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Методика визначення комплексних модулів для полікарбонатного пластика при гармонічному навантаженні

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A procedure for complex moduli determination for polycarbonate plastic under harmonic loading

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Досліджується циклічна поведінка аморфного полімеру – полікарбоната – в умовах гармонічного навантаження. Для моделювання нестаціонарної фізично нелінійної поведінки матеріалу використовуються еволюційні рівняння Заїрі. В умовах гармонічного кінематичного навантаження будуються амплітудні фізичні співвідношення, які пов'язують амплітуди основних польових величин і використовують концепцію комплексних модулів. Для знаходження дійсної та уявної частини цих комплексних модулів (модулів накопичення і втрат) використовується модифікована схема методу еквівалентної лінеаризації з використанням циклічних діаграм. Побудовано залежності комплексних модулів від амплітуди інтенсивності навантаження. Показано, що стандартна схема методу еквівалентної лінеаризації завищує значення амплітуди напруження більше ніж на 10%.

Ключові слова: гармонічне навантаження, амплітудні співвідношення, непружна деформація, комплексні модулі.

The problem of characterization of material response to harmonic loading is addressed. In the present research, Zaïri unified constitutive model is used to predict the time dependent inelastic response of amorphous glassy polymer, a polycarbonate (PC). The approach that uses the complex-value amplitude relations is preferred rather than direct numerical integration of the complete set of constitutive equation for the material. The key point of the approach adopted lays in determination of complex moduli, i.e. storage and loss moduli under harmonic loading. It is usually done by making use of equivalent linearization technique. It is shown that this technique leads to overestimation of stress amplitude. To avoid this, the modified equivalent linearization technique is used. It relies on special procedure for determination of storage modulus which based on the usage of cyclic stress–strain diagram. Obtained histories of main field variables evolution were used to find the stress–strain cyclic diagram and real as well as imaginary parts of complex shear modulus with making use of both standard and modified equivalent linearization techniques. The prediction of stress amplitude obtained in the frame of the former scheme overestimates the actual value for more than 10% while the latter scheme gives it with desirable accuracy.

Key Words: harmonic loading, amplitude relations, inelastic deformation, complex moduli.

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1. Introduction

Cyclic loading is one of the most important and widely used types of loading imposed on structural elements. Materials of structures and their members experiencing cyclic deformation can exhibit specific time dependent properties and can be deformed inelastically being exposed to high stress levels. Inelastic deformation of the material is accompanied by heat generation caused by the internal mechanisms of mechanical energy dissipation. This phenomenon is usually called the "dissipative heating" [1,2]. It's important to notice here that, under some conditions, the dissipative heating, being small over one separate cycle of vibration, can lead to overheating for long term processes causing the change of mechanical properties, degradation of performance and durability of the structure.

At the present, there are two approaches to address this issue. In the frame of the first approach, the complex set of constitutive equations governing response of numerous internal parameters is introduced. For polymers, the constitutive modeling utilizes, either directly or with some modifications, viscoplastic constitutive equations which have been developed for metals. The Schapery single integral form has been widely used to characterize the nonlinear (stress or strain dependent) viscoelastic behavior of polymers. In general, the models can divided into two categories. The first category additively combines linear viscoelastic and plastic constitutive relations (see, for example, [3]). In this category, the viscoelastic strain rates depend upon loading histories and time, and the plastic strain rates depend only upon loading path histories. Second category combines linear elastic and viscoplastic constitutive relations, such as the models proposed in [Perzyna, Perzyna and Wojno, Bodner and Partom , Frank and Brockman, Goldberg and Roberts, Gilat and Zaïri [4–6]. To describe the material time dependent behavior accounting for different features and peculiarities over the cycle of vibration, a direct integration of the set of constitutive equations is necessary. Usually it appears to be time and resource costly for multi-cyclic processes.

