

Dielectric studies of nitrocellulose–nitroglycerine mixtures

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Dielectric measurements are reported over a frequency range from 10 Hz to 10^7 Hz and over a temperature range from ~ 220 – 280 K for nitrocellulose (NC) (12.2% nitrated) with varying levels of nitroglycerine (NG), up to 60 wt% NG. A dipolar relaxation is observed and its variation with concentration of NG, temperature, with the presence of stabilizer and method used in preparation of samples are reported. It is observed that the amplitude of the dipolar relaxation increases slowly with the addition of NG up to $\sim 30\%$, whereupon it increases markedly with further addition of NG. The activation energy for the relaxation process is similarly observed to be sensitive to the level of NG in the system and depends critically on the concentration up to 30%, whereupon it becomes independent of concentration. Comparison of the dielectric data reported here with absorption measurements and nuclear magnetic relaxation studies indicates that these observations can be interpreted in terms of a critical adsorption model. At low concentrations, the NG is adsorbed onto the surface of the microcrystallite structures present in the NC system. Monolayer coverage is believed to occur at $\sim 30\%$ and the marked changes in the dielectric behaviour are consistent with the formation of a multilayer structure.

(Keywords: nitrocellulose; nitroglycerine; dielectrics; relaxation; microstructure; absorption)

INTRODUCTION

The basic ingredients in double base propellants are nitrocellulose (NC) and nitroglycerine (NG). Often other ingredients are added to alter the ballistic performance of the simple mixture. Little is known concerning the manner in which a plasticiser, such as nitroglycerine, is dispersed in the NC matrix. Varying the content of the NG has a profound effect not only on the burning rate of the propellant, but also on such physical properties as its brittleness, its ultimate tensile strength and total strain capability at different temperatures. A knowledge of the interaction in the NG/NC system, therefore, is of considerable technological significance.

Nitrocellulose may be considered to be a partially crystalline polymer; hence, whether it contains plasticizer or not, its dielectric spectrum would be expected to reflect the presence of ordered regions within the sample¹. Such order may exist at a number of levels; extending over a few Angstroms and associated with the ultimate crystalline microfibril of the cellulose precursor or associated with the incompletely disintegrated fibres, as is frequently observed in thin sections of propellant in the polarizing microscope.

Dynamic mechanical analysis has shown the existence of two major relaxation processes, one occurring at high temperature (α), the other at low temperature² (β). These

have been designated as the alpha and the beta processes, *Figure 1*. It is clear from the data that the maximum loss in modulus of the system occurs at the alpha peak, and would normally represent the T_g of the sample. For years, the T_g for double base propellants, with NG contents of $> 40\%$ has been assumed to occur at about -40°C . It is only in this work that we are able to show that this transition temperature is associated mainly with the plasticizer and is not primarily a property of nitrocellulose in a highly plasticized state.

Dielectric measurements have shown the existence of

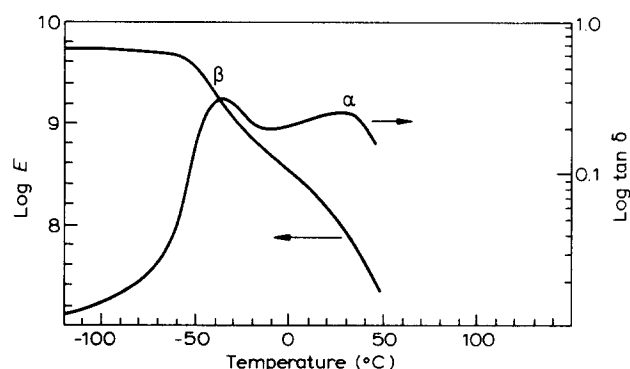


Figure 1 Mechanical relaxation spectrum for a (12.2%) nitrocellulose–(40%) nitroglycerine system. The curve was obtained using a Dupont Dynamics Analyser, $\beta \sim 25$ Hz and $\alpha \sim 5$ Hz

