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Effect of mechanical stress on optical properties of polydimethylsiloxane

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ABSTRACT

In this paper we present results of our investigation of the effect of mechanical stress on the coefficient of absorption and the refractive index of polydimethylsiloxane (PDMS) in the NIR region. We study optical transmittance and optical paths of PDMS samples compressed up to a length expressed by the value of the relative stress −0.5. The experimentally obtained results imply that the stress-induced changes of the absorption coefficient and the refractive index of PDMS are due to a change of the density of dimethyl-siloxane groups rather than a change of the PDMS's molecular structure. Since we performed measurements for high stresses, we modified the Poisson's relation to obtain its generalized form that holds for any stress and that we named generalized Poisson's relation. To obtain this relation we assumed that an elementary increase of each of the two lateral dimensions of a sample is determined by the Poisson's constant and the actual longitudinal dimension of the sample which is subject to change during the process of deformation. Then to express the change of the density of the electric dipoles in a PDMS sample we used this relation. The realized measurements indicate that the deformation dependent changes of the optical transmittances and the optical paths of the samples are in a good agreement with the values calculated using the assumption of the dominant influence of the density of the elementary dipoles and the validity of the generalized Poisson's relation.

The deformation affects the optical transmittance and the refractive index so strongly that it is necessary to take it into account when the PDMS is used as a medium for optical applications. The transmittance at the wavelength of 1700 nm and for the relative stress −0.5 decreases about three times and the change of the refractive index at the wavelength of around 1500 nm reaches a value of about 0.05. These values imply that it is possible to utilize the PDMS for constructing optical sensors that could be used for measuring stress or mechanical displacement.

1. Introduction

Polydimethylsiloxane is known as an elastomer having unique mechanical properties such as a small value of the shear modulus [1], high compressibility [2] and good stability in a wide range of temperatures [3]. In addition to unique mechanical properties, the PDMS possesses also interesting optical properties, e.g. the value of its refractive index is close to that of glass, it exhibits photoelasticity [4,5] and has rather low dispersion in the VIS–NIR region [3,6]; it is almost transparent in the VIS and, on the other hand, it significantly absorbs at some wavelengths in the NIR [7]. The large number of papers investigating the mechanical and optical properties of the PDMS [e.g. 8–16] and its applications [e.g. 17–22] published up to date confirms that the interest in this material is not fading away. But as far as we know, only a small part of the works concerning the PDMS has been devoted to the investigation of the effect of the mechanical deformation on its refractive index (except for birefringence) and its coefficient of absorption. This is in spite of the fact that the PDMS exhibits spectral regions with high values of the coefficient of absorption, which means that a small change of a sample's thickness may imply a significant change of the intensity of light that has passed through a layer of the material. If so, then the PDMS may be utilized for constructing mechanical displacement or stress sensors. Besides, there are rather big differences between data reporting on high losses occurring in the PDMS in the VIS spectral region [22,23] and between values of the stress–optical coefficient listed up to date [24,25]. This has led us to study the effect of the mechanical deformation on the optical properties of the PDMS.

2. Effect of deformation on optical parameters

Changes of optical parameters caused by deformation can be due to the changes of the configuration of the elements from which a material consists and/or the changes of the properties of the elementary dipoles that determine the values of the optical parameters characteristic for this material [26]. In both cases the

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deformation affects both the refractive index and the coefficient of absorption.

When describing the effect of deformation on the optical parameters of the PDMS, we assumed that the deformation does not affect the properties of the elementary dipoles that are responsible for the optical properties of the PDMS. We also assumed that the changes of the coefficient of absorption and the refractive index are due to a change of the density of the dipoles. The effect of the latter mechanism may be evaluated by comparing the results of the theoretical calculations performed under this assumption with those obtained experimentally. This comparison will allow for evaluating the involvement of the above mentioned mechanisms on the optical parameters of the PDMS.

According to the assumption that the coefficient of absorption α is proportional to the density of the medium we can write

$$\alpha(\rho(\varepsilon_l)) = \alpha_0 \frac{\rho(\varepsilon_l)}{\rho_0}, \tag{1}$$

where α_0 is the coefficient of absorption of the non-deformed medium, ρ is the density of the medium, $\varepsilon_l = \Delta l/l_0$ is the relative change of a sample's length (relative deformation), l_0 is its original length and Δl is the change of the length due to deformation. The density of the elementary dipoles in the sample deformed by tensile (or compressive) stress depends not only on the longitudinal deformation but also on the transverse contraction (or extension). Then the density for a uniaxial strain is expressed by the formula

$$\rho(\varepsilon_l) = \frac{\rho_0}{(1+\varepsilon_l)(1+\varepsilon_t)^2}, \tag{2}$$

where $\varepsilon_t = \Delta h/h_0 = (h(\varepsilon_l) - h_0)/h_0$ is the lateral deformation and h_0 and Δh denote the transverse dimension of the sample prior to the deformation and its change due to the deformation, respectively. If the deformation ε_l and the dependence of ε_t on ε_l are known, then, assuming that the density of the medium is responsible for its optical properties, the value of the coefficient of absorption can be expressed using Eqs. (1) and (2) .

