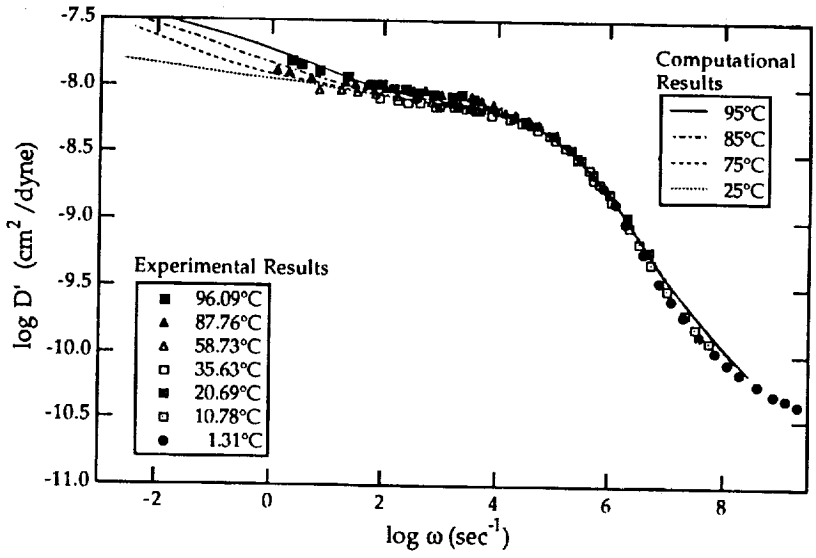
Upon comparing the computations to experiments for a Styrene-Butadiene-Styrene block co-polymer, one finds that the agreement with the experiment is not satisfactory for a two-phase solid. However, by considering a third phase surrounding the hard inclusions, the properties of which can be initially estimated roughly, the agreement between analysis and experiment is rather good.

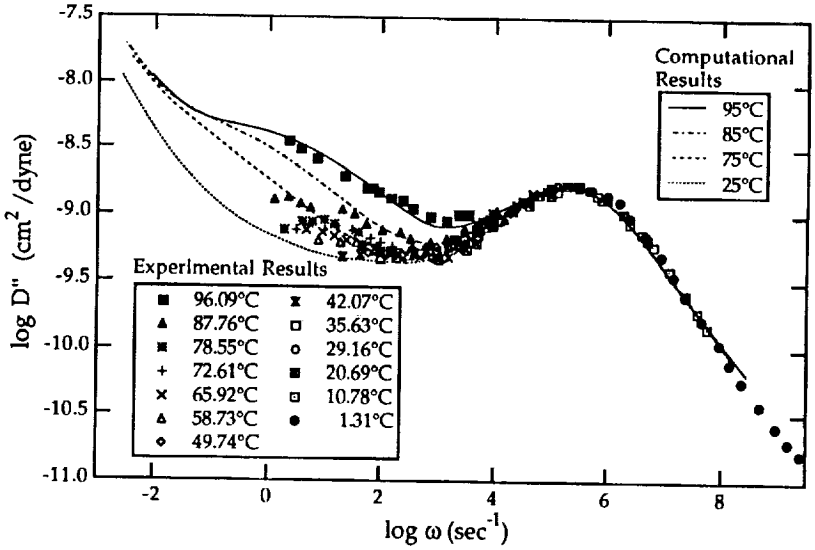


VISCOELASTIC (DYNAMIC) PROPERTIES INCORPORATING VISCOELASTIC PHASE BOUNDARIES INTO COMPOSITE

One can then refine that initial estimate and "back-fit" a three-phase model to the experimental data without violating the boundaries imposed from fundamental but less detailed analysis by fine-tuning the computational model. The resulting material properties have thus been determined experimentally with the aid of a fairly refined material model. The computations also point out the range of frequency measurements one needs to perform in order to improve on the precision with which such phase property determinations can be performed.

This description concludes the example of how computations can assist in refined analyses of property domains that are difficult to access by direct physical test procedures, although such procedures are now being developed. It is of interest to point out that although the model is conceived on the macroscopic scale, its application is made here to the sub-micron range of inclusion sizes.