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three and in some cases four relaxations. For a sample containing 50% of NG (at room temperature) two relaxations will be observed below 100 Hz (Figure 2). A large peak centred around 10^{-5} Hz and a smaller feature centred around 0 Hz. The precise origins of these relaxation features are undefined but may be ascribed to large scale cooperative dipole motion of the NC chain and/or of space charge migration. A third feature is observed at approximately 10^7 Hz, ascribed to the beta relaxation and will be the main topic of discussion of this paper. Published n.m.r. data^{3,4} have shown that within the temperature range of -100° to $+80^\circ\text{C}$ the mobile species, as observed by the T_2 relaxation measurement, was due almost entirely to the nitroglycerine, there being hardly any movement from the nitrocellulose matrix. Motions associated with the NC are therefore ascribed to the lower frequency dielectric relaxations. These observations have been confirmed by the work carried out by Foland⁵ and are consistent with the d.m.a. data². This paper will attempt to show that the beta peak, as measured by dielectric spectroscopy, is identical to the relaxation observed in the n.m.r. studies and that it is associated with the beta relaxation observed by d.m.a.

EXPERIMENTAL

Materials

The nitrocellulose used in this study was a commercial sample of the type used in rolled solventless propellant. It was prepared by immersion of purified wood pulp in mixed nitric–sulphuric acid and stabilized by the normal procedure of extended boiling in a succession of aqueous media. Its nitrogen content as measured by a Lunge nitrometer was 12.2%, and its molecular weight, measured viscometrically, was approximately 250 000 with a polydispersity in the range 5–6.

Sample preparation

Nitrocellulose, a fibrous material, is made into a slurry with water and to this is added the nitroglycerine. The water is filtered off and the resultant wet 'paste' is subsequently dried.

Flat discs of the propellant approximately 25 mm in diameter were formed in two ways.

Samples with NG content in excess of 30% were cut from sheets formed by passing the dried paste through a hot rolling mill. The schedule was thirty passes through a nip of 1.0 mm, five more at a nip of 0.5 mm, and, finally, four passes at a nip of 2.5 mm. The samples contained one per cent of diphenyl–diethylurea as a stabilizer.

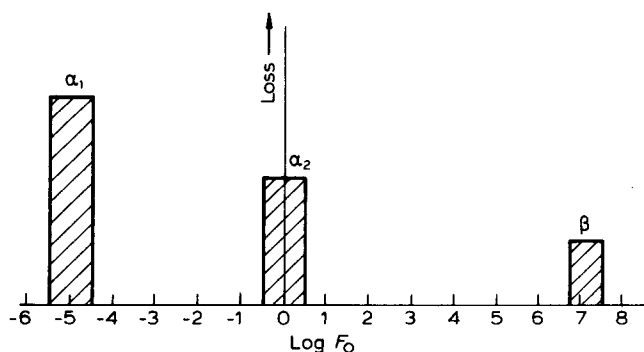


Figure 2 Histogram of the locii of relaxations in the nitrocellulose–nitroglycerine system at room temperature

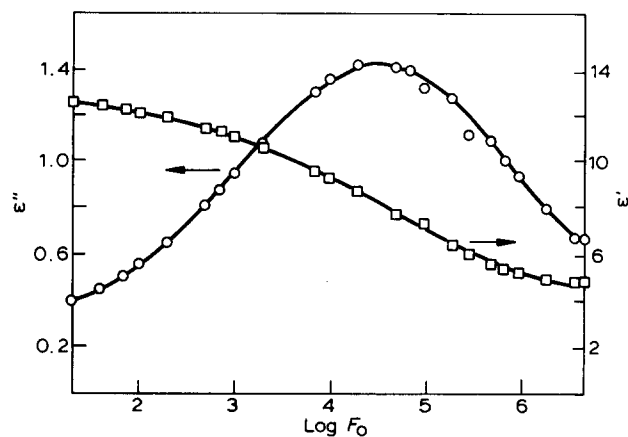


Figure 3 A typical dielectric response—real (ϵ') and imaginary (ϵ'') put as a function of frequency for a (50%) nitroglycerine–(12.2% N) nitrocellulose sample

To test whether or not the rolling process affected the measurements, samples were made in which the dry paste was loaded into a press and subjected to a pressure sufficiently high to produce discs 4 mm or less in thickness. The discs so formed ranged from a hard biscuit at 35% nitroglycerine to a friable product at a 60% loading. Care had to be exercised at concentrations greater than 40%, since above this level the NG was easily expressed from the dry paste.

