

Structural analysis of polydimethylsiloxane samples

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Abstract

This work presents a structural analysis of polydimethylsiloxane (PDMS) samples through the study of the mechanical properties of a soft material. For this, the dimensions of the crosslinking samples were modified taking a cure ratio as a reference, to determine the stress-strain, applying the Prony model which the Ansys-Mechanical platform offers. Experimental data was collected from the literature and a force test was performed on three different cylindrical samples (10:1 ratio) of PDMS with a curing agent. Consistent results of the modulus of elasticity as a function of time were obtained. Finally, using the Neo Hookean model, with consideration of hyperelastic material, and employing longer relaxation times, the results showed interesting findings in the parameters of total and directional deformation and other viscoelastic properties for this type of material.

Keywords: Structural Analysis, Mechanical properties in Polymers and Viscoelasticity Effects

Resumen

Este trabajo presenta un análisis estructural de muestras de polidimetilsiloxano (PDMS) a través del estudio de las propiedades mecánicas de un material blando. Para esto, se modificaron las dimensiones de las muestras de reticulación tomando como referencia una relación de curado, con el fin de determinar la tensión-deformación, aplicando el modelo de Prony el cual ofrece la plataforma de Ansys-Mechanical. Los datos experimentales fueron colectados a partir de la literatura y se realizó una prueba de fuerza sobre tres diferentes muestras de forma cilíndrica de proporción 10:1 de PDMS con un agente de curado. Se obtuvieron resultados consistentes del módulo de elasticidad en función del tiempo. Finalmente, usando el modelo de Neo Hookean, con una consideración de material hiperelástico, y empleando tiempos de relajación mayor, los resultados mostraron interesantes hallazgos en los parámetros de deformación total y direccional y demás propiedades de viscoelasticidad para este tipo de material.

Palabras claves: Análisis Estructural, Propiedades Mecánicas en Polímeros, Efectos de Viscoelasticidad.

I. INTRODUCTION

Viscoelastic materials are characterized by a combination of elastic and viscous behaviors. The former is responsible for storing energy during deformation. On the other hand, the latter is responsible for dissipating energy during deformation. The elastic behavior is rate-independent and represents the recoverable deformation due to mechanical loading. The viscous behavior is rate-dependent and represents dissipative mechanisms within the material. For instance, a wide range of materials exhibits viscoelastic behavior, including polymers, glassy materials, soils, biologic tissue, and textiles.

The following are descriptions of the viscoelastic constitutive models, which include both small and large formulations. We also present the time-temperature

superposition for simple thermoreological materials and a viscoelastic model of the harmonic domain.

The viscoelastic properties were calculated by choosing a specific polymeric material and the results were included in this study. This polymer is polydimethylsiloxane (PDMS). The basic concepts of viscoelasticity are described at the beginner level, considering that PDMS under glass-transition temperature exhibits high entropic elasticity. The analysis of stress-strain for some polymeric materials is shortly described. Dielectric and dynamic mechanical behavior of aliphatic, cyclic saturated and aromatic substituted poly(methacrylate)s are explained. An interesting approach to the relaxational processes is presented. The viscoelastic behavior of poly(itaconate)s with mono- and disubstitutions and the effect of the substituents and the functional groups are extensively discussed. The viscoelastic behavior of different poly(thiocarbonate) is also analyzed.

The mechanical properties of polymers are also influenced by the architecture of the molecules, whether they consist of linear chains, cross-chains, or cross-linked chains. In particular, extensively cross-linked polymers might have one single super-molecule in a container: PDMS is an example of such a polymer. The Young's modulus of polymers is highly dependent on their chemistry as well as the temperature. The value of E for these materials increases as covalent bonds aligned to the loading axis increases, with cross-linked polymers having Young's modulus values between 50 to 100 GPa.

Some works related to mechanical analysis with Computation Fluid Dynamics (CFD) for PDMS analysis are here mentioned. Lin *et al.* [1] reported numerical modeling of the PDMS elastomer at the microlevel for biological applications. They emphasized the importance of modeling PDMS as a viscoelastic material. Furthermore, they also compared the performance of biological components with and without viscoelastic consideration.

Dragatogiannis *et al.* [2] described a modified model from the finite element method (FEM) for the PDMS nanoindentation. The suggested model, based on the Sneddon equation, takes into account the finite dimensions of the specimen and the indenter's curvature.

Load-displacement curves from FEM analysis were obtained and compared with the experimental and calculated (Sneddon equation) data. Sneddon's solution and FEM analysis deviated from the experiment. Thus, a new analysis was applied by Dragatogiannis *et al.* [2] considering the finite tip radius effect.

A fitting analysis of a typical nanoindentation creep curve is here performed using the Maxwell two-element model to obtain information about the time-dependent properties of untreated and ultraviolet treated PDMS.

Gidde *et al.* [3] investigated that the micropumps are the most important components of lab-on-a-chip devices, which are recently becoming popular due to their outstanding advantages. Among the different designs of micropumps, the nozzle-diffuser valveless design is the most preferred one due to simplicity in manufacturing. For the simulation of these pumps, local fluid-structure interaction modeling is important to obtain performance accuracy. To capture fluid-structure interaction accurately, an appropriate selection of the fluid as well as the structural modeling approaches are very essential.