THE NONLINEARLY VISCOELASTIC CONSTITUTION OF STRUCTURAL POLYMERS

A third example leading to the need for still smaller size scales is illustrated next. The motivation for this work is the need to better understand the time-dependent behavior of polymers (durability), their long-term fracture behavior, how it is to be studied in accelerated tests, as well as a host of problems related to composite manufacturing. It is of basic interest to generate constitutive behavior that incorporates the material behavior of the matrix material as it progresses through the manufacturing process, as it ages physically, as it is stressed to moderate and high levels, as, for example, at the tip of a crack. It appears that we meet here a (temporary) limit of continuum mechanics, because the parameters which govern the dominant microscopic (molecular) details and their definite influence on the macroscopic constitutive response are not yet known.

The model starts from linear viscoelasticity, but includes the effect of small volume changes that result from either thermal expansion, solvent diffusion or mechanically induced dilatation, as it influences the time-dependent behavior of the polymer. In contrast to the linearity assumption, this material description couples shear and dilatational behavior, and renders a large effect of small volume changes on the time scale of the material response.

NONLINEARLY VISCOELASTIC BEHAVIOR

$$s_{ij} = \int_{-\infty}^{t} 2\mu\left(t^*(t) - \xi^*(\xi)\right) \frac{\partial e_{ij}\left(\underset{\sim}{x}, \xi\right)}{\partial \xi} d\xi$$

$$\tau_{kk}\left(\underset{\sim}{x}, t\right) = 3\int_{-\infty}^{t} K\left(t^*(t) - \xi^*(\xi)\right) \frac{\partial \varepsilon_{kk}\left(\underset{\sim}{x}, \xi\right)}{\partial \xi} d\xi$$

INTERNAL TIME

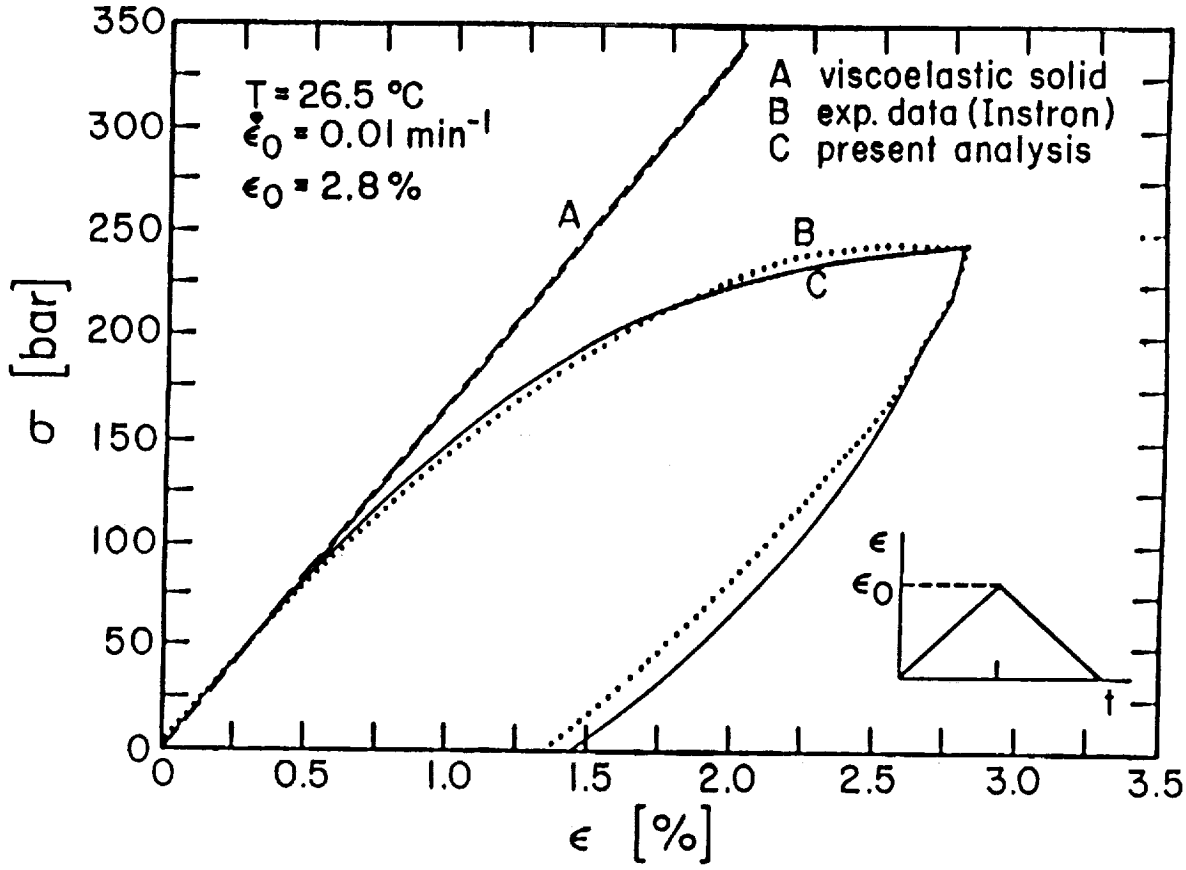
$$dt^* = \frac{dt}{a\left[T\left(\underset{\sim}{x}, t\right), \varepsilon_{kk}\left(\underset{\sim}{x}, t\right)\right]}$$