Pastes containing less than 35% NG cannot be rolled. The samples were prepared, therefore, by loading the wet paste into a small press, and subjecting it to a pressure of 90 MPa for at least 15 min. During this time the excess water was expressed from the sample and removed. The biscuit so formed was extracted from the press and subsequently dried for two weeks in an oven maintained at 45°C . It was found that the mass of the disc reached a constant value within this period. The dried biscuits were stored in a desiccator. For reasons explained in the text, samples were made with and without the addition of 1% stabilizer.

Dielectric measurements

The real and imaginary parts of the dielectric permittivity were measured using a three terminal cell, which could function over the temperature range -70° to $+60^\circ\text{C}$.

The measurements were made using a Teradyne bridge-C357 operating at a frequency of 1 kHz⁷, and a General Radio A.C. Bridge 1616 driven by a Rohde and Schwartz R.C. Generator Type BN 40581. The latter combination gave an effective frequency range of 10 Hz to 100 kHz. Higher frequencies were obtained by using a Wayne Kerr A.C. Bridge B602 driven by a Wayne and Kerr Source and Detector SR268, thus extending the range from 100 kHz to 5 MHz.

RESULTS

A typical dielectric spectrum of the beta process, showing the variation of the permittivity ϵ' and the loss process ϵ'' as a function of frequency is given in Figure 3. The position of the loss peak is strongly dependent on the concentration of the nitroglycerine and also on the temperature, but independent of whether or not the material had been rolled. Such behaviour was observed also for the re-

relaxations measured using pulse n.m.r. techniques⁵. Similarly, the d.m.a. studies showed that the position of the beta peak did not depend on whether the sample was made from rolled sheet or formed by solvent incorporation². The latter process involves mixing the dry ingredients with the solvent in an incorporator, followed by extrusion and subsequent drying. This relaxation is therefore independent of the method of preparation of the sample and is dependent only on the nitroglycerine content. Thus, dielectric spectroscopy, n.m.r. and d.m.a. are observing relaxation phenomena derived from the same source, that is the interaction of NG with NC.

Variation of the dielectric loss with NG content

The variation of the frequency of the dielectric loss peak as a function of NG concentration is shown in Figure 4. The minimum at ~27% indicates that the dipoles experience their greatest hindrance to motion at this concentration. It was observed also that, within experimental error, the position of the peak was unaffected by the presence of 1% stabilizer. The decrease in frequency as the NG content was increased can be explained by a concentration dependent Kirkwood 'g' factor⁸. From n.m.r. studies carried out by R. Foland and supported by the observations made by both French and Russian workers^{3,4}, it is clear that the mobile fraction is due almost entirely to the nitroglycerine molecules. N.m.r. data further support the observation that there is a marked

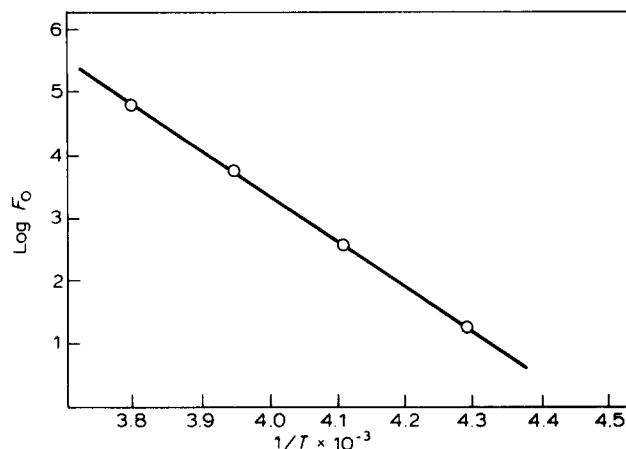


Figure 5 Variation of the relaxation frequency with reciprocal temperature for a (40%) nitroglycerine-(12.2% N) nitrocellulose sample

increase in the mobility of the relaxing species at a nitroglycerine concentration greater than 27%.

Variation of the dielectric loss with temperature

Varying the temperature of the observations gave a linear plot of $\log(F_0)$ against $1/T$; a typical example is shown in Figure 5. The linearity indicates that the relaxation corresponds to a simple thermally activated process as described by Arrhenius. The change in the activation energy as a function of NG content is shown in Figure 6.