As stated earlier, PDMS materials behave as viscoelastic material. However, most of the earlier studies on PDMS micropump modeling have considered PDMS as a linear elastic material. In this study, a nozzle-diffuser-based valveless micropump is modeled using a fluid-structure interaction approach along with a linear viscoelastic model for PDMS. The mechanical properties of the PDMS material are experimentally obtained using dynamic mechanical analysis for the range of micropump operating frequencies. The viscoelastic properties of PDMS, with a proportional variation of curing agent, are introduced in the fluid-structure interaction model of micropump using the Kelvin-Voigt model. The results are presented in the form of micropump performance

parameters such as diaphragm deflection, von-Mises stresses, swept volume, and fluid flow rate.

In this context, we also aim at examining some variables, such as tensile strength, Young's, and Poisson's modulus. Some PDMS samples were collected and the structural mechanical analysis tools of the Ansys platform were employed. Load compression data previously obtained by Fincan [4] were used.

II. MECHANICAL PROPERTIES OF PDMS

PDMS is a highly cross-linked semi-crystalline thermoplastic material. It is unique among polymers because it has a silicon-oxygen backbone instead of a carbon backbone, which is more commonly found. Consequently, it has a lower glass transition temperature of $-125\text{ }^{\circ}\text{C}$, which in turn makes it less temperature-sensitive than other rubber-like polymers. It is used in membrane oxygenators because of its high oxygen permeability. PDMS is highly flexible and biologically stable, which is why it is often used in sensitive medical equipment, such as catheter and drainage tubing, and insulation for pacemakers. Furthermore, it is used in prostheses, such as finger joints, blood vessels, heart valves, and other implants.

Commercially available PDMS is known by various names, including siloxanes, silicone fluids, dimethicone, and E900. It is manufactured commercially by the reaction of elementary silicon and methyl chloride (CH_3Cl). The reaction yields dimethyldichlorosilane ($\text{Si}(\text{CH}_3)_2\text{Cl}_2$), which is distilled and hydrolyzed to form linear siloxanes and is further polymerized. Smaller molecular weight siloxanes are removed by thermal treatment, or through solvent extraction.

III. VISCOELASTICITY OF POLYMERS

Polymers deform elastically at low temperatures and like a viscous liquid at high temperatures. Amorphous polymer: glass at low temperatures, rubber at intermediate temperatures, viscous liquid at high T. Low temperatures: elastic deformation at small strains ($\sigma = E\varepsilon$). Deformation is instantaneous when the load is applied. Deformation is reversible. High temperatures: viscous behavior. Deformation is time-dependent and not reversible. Intermediate temperatures: viscoelastic behavior. Instantaneous elastic strain followed by viscous time-dependent strain. Viscoelastic behavior is determined by the rate of strain (elastic for rapidly applied stress, viscous for slowly applied stress) Under intermediate temperatures, they exhibit a behavior that is similar to a rubbery solid, known as viscoelastic deformation. This is a very important property for polymers and most biological materials because they possess cross-linked crystalline structures that are somewhat viscoelastic.

B. Prony series

In a three-dimensional relaxation test, the material is subjected to a sudden strain that is kept constant throughout the test, and the stress is measured over time. The initial stress is due to the elastic response of the material. Then, the stress relaxes over time due to the viscous effects of the material. Typically, either a tensile, compressive, bulk compression or shear strain is applied. The resulting stress vs. time data can be fitted with several equations, the so-called models. Only the notation changes depending on the type of strain applied:

$$G' = G_0 \left[1 - \sum_{i=1}^{n_G} \left(\alpha_i^G - \frac{\alpha_i^G (\tau_i^G \Omega)^2}{1 + (\tau_i^G \Omega)^2} \right) \right],$$

$$G'' = G_0 \sum_{i=1}^{n_G} \left(\frac{\alpha_i^G (\tau_i^G \Omega)^2}{1 + (\tau_i^G \Omega)^2} \right), \quad (1)$$

$$K' = K_0 \left[1 - \sum_{i=1}^{n_K} \left(\alpha_i^K - \frac{\alpha_i^K (\tau_i^K \Omega)^2}{1 + (\tau_i^K \Omega)^2} \right) \right],$$

$$K'' = K_0 \sum_{i=1}^{n_K} \left(\frac{\alpha_i^K (\tau_i^K \Omega)^2}{1 + (\tau_i^K \Omega)^2} \right). \quad (2)$$

The input of the Prony series parameters follows the input method for time-domain viscoelasticity (Eq. (1) and (2)) for a viscoelastic material in harmonic analyses. This is convenient when the elastic shear modulus obtained from data is independent of relaxation data.

Since PDMS has hyperplastic properties, it is easier to get information, because plenty of data are available as (hyperplastic) compliance vs. time. Unfortunately, there is no known closed-form for compliance in terms of the coefficient of the Prony series. So, if one has hyperelastic data, it is not easy to get the coefficients of the (relaxation) Prony series, which are needed for example in materials such as polymers, viscoelastic materials. Such materials have two well-defined components that interact with each other, which are the elastic and viscous components. The combination of both components would result in a more rigorous model to simulate the PDMS. Then, it would be possible to obtain more characteristics of the system than other models.

IV. RESULTS AND DISCUSSION

To determine the mechanical properties of PDMS 10:1 (curing agent ratio), different samples were tested. Different simulations in steady-state were carried out to determine: total deformation, the maximum shear elastic strain, and the shear modulus.

Figures 2–4 depict the results generated using the engineering data. In this section, we do not take into account the Neo Hookean model, but the Poisson's modulus data found in Table I.

Viscoelasticity is defined as the response of a fluid or solid, which is a combination of viscous and elastic behavior, as determined by the rate of deformation relative to the relaxation time of the material. It can be both linear and non-linear, but linear viscosity is an especially useful area of study for many engineering applications of polymers and composite substances.