$$\log_{10}(a) = \frac{B}{2.3}\left[\frac{1}{f} - \frac{1}{f_0}\right]$$

$$f = f_0 + A_1\alpha^* dT + A_2 K^{-1} * d\tau_{kk}$$

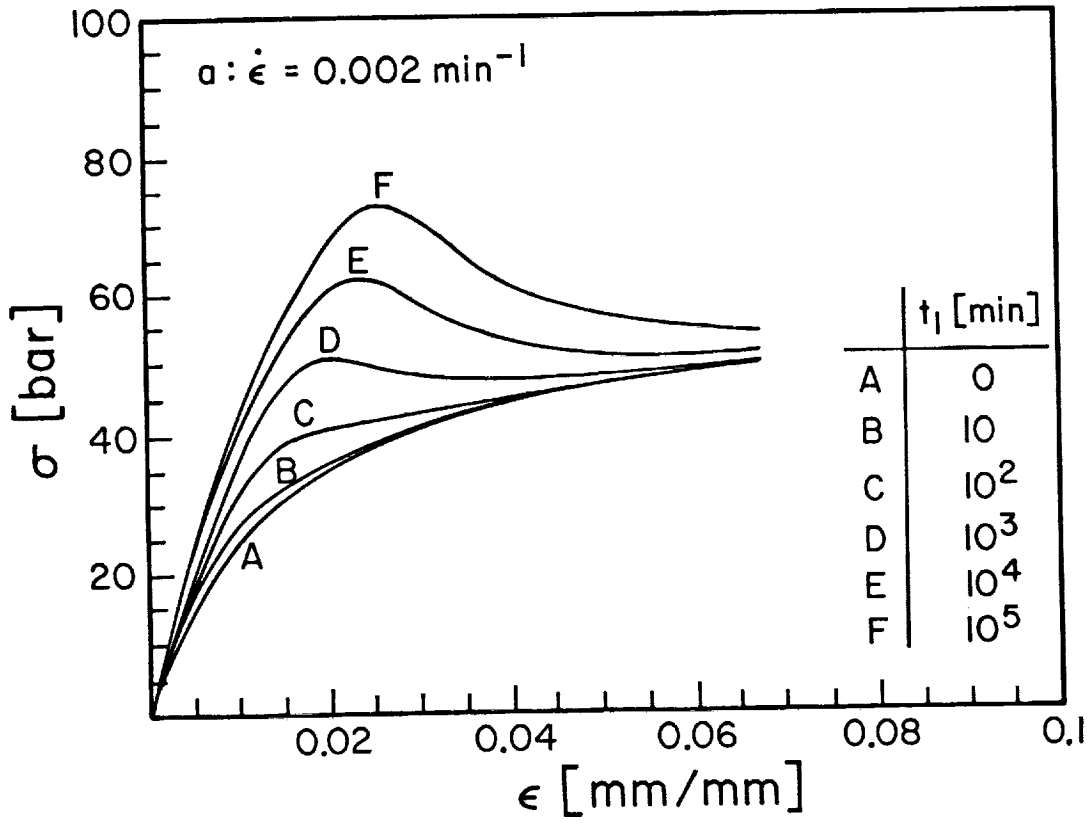
NONLINEAR MATERIAL MODEL: CONSTANT STRAIN RATE LOADING AND UNLOADING

Illustrated below is an example of the model characterizing a loading-unloading sequence as compared with a) linearly viscoelastic prediction, and b) experiments.



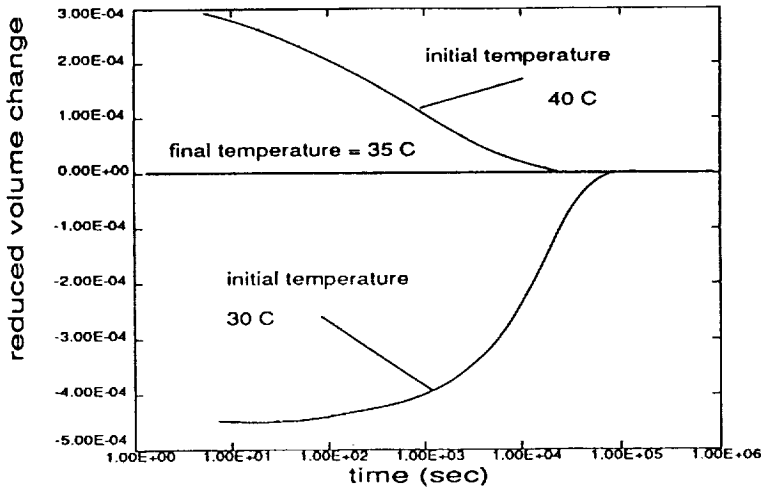
NONLINEAR MATERIAL MODEL: PHYSICAL (PRESSURE) AGING

An example of the model illustrates how time-dependent solidification of the material influences the subsequent stress strain behavior in a constant strain rate test: As the material solidifies