Analysis of the distribution of the dielectric losses

The dielectric loss peaks were analysed using the Havriliak–Negami formula⁹,

$$\epsilon^* = \epsilon_0 - (\epsilon_0 - \epsilon_\infty) \left\{ (i\omega\tau_0)^{1-\gamma} / 1 + (i\omega\tau_0)^{(1-\gamma)} \right\}^\delta$$

where ω is the frequency of observation in radian, and τ_0 is the relaxation time, ϵ_0 is the static dielectric constant and ϵ_∞ is its limiting value at high frequency. The variables γ and δ are a measure of the broadness and skewness of the loss peak. The analysis was executed quickly and easily using a microcomputer⁶. In all cases, the data could be fitted using only the parameter gamma. Furthermore, the breadth of the peak as measured by gamma was dependent on the NG content, having a maximum at ~15% NG. Gamma also increased with decreasing temperature, indicating that the distribution of relaxation times broadens as the temperature is lowered, Figure 7. The significance of these observations will be discussed later.

The Havriliak–Negami analysis also gives an estimate of the constants ϵ_0 and ϵ_∞ . The difference between these two components, defined as the dielectric increment, is proportional to the number of dipoles taking part in the relaxation process and also their effective activity. If we assume that the dipolar relaxation process is attributed to the motion of the NG dipole, the restrictions on its free rotational motion arising as a consequence of interaction with the polymer matrix will be reflected in the magnitude of the Kirkwood 'g' factor. The Kirkwood equation describes deviations in the dielectric response from the ideal free rotation condition and indicate the extent of correlation of motion of a dipole with its surrounds. To correct for the variation in bulk density from sample to sample the experimentally determined increments were

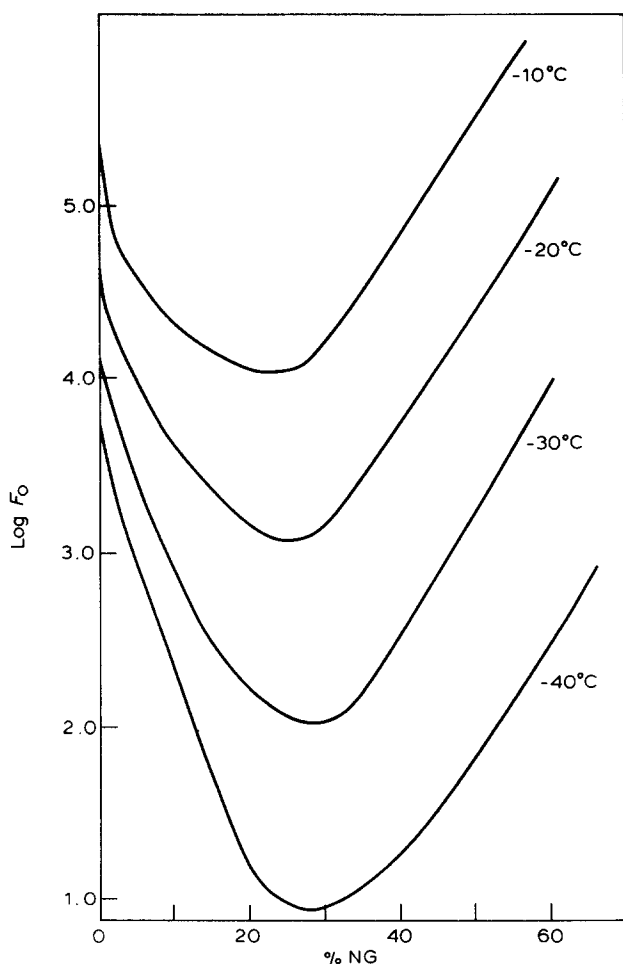


Figure 4 A variation of the frequency of the dielectric loss peak as a function of the nitroglycerine concentration at various temperatures for a 12.2% nitrocellulose sample