PDMS is a semi-crystalline thermoplastic, implying that it can be repeatedly softened by the application of heat and solidified by the removal of heat. The storage (E') and loss modulus (E'') in viscoelastic materials measure the stored energy (elastic portion), and the energy dissipated as heat (viscous portion), respectively. Table I lists the physics materials that were selected for these simulations.

TABLE I. Macroscopic compression tests result for PDMS Poisson's ratio.

PDMS 10:1	Poisson's Ratio
Sample 1	0.433
Sample 4	0.427
Sample 6	0.382

A. Macroscopic Test for Determining PDMS 10:1 Elastic Modulus

A general overview is here given regarding the elastic modulus, viscoelasticity, and other mechanical properties of materials before discussing the corresponding properties of PDMS. One of the main characteristics of any material is how it behaves when it is subjected to an externally applied force. Under such conditions, the material deforms either elastically or plastically. The deformation under elastic conditions is reversible in normal conditions and it is linear for many materials. Linear deformation usually obeys a relation that is called Hooke's law, which states that the applied stress is proportional to the strain. The constant of proportionality is called Young's modulus.

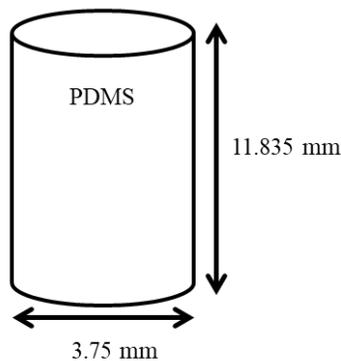


FIGURE 1. A scheme of the cylindrical PDMS samples for compression tests.

Static structural analysis was performed to solve the parameters, such as total deformation and the shear elastic strain. For that, we employed appropriate solvers to perform the finite element analysis (FEA)s. The tool we used to calculate FEA was the Ansys Mechanical ADPL (The generalized model of Maxwell). The relation between the coefficient of viscosity and the modulus of elasticity, in the Maxwell model, is called relaxation time $\tau = \eta/Y$. It

corresponds to the duration of stress to reduce to 1/e of its initial value. We employed this software due to its many features, such as parameterization, macros, branching and looping, and complex math operations. All these benefits are accessible within the Ansys Mechanical APDL user interface and were here used to determine the physical parameters.

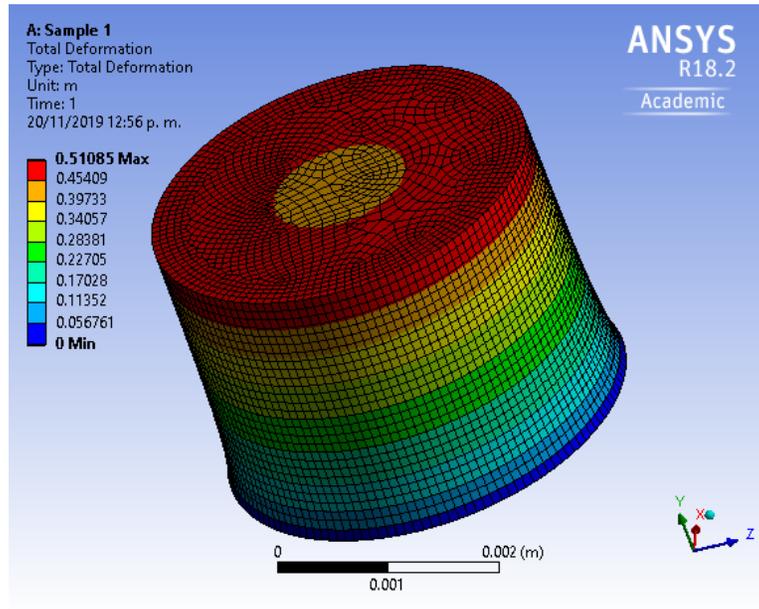


FIGURE 2. Total deformation simulation sample 1.

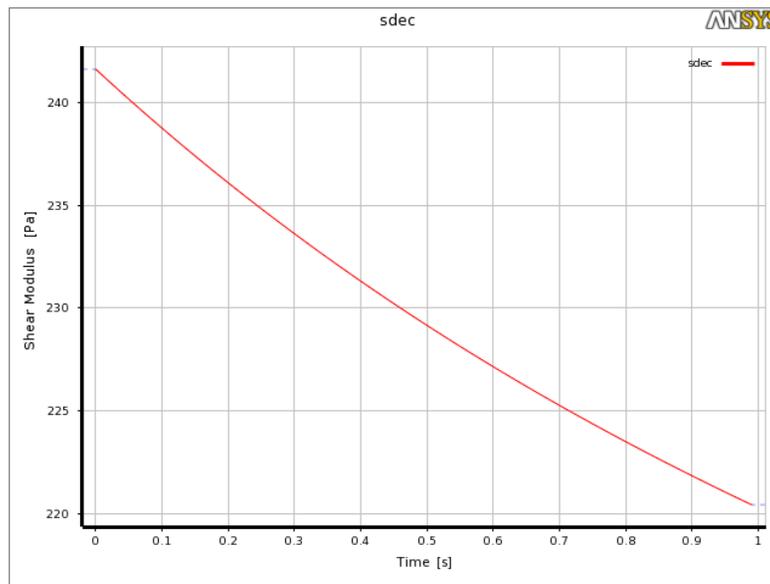


FIGURE 3. Plot of Shear modulus sample 1 at different relaxation times.