Since the number of the molecules in a unit volume depends on the sample deformation, the refractive index dependence on the strain of the medium is given by the formula following from Clausius–Mossotti equation [27].

$$n = \sqrt{1 + \frac{N(\rho)a}{1 - \frac{N(\rho)a}{3}}}, \tag{3}$$

where $N(\rho)$ is the number of atoms per unit volume and a is atomic polarizability.

The fundamental description of the tensile (compressive) deformation is based on the assumption that the transverse (lateral) contraction (extension) is directly proportional to the longitudinal extension (contraction) induced by the deformation, i.e.

$$\Delta h = -\nu h_0 \frac{\Delta l}{l_0}, \tag{4}$$

where ν is the Poisson's constant, Δh, Δl, l_0 and h_0 are the increments of the transverse and the longitudinal dimensions and the original length and the thickness of the sample, respectively.

However, for large deformations which are feasible due to the wide region of elasticity of the PDMS, the transverse contraction (extension) does not need to depend linearly on the deformation as expressed by Eq. (4). The dependence of the transverse dimensions on the tensile (compressive) deformation can be derived from Eq. (4) if one assumes that it is valid in a differential form in each moment of the deformation, i.e.

$$dh = -\nu h \frac{dl}{l}, \tag{5}$$

where l is the length of the sample during the deformation. Solving Eq. (5) we get for the dependence of the transverse dimensions of the sample on the change of its length Δl

$$h(\Delta l) = h_0\, l_0^{\nu} (l_0 + \Delta l)^{-\nu}, \tag{6a}$$

or

$$\varepsilon_t = (1+\varepsilon_l)^{-\nu} - 1. \tag{6b}$$

The first two terms of the Taylor series of the function $\varepsilon_t(\varepsilon_l)$ defined by Eq. (6b) give for weak deformations equation $\varepsilon_t = -\nu\varepsilon_l$. This expression is in accordance with the commonly used expression for the transverse deformation in case of weak deformations given by Eq. (4). For the transverse deformation expressed by Eqs. (6a) and (6b) (Eq. (4), alternatively), Eqs. (1) and (3) describe the strain (stress) dependence of the coefficient of absorption and the refractive index.

3. Measurement and comparison between measured and calculated dependences

We studied the effect of deformation on the coefficient of absorption, the refractive index and the birefringence in samples of PDMS Sylgard® 184 (Dow Corning Corporation) prepared by cross-linking the pre-polymer with the curing agent in the ratio 10:1 of weight. Both parts were well mixed and the mixture was poured into small cuvettes with thicknesses 1 mm, 2 mm and 5 mm and transverse dimensions 10 mm and 20 mm. The PDMS was then cured at the room temperature for 48 h. The prepared samples were homogeneous enough since they were well transparent and we did not observe any scattering or a distortion of the used He–Ne laser beam. Before starting the measurement we optimized the transverse dimensions of the samples by slicing them in order to fit a sample into a screw preparation by which the deformation was generated.

3.1. Absorption–stress dependence

We determined the coefficient of absorption of the PDMS by means of the transmittance measurements using the set up schematically shown in Fig. 1. The spectral dependence of the coefficient of absorption was determined by measuring the spectral optical transmittance of non-deformed samples with thicknesses 1 mm, 2 mm and 5 mm. We used the NIRQuest512-2.2 (Ocean Optics) spectrometer with an optical resolution of about 4 nm and Anritsu MS9710B with an optical resolution of about 1 nm as optical spectrum analyzers. The samples were inserted into the screw preparation, which made it possible to realize compressive deformation during the measurement. The optical signal after

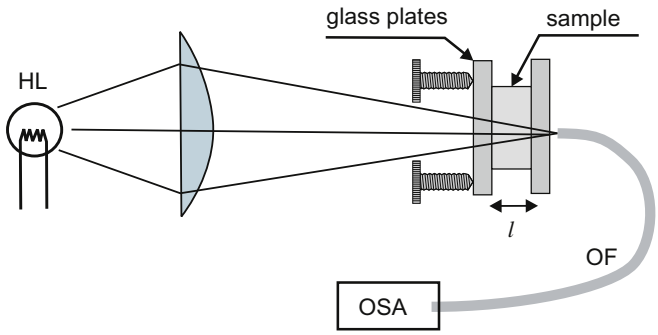

Fig. 1. Experimental setup used for measuring the coefficient of absorption and the stress-induced changes of absorption. HL – halogen lamp, OF – optical fiber, OSA – optical spectrum analyzer.