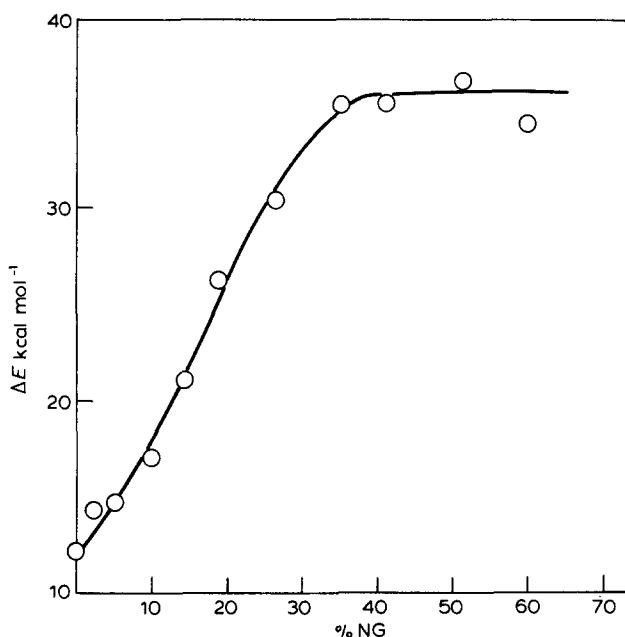


Figure 6 Variation of the activation energy with nitroglycerine concentration

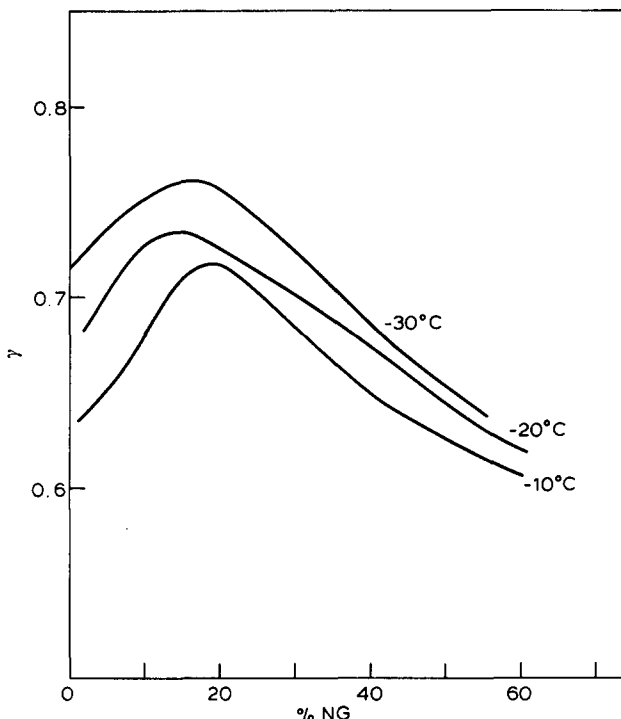


Figure 7 Variation of the gamma distribution parameter with nitroglycerine concentration and temperature

normalized to the theoretical density expected for each sample. A plot of the normalized increment against nitroglycerine concentration is shown in Figure 7. The curve shows that the number of dipoles responding to the electric field increased markedly after the addition of 30% of plasticizer. This is in accordance with the n.m.r. findings¹⁰.

DISCUSSION

Comparison of the dielectric data with those obtained from d.m.a. indicates that the feature being observed above 10 Hz at room temperature is the so-called beta

relaxation. It had been supposed from n.m.r. and d.m.a. studies, that the beta peak was due entirely to the nitroglycerine component of the system. The strength of the T_2 signal in the n.m.r. was proportional to the number of hydrogen atoms contained by the plasticizer, provided it is assumed that approximately 12% of the NG is tightly bound to the NC and did not contribute to the signal⁵. The present study shows this to be an over-simplification. It is observed that the beta peak exists in pure nitrocellulose, and that there is a continuous change in its position and magnitude as more nitroglycerine is added to the matrix. To interpret this, it is of interest to consider the relaxation in the nitrocellulose.