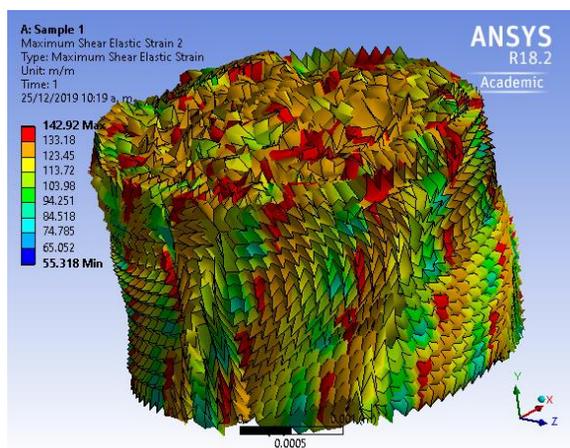


FIGURE 4. Maximum Shear Elastic Strain Sample 1.

The simulations depicted in Figures 2–4 were carried out at room temperature, for a time interval of 1 min. The total deformation reached 50% and the shear modulus decreased from 245 to 220 Pa. For this variety of polymer, various orientations with the force of 1 N were applied to this material, resulting in deformation responses. In the case of maximum shear stress, it reached 142.92 Pa, deforming the initially established geometry.

A. Stress-Strain Behavior of Polymers

Many polymers exhibit stress-strain behavior that is somewhat similar to solids. However, an important characteristic of such materials is that their mechanical properties vary with the rate of developed strain, as well as temperature. As discussed earlier, deformation can occur through brittle, plastic, or highly elastic routes. The values of Young's modulus and tensile strength for polymers are much lower than metals, while some polymers can elongate by as much as 1,000% of their original length. Also, the mechanical properties of many polymers change significantly with temperature, from brittle to highly elastic behavior as temperature increases.

An important characteristic of the plastic flow regime in polymers is the principle of maximum plastic dissipation. According to this principle, the state of stress present in a sample for a given plastic strain increase results. This increment is either equal to or greater than the work done by the plastic strain increase with any other state of stress, within or on the yield surface. This principle gives rise to the associated flow rule, which states that each plastic strain increase is proportional to the component of an outward stress vector acting normal to the yield surface. The Young's modulus of polymers is highly dependent on their chemistry as well as the temperature. The value of E for these materials increases as covalent bonds aligned to the loading axis increases, with cross-linked polymers having Young's modulus values.

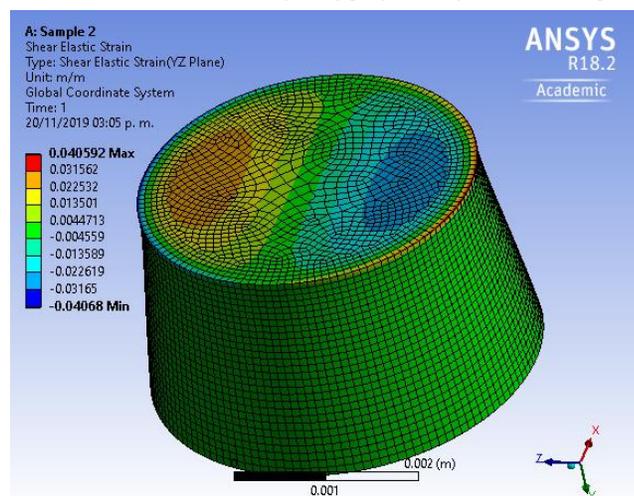


FIGURE 5. Shear elastic strain of Sample 2.

Examples of these parameters are illustrated in Figures 5 and 6. Two types of samples were tested for maximum shear elastic using Samples 2 and 6 (See Table I).

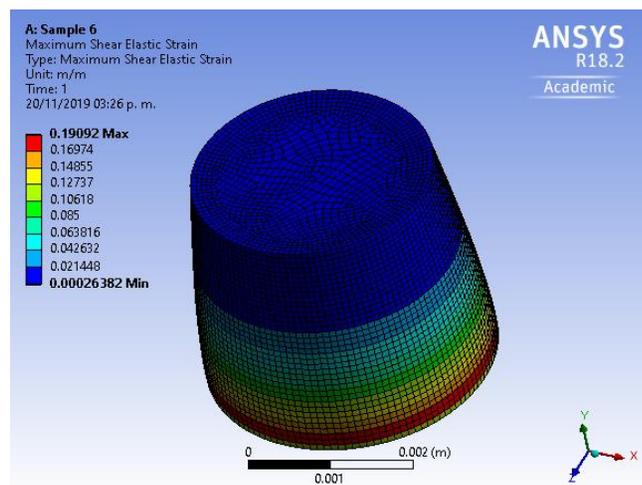
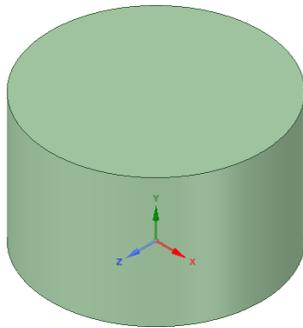


FIGURE 6. Maximum Shear Elastic Strain Sample 6.

B. Compressive Strength Testing of PDMS

Tests were performed to analyze the compressive strength of the PDMS samples (ratio 10:1) (Figure 7), by applying 400 or 700 Pa. We employed the elastic modulus (Young and Poisson), and shear and bulk data. The data were then fed into the Ansys mechanical analysis program.



ANSYS
R18.2

Force orientation was made towards the direction of gravity, as shown in Figure 8. Figure 9 shows how the sample undergone to a resistance of 400 Pa. Figures 9a and 9b depict how the size of the sample decreased, reaching a maximum deformation of 0.0014172 m. Under higher pressure of 700 Pa, we observed a much higher deformation of the sample, achieving a maximum deformation of 0.00248 m.

FIGURE 7. Cylinder sample.