more and more (curves A -> F), a yield behavior emerges which is the result of delayed viscous response as the stress level increases.

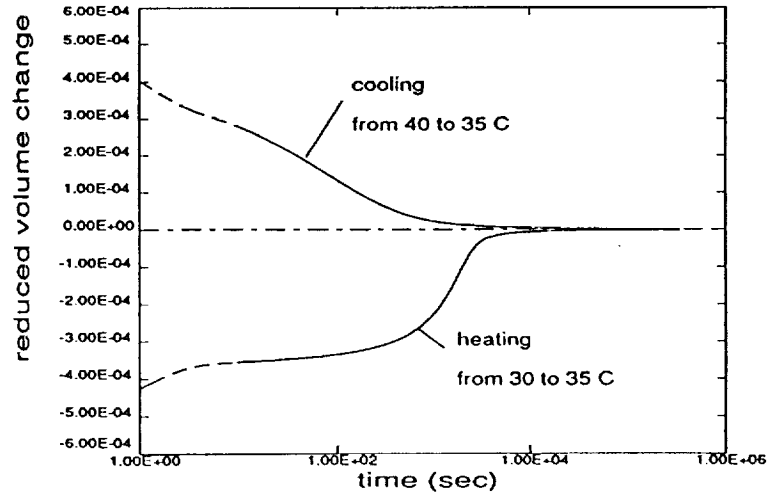


NONLINEAR MATERIAL RESPONSE: EXAMPLE OF COOLING THROUGH THE GLASS TRANSITION

Another example and comparison with experiments of the time-dependent change in volume of a material quenched suddenly from above and below the glass temperature is illustrated. Considering that the detailed properties of the material for the test configuration were not available to us and needed to be estimated (especially the important bulk modulus in its time dependency), the agreement is better than merely qualitative.