Nitrocellulose is a very polar molecule, each nitrate ester on the pyranose ring having a dipole moment of 2.95 Debye¹⁰. Yet the corrected dielectric increment for the polymer is only 0.57, a very low value. An estimate of the effective dipole moment of the ring can be made by applying the Kirkwood equation⁸,

$$\mu_{\text{eff}}^2 = g\mu^2 = \left(\frac{M}{d}\right) \frac{9kT}{4\pi N} \frac{(\epsilon_0 - \epsilon_\infty)(2\epsilon_0 + \epsilon_\infty)}{\epsilon_0(\epsilon_\infty + 2)^2}$$

where d the density of the sample, k Boltzmann constant, N Avogadro's Number, T the temperature of the sample, and M the molecular weight of the substituted pyranose ring unit, i.e. 267. Calculation gives the value of the effective dipole moment as 0.8 Debye. This would imply a severe restriction on the freedom of the dipoles on the pyranose ring to rotate. By the application of simple vector analysis the magnitude and direction of the resultant dipole acting on the ring can be calculated, Appendix 1. The results depend on whether the tg , gg or gt structures as defined by Meader *et al.*¹¹ are present. It has been shown by analysis of birefringent data that only the gt and tg structures are possible for nitrocellulose¹². The *trans-gauche* structure is the one where the O(6) atom on the primary linkage is *trans* and *gauche* to the ring oxygen O(5) and the C(4) position, respectively. The results of the vector analysis for the trinitrated cellulose show that both the tg structure and the gt structure give resultant dipoles lying some 80° to the Z axis, but acting in opposite directions. The value for the gt structure being 2.5 Debye and for the tg structure 2.29 Debye. Studies of the electro-optic scattering from nitrocellulose solutions have indicated that the main chain backbone is extremely stiff and extended. Dipole moment calculations for the pyranose ring gave a value of 2.3 Debye¹³. Since the nitrocellulose molecule forms a helix¹¹, then over a large number of rings the x and y components of the resultant dipoles would tend to cancel leaving only the z components of the ring dipole. Should there be structures in which the tg and gt forms alternate, then the overall dipole moment will approach a value of zero, and hence give a low value for the dielectric increment.

The above analysis has assumed that the ring can rotate. If, however, this cannot occur, then the contribution to the polarization is from the moment of the nitrate esters and hydroxyl groups only. The low value of the dielectric constant would indicate that there is considerable restriction to the movement of these groups.

Addition of as little as 2% of nitroglycerine is sufficient to significantly slow down the NC relaxation process, thus indicating a very strong coupling between the plasticizer and the nitrocellulose. Concomitant with this decrease is the increase in the dielectric increment of the system in

accordance with the addition of the nitroglycerine. As the concentration of the plasticizer is increased further, the relaxation frequency is lowered until it reaches a minimum at 27% loading. Further increases in nitroglycerine content cause the relaxation process to increase in frequency. N.m.r. data show that above the 27% NG level the magnitude of T_2 increases markedly³. The dielectric increment also increases sharply and the activation energy rises to a plateau at approximately 35% NG concentration. All of this indicates that above a concentration of 27% NG the interaction between the plasticizer and the matrix is considerably weakened.

By assuming that the molecular weight of the NC/NG system is given by:

$$M = x M_{\text{NG}} + (1 - x) M_{\text{NC}}$$

where x is the concentration of the nitroglycerine, M_{NG} the molecular weight of the NG, and M_{NC} that of the nitrocellulose, the effective dipole moment of the system as a function of NG content can be calculated via the Kirkwood equation. The results are presented in Figure 8. It is evident that there is a smooth increase in the dipole moment as the content of plasticizer is increased, levelling off to the value expected for pure nitroglycerine.

Examination of the Havriliak–Negami parameter, γ , as function of nitroglycerine content, showed that it reached a maximum at a concentration of ~15%. N.m.r. studies on similar systems have indicated also that the distribution of relaxation times increases as the content of the plasticizer was lowered^{5,10}. Unfortunately, the studies were not carried out at sufficiently low concentrations to confirm the existence of a maximum in the distribution parameter⁴.

Before attempting to discuss in detail the effects observed with the dielectric probe, consideration should be given to any evidence pertinent to the morphology of the system. If it is assumed that the cellulose structure is preserved in the manufacture of NC, then it can be supposed that the morphology of nitrocellulose involves crystalline microfibrils, of the order of 5 nm in diameter,