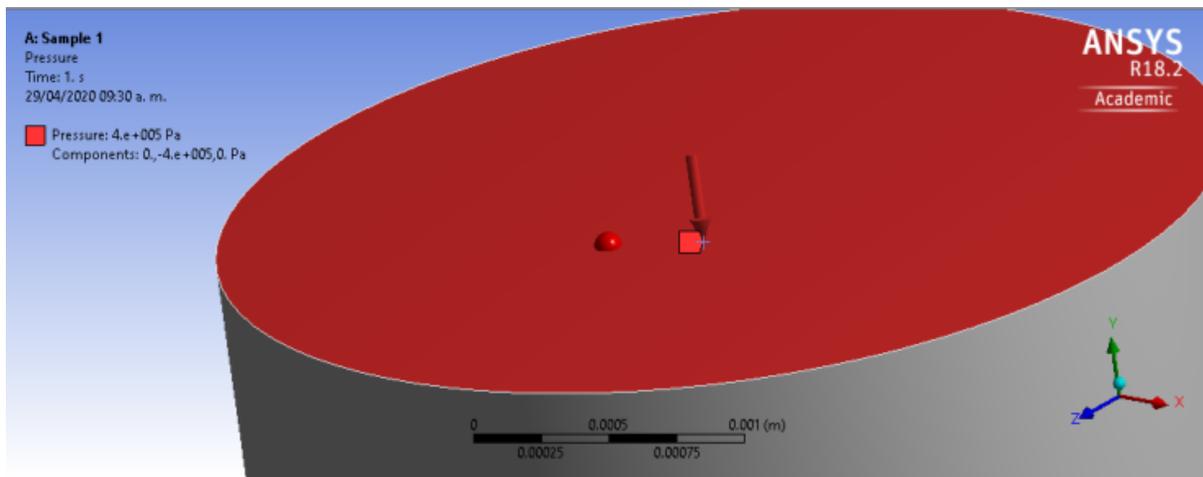


FIGURE 8. Pressure and force orientation of the sample.

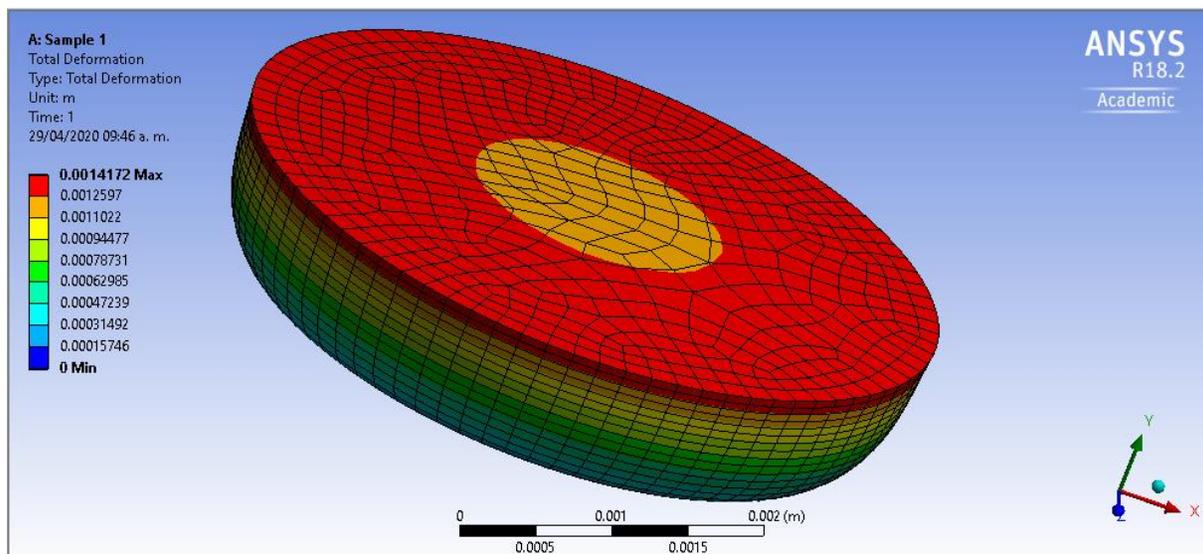


FIGURE 9a. Total deformation at 400 Pa.