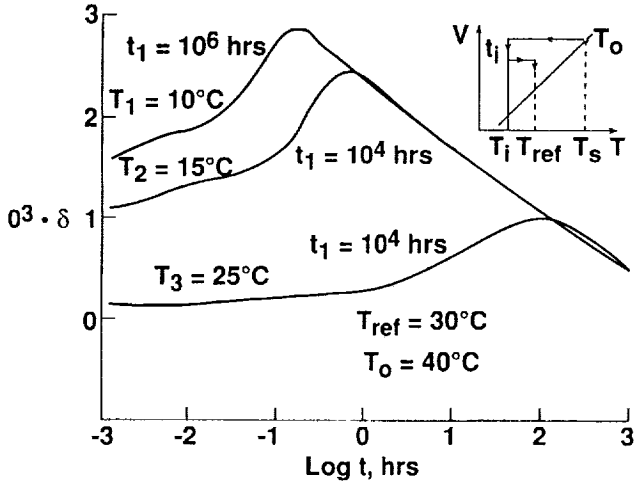
Reduced volume change $\frac{V-V_\infty}{V_\infty|\Delta T|}$ of PVAc, plotted vs. time; data obtained by Kovacs (1963).

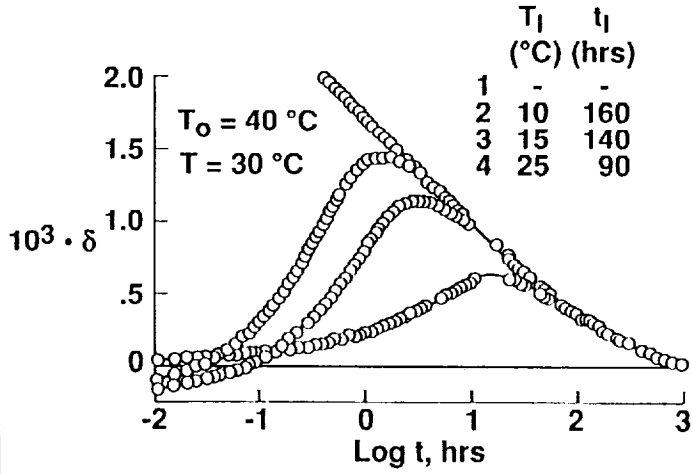


Reduced volume change $\frac{V-V_\infty}{V_\infty|\Delta T|}$ for the 1 mm radius sphere cooled from 40 to 35 C and heated from 30 to 35 C (thermorheological model, "modified" bulk modulus).

COMPLEX COOLING HISTORIES NEAR THE GLASS TRANSITION AND THEIR EFFECT ON VOLUME BEHAVIOR

A final comparison addresses more complex temperature histories as outlined in the insert to the figure on the left. The qualitative comparison to the experiments supplied by Kovacs is shown in the figure on the right.





CONCLUSIONS

Progress is being made in understanding the thermorheological behavior of polymers with respect to:

a) complex temperature histories of interest in high-temperature applications and manufacturing processes;

b) elevated stresses and nonlinear material behavior of vital importance in understanding the material behavior at the tip of cracks and how that influences their evolution and growth in a time-dependent manner, giving rise to improved understanding of what governs the long-range durability of these materials. Moreover, this understanding makes it increasingly possible to evolve acceleration test schemes because the physics underlying these schemes are becoming clear.

It is also becoming clear that mere continuum concepts are insufficient to characterize the diversity of material behavior at the molecular level and how that diversity influences the macroscopic behavior. As a consequence it becomes increasingly important to devote computational efforts to molecular and supramolecular domains in an effort to better understand the influence of molecular parameters on the mechanical continuum behavior of these materials. With the arrival of supercomputers, significant advances can be established from this perspective to provide guidance on what improvements can be made, if any, in the macroscopic and phenomenological description of matrix material constitutive behavior.