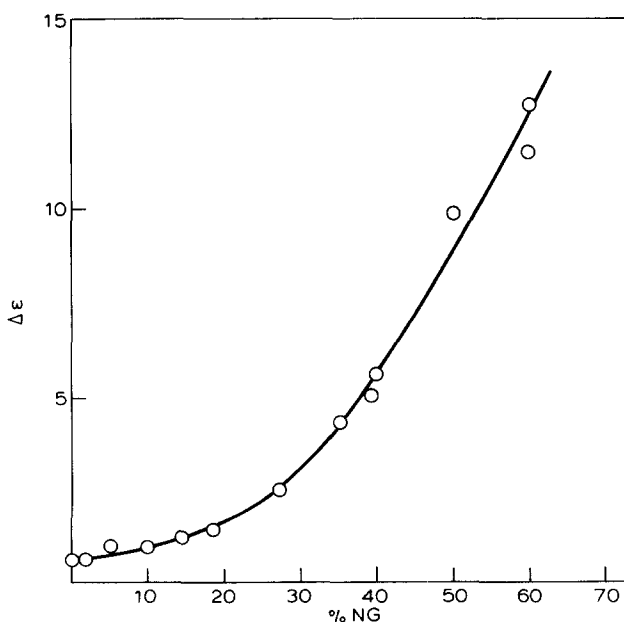


Figure 8 Variation of the normalized dielectric increment of the nitroglycerine–nitrocellulose with nitroglycerine content

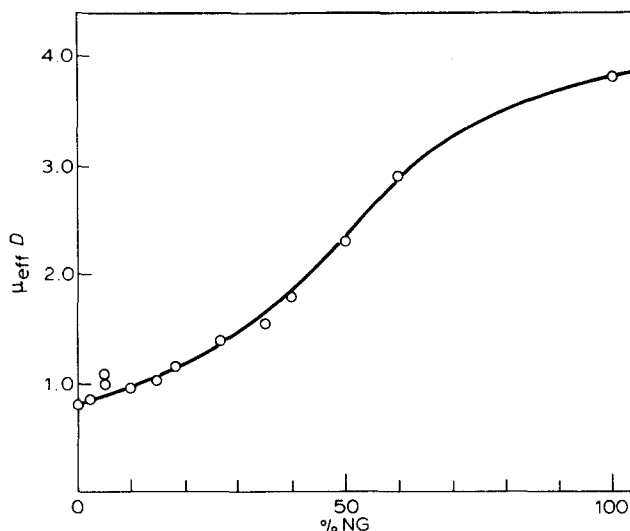


Figure 9 Variation of the effective dipole moment of the nitroglycerine–nitrocellulose system with nitroglycerine content

which can provide stable surfaces¹⁴. It would not appear unreasonable, therefore, to assume that a model for this system might be based on specific site interactions. Such a model has been used to interpret the n.m.r. data, and is supported also by work on the vapour phase absorption of nitroglycerine on nitrocellulose¹⁵.

When discussing the dielectric properties of a system in which the bulk dielectric constant is changing significantly with concentration, the effects of polarity on the local electric field must not be ignored. It has been pointed out by Powells¹⁶ that the effective relaxation frequency, τ_{eff} , can be correlated with the theoretical value in the presence of the local field effect by:

$$\tau_{\text{eff}} = [(2\epsilon_0 + \epsilon_\infty)/3\epsilon_0]\tau$$

Application of this equation to the NG/NC data indicates that the relaxation time would tend to decrease with the addition of NG. The magnitude predicted by the above relationship is significantly smaller than observed in practice, and is totally contrary to the trends observed at high NG levels. The data are, therefore, inexplicable in terms of simple local field effects.

Distribution of dielectric relaxation processes

The specific site interaction model assumes that there exist a limited number of sites possessing high interaction energies. The n.m.r. analysis of this situation has been described by Resing¹⁷, who assumes that the molecules are 'adsorbed' onto the sites but are free to both translate and rotate. The assumption made here is that it is these sites which are responsible for the beta relaxation process. The observations from the dielectric study are consistent with the NG molecules progressively occupying these sites. The tight binding reduced the extent of rotational motion of NG compared with its value in the pure liquid, thereby decreasing its dielectric increment and restricting its motion. The fact that the NG is interacting closely with the NC derives from the observation that only one dielectric feature is evident for the binary system, implying that considerable cooperation is occurring between the two relaxation processes. As further nitroglycerine is added, so the site occupancy is increased towards monolayer coverage. According to the data of Lotmentsev et