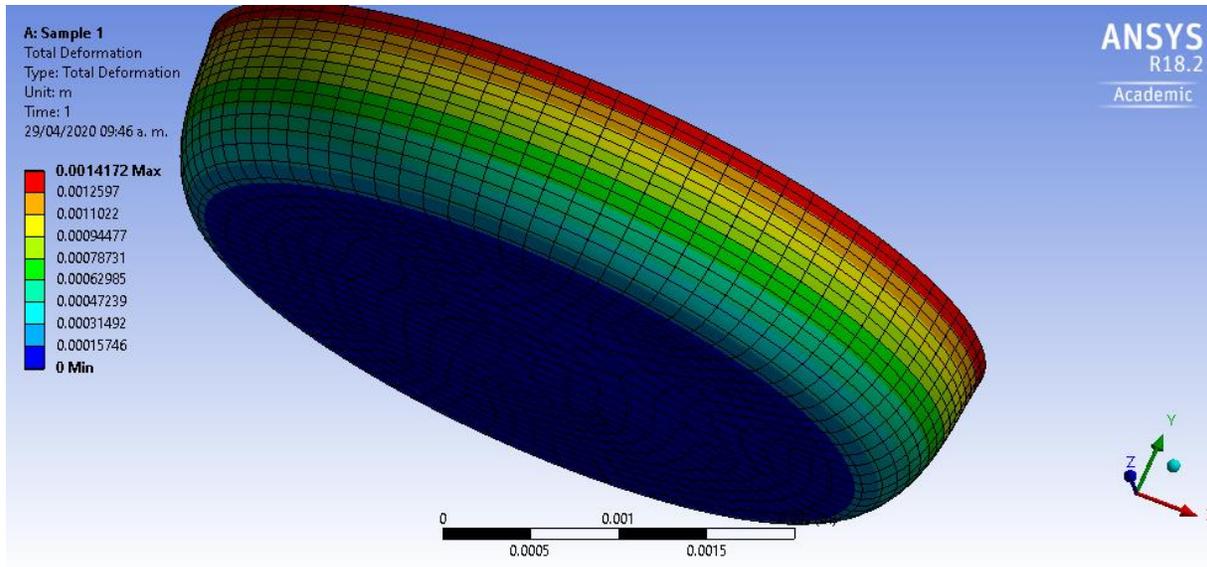


FIGURE 9b. Total deformation at 400 Pa.

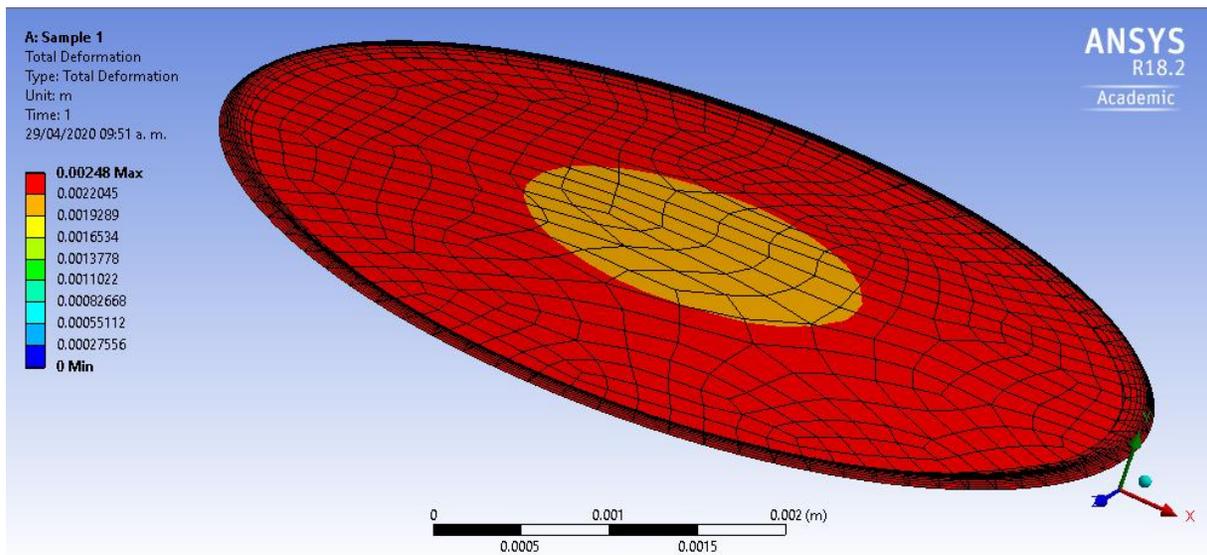


FIGURE 10. Total deformation at 700 Pa.

V. RESULTS OF HYPERELASTIC MATERIAL MODEL

Simulations were performed employing Young’s modulus curve vs. the relaxation time. For this study, it was necessary to get the initial Shear modulus (G) (Eq. 3) and the incompressibility parameter named $D1$.

$$G = \frac{E}{2(1+\nu)}, \quad (3)$$

where G is the Shear modulus for the isotropic material and is expressed in terms of Young’s modulus (E) and the Poisson’s ratio (ν).

The $D1$ refers to the incompressibility factor. The lowest the value, the more incompressible the material. Divergence may occur when this value is too low.

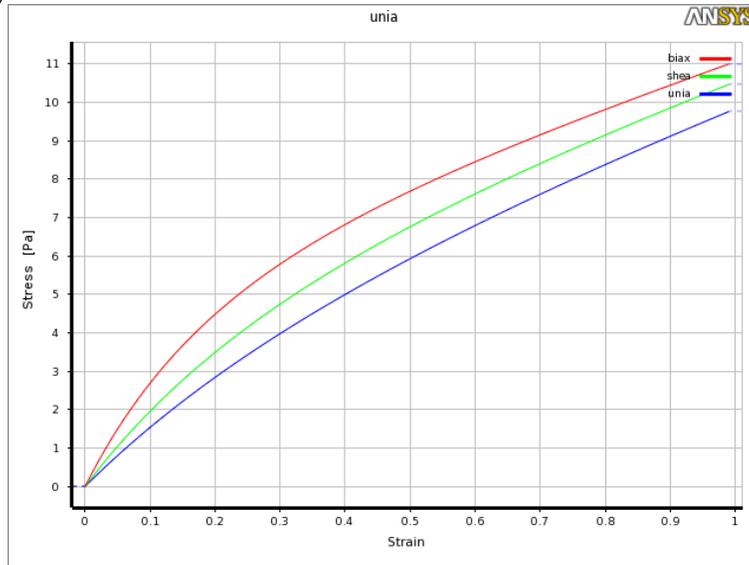


Figure 11. Strain vs Stress Curve.

An important characteristic of the plastic flow regime in polymers is the principle of maximum plastic dissipation. This principle gives rise to the associated flow rule, which states that each increase in plastic strain is proportional to the component of an outward stress vector acting normal to the yield surface.

The stress/strain curve simulation was performed considering room temperature. The strain values presented have been corrected using the correction factor.

The strain stress curve, for the hyper-elastic material

(See Figure 11) is required for these kinds of materials, such as our material (polymer at a 10:1 – curing agent). With this information, we were able to determine the viscoelastic parameters.

The strain vs. stress curve, represented in Figure 11, shows the uniaxial, biaxial, and shear modulus results. They were necessary to build the model. The results shown were made by employing 10.5 Pascal as a function of stress or deformation. Note that elastomers deform much more than metals, elastomer: 20 to 100% and metal: 10 to 15%.

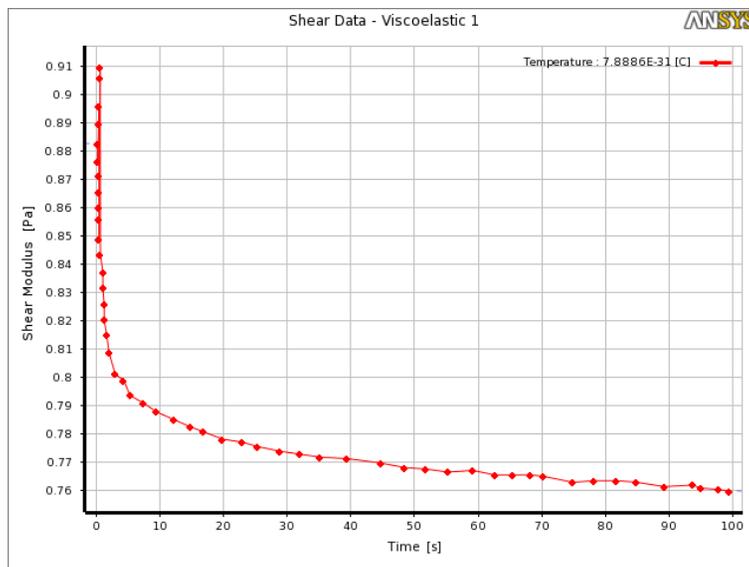


FIGURE 12. The shear modulus curve vs. the relaxation time.

Employing the Pronyx relaxation model, two tests were performed to converge the shear modulus curve vs time (Figure 12).

We run a viscoelastic analysis of a 3D hyperelastic cylinder with viscoelastic curve-fitting using the Prony

Shear Relaxation cell. The coefficients related to the relative modulus was initialized with a time of 1s (Figure 13). Figure 13 shows that the curve at 1 s of relaxation time failed to fully adjust. As a result, another test was made with 8 s of relaxation time. In this case, the shear module was

A larger deformation with a time step of 7 s was then selected with their respective sub-steps. A convergence of the results was achieved, as shown in Figure 15.

fitted accordingly (Figure 14). Note that it can be observed the results of the total and directional deformation. Afterward, time was increased to 8 s, as shown in Figure 14. Once the curve was successfully fitted, the simulations provided us with information about the directional and total deformation.

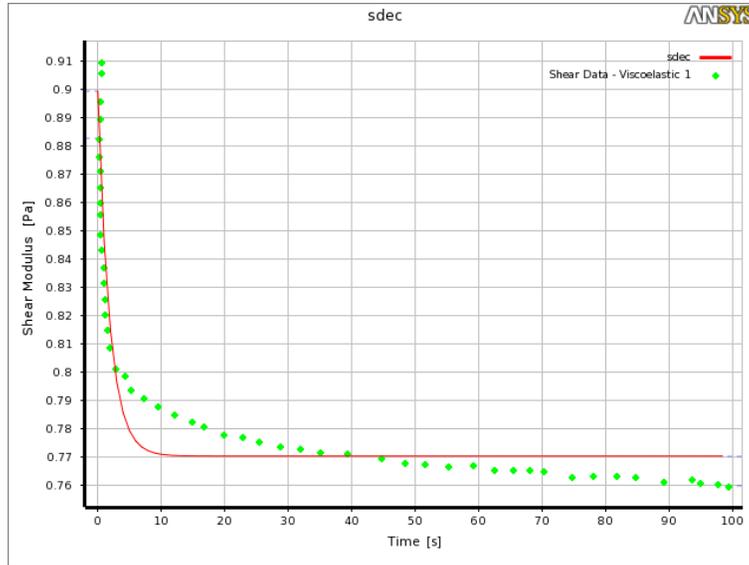


FIGURE 13. Curve fitting of Shear modulus vs time

The force selected was based on the work of Finca (2015), who employed -0.98 N on the Y direction. Figure 16 highlights that the maximum deformation was up to 0.03024 m. It shows how this hyperelastic property influences the structure of this polymer that has a high molecular weight. Materials under the application of forces may deform through three principal mechanisms: by transmitting the applied force directly to intermolecular bonds and interatomic interactions; by undergoing

substantial shape changes; or by deforming either semi-permanently or permanently.

Figure 17 depicts that, in 1 s of simulation, the total deformation was 0.29755 m, which is considered as a semi-permanent deformation. This is usually observed in amorphous polymers and many other materials at high-stress levels. Polymeric materials under these conditions may undergo plastic deformation, also called plasticity or ductility, and then experience ductile failure with yield.