*al.*¹⁵, monolayer coverage is anticipated at an NG concentration of approximately 25%, which agrees well with the observed variation of the dielectric parameters. The data suggest, also that as the sites are filled, so the extent of cooperative dipolar interaction increases. This is made evident by an increase in the value of γ and by the increase in the activation energy. Addition of NG in excess of 27% leads to multilayer adsorption. These molecules will be more free to rotate than those in the first layer, hence the dielectric increment approaches that of the pure liquid, *Figure 9*. The NG molecules in the multilayers, although not intimately interacting with the NC, are clearly exhibiting a very high degree of cooperativity in their motion, as evidenced by both the high value of the activation energy, 35 kcal mol^{-1} and the magnitude of the distribution parameter. The concentration dependence of the latter indicates that for high levels of NG the narrowing of the dielectric distribution is consistent with the molecule obtaining a 'liquid'-like environment in the multilayer.

In order to determine the validity of this interpretation we must consider what evidence exists for such sites. Since the molecular mass of nitroglycerine is almost the same as that of the pyranose ring, then the changes in the properties indicated above are consistent with there being three molecules of NG interacting with every seven rings. In molecular terms this is very similar to the amount of isopropyl nitrate found 'permanently absorbed' in vapour sorption experiments¹⁸. If the ultimate crystalline microfibril which exists in cellulose persists in the NC, then the 27% sorption obtained for NG may be interpreted as adsorption on the surface of such fibrils. It has been suggested that these ultimate microfibrils in cellulose consist of a cross-sectional array of 12×8 cellulose chains¹⁴. Of these, 10×6 will be internal, leaving 37.5% of the chains accessible for adsorption. The data reported herein would appear therefore to be consistent with NG being selectively adsorbed onto the surface of these crystalline fibrils, and dispersed in disordered regions in the polymer. This conclusion is in agreement with the calculations of Derinovskii *et al.*⁴, who state that the nitroglycerine molecule occupies sites which are no bigger than 3 nm, holding up to one hundred molecules.

CONCLUSION

The dielectric studies discussed in this paper can be divided into two regions. For NC levels below $\sim 30\%$ the behaviour is characteristic of specific site adsorption characteristic of strong interaction between the NC and NG. Above 30%, the available sites are completely filled and the relaxation is characterized by properties more typical of a fluid phase. The concentration variations reported in this paper reflect the relative importance of these various contributions and are consistent with an adsorbate–absorbent system.

This interpretation appears to be consistent with n.m.r., and vapour phase adsorption studies. The specific sites probably exist at the surface of the microfibrils or in areas of disorder in the microfibrillar structure of NC. On the assumption that one nitroglycerine molecule is adsorbed per pyranose ring, then 43% of the rings can act as

adsorption sites for the NG. This estimation of the number of accessible sites correlates well with that obtained from measurements of the absorption of isopropyl nitrate in NC. The dielectric data further indicate that the nitrocellulose molecule exists as a very stiff chain and this observation is consistent with the observations of NC solutions using light scattering methods.

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APPENDIX

The Cartesian coordinates for the oxygen and nitrogen atoms of the fully nitrated cellulose structure have been reported by Meader *et al.*¹¹ The position vector for each of the atoms is defined as:

$$\vec{R} = x\vec{i} + y\vec{j} + z\vec{k}$$

where i, j, k are unit vectors and the values of x, y and z are given by Meader *et al.* Using the above equation to define the principal vectors, the resultant vector for the oxygen and nitrogen atoms in the pyranose ring can be computed. The resultant position vector for the –O–N bond for the ring in the *gt* conformation is given by:

$$\vec{R}(gt) = R\vec{N}(gt) - R\vec{O}(gt) = -0.0864\vec{i} - 0.669\vec{j} + 0.0378\vec{k}$$

giving the magnitude of the resultant bond vector as 0.1156. Assuming that the dipole moment is proportional to the bond length, and taking Meader *et al.*'s value for the –O–N bond as 0.137 nm, then the magnitude of the resultant dipole moment per repeat unit is given by:

$$\mu = 0.1156/0.137 \times 2.95$$

and its orientation with respect to the principal axes is $\alpha = 138.4$, $\beta = 125.4$ and $\gamma = 70.9$. A similar calculation for the *tg* conformation gives a dipole moment of 2.29 Debye with direction angles of $\alpha = 141.5$, $\beta = 58.9$ and $\gamma = 110.2$ to the principal axes.