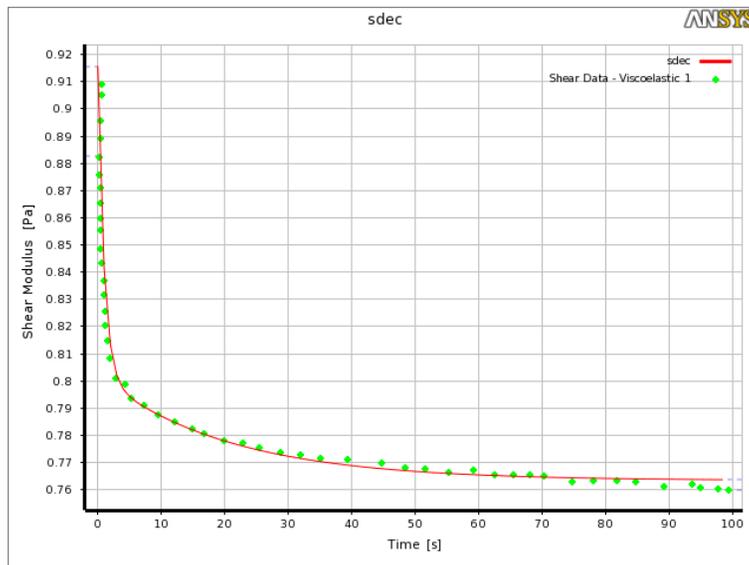


FIGURE 14. Shear modulus vs time.

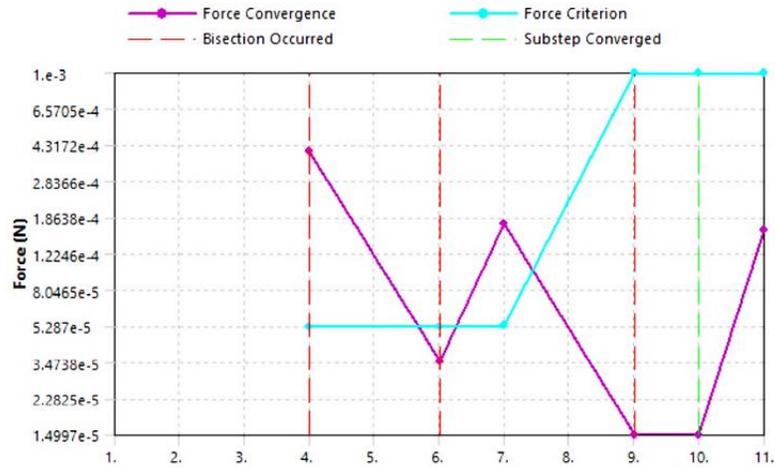


FIGURE 15. Convergence plot.

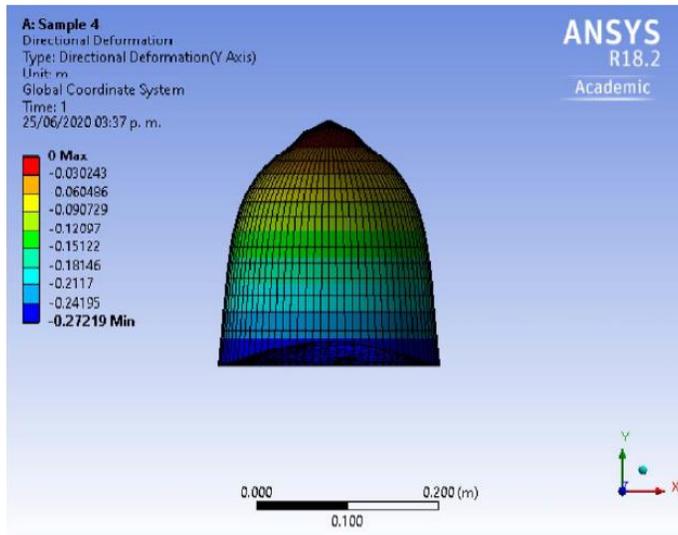


FIGURE 16. Directional deformation without elements.

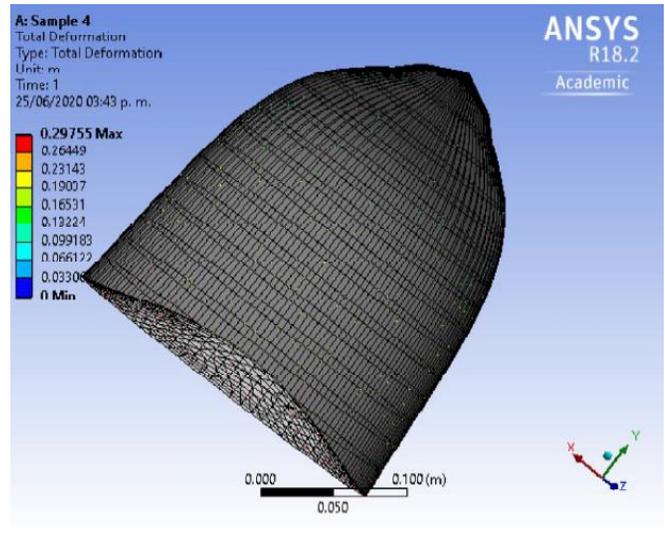


FIGURE 17. Total deformation.

VI. CONCLUSIONS

The main purpose of this study was to use a simple method to obtain the mechanical properties by using the structural analysis of a soft material called polydimethylsiloxane (PDMS). The experimental data were taken from literature, including elastic modulus and the base/agent ratio. We were able to apply viscoelasticity models to evaluate the theoretical deformations of the PDMS samples in environmental conditions with short simulation time.

Some experimental conditions were tested to determine the compression of PDMS. The results showed a reduction in size, particularly under 700 Pa (the uppermost pressure

used), which resulted in a maximum deformation of 0.00248 m.

Under the application of the hyperelastic model for the PDMS, a different behavior was observed. In such cases, the Neo Hookean solid model was able to fit the curve of the shear module vs. time, considering a large deformation of the domain.

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