Within the second approach, the approximate amplitude relations are used to characterize the cyclic response of the material, i.e. the relations between amplitudes of the main mechanical field parameters over the cycle [7]. Naturally, the application of this technique is justified for the class of problems where there is no need for detailed information on the material response during the cycle (life prediction of the structure, failure due to overheating as a result of internal dissipation etc.). The key point of the amplitude theories is concept of complex moduli [7]. For an inelastic (particularly viscoelastic) material, the modulus governing the relation between strain and stress amplitudes is represented by a complex quantity with real and imaginary parts referred to as storage and loss modulus respectively. The former characterizes elastic response of material and the latter one defines the dissipative ability of the material [2]. In other words, the energy is stored during the loading part of cycle and released under unloading phase, whereas the energy loss occurs during complete cycle due to dissipative properties of the material. The drawback of the approach was the overestimation of stress amplitudes as a result of making use of standard equivalent linearization technique for calculation of both storage and loss moduli. To overcome this difficulty, the modified scheme was proposed in [2,7]. But applicability of the method should be verified for each particular type of the material.

This paper is devoted to investigation of the technique applicability to the typical elastic-viscoplastic materials such as Polycarbonates (PC), and to determination of complex moduli for isothermal loading case for wide range of loading amplitudes. Particular attention will be paid to simulation of cyclic response of pure polymer material (PC) to monoharmonic kinematic loading in the frame of the second approach.

2. Constitutive relations

To accurately predict an overall performance and lifetime of polymer, it is necessary to model time dependent and inelastic responses. Viscoelastic materials such as polymer materials have the particularity of possessing viscous, elastic and, under some conditions, plastic behavior. Constitutive material models of viscoelastic solids have been proposed for isotropic materials undergoing small deformation gradients whereas the inelastic strain can be calculated as the difference of the total strain and elastic strain. In order to determine the viscoelastic-viscoplastic response of the polymer, Zaïri et al. [5] proposed a model for predicting the viscoplastic response of neat polymers, utilizing a set of state variables as an indication of the resistance of polymeric chains against flow. It should also be mentioned that polymer’s mechanical properties and loading/strain rate are the two main parameters that govern the nonlinear response of the polymer. Bodner and Partom model [4] is a typical representative of the class of constitutive theories that constitutes a state variable approach with no yield surface. In the frame of this model, the viscoplasticity contribution exists at all non zero stress levels, and it is found to be the more adequate for the viscoplastic part. The model is modified in order to include strain softening immediately after yield and subsequent re-hardening in [8]. Accordingly, the viscoplastic strain component can be expressed in terms of the deviatoric stress components as follows:

$$\dot{\boldsymbol{\varepsilon}}^{vp} = \sqrt{3} D_0 \left(\frac{\sigma_e}{Z_1 + Z_2} \right)^{2n} \frac{\boldsymbol{\sigma}'}{\sigma_e}, \qquad (1)$$

where $\dot{\boldsymbol{\varepsilon}}^{vp}$ is the viscoplastic strain rate which can be defined as a function of deviatoric stress; the internal state variable Z_1 was initially introduced in [8] to account for the horizontal plateau upon yield and the subsequent strain hardening exhibited by a glassy polymer and Z_2 is internal variable to account for the effect of strain softening. The equivalent (effective) stress is given by expression: $\sigma_e = (3/2\boldsymbol{\sigma}':\boldsymbol{\sigma}')^{1/2}$, where $\boldsymbol{\sigma}' = \boldsymbol{\sigma} - tr(\boldsymbol{\sigma})\boldsymbol{I}/3$ is the deviatoric part of the Cauchy stress, $\boldsymbol{\sigma}$. Moreover, D_0 and n are material constants; D_0 represents the maximum inelastic strain rate and n is the strain rate sensitivity parameter controlling the viscosity of flow. The rate of change of the other two internal state variables, Z_1 and, Z_2 can be determined using the following evolution equations:

$$\dot{Z}_1 = m\left(\frac{Z_1 - (1-\alpha)Z_{10}}{Z_{10}}\right)\dot{W}^P, \tag{2}$$

$$\dot{Z}_2 = h(Z_{2s} - Z_2)\dot{W}^P - AZ_{2z}\left(\frac{Z_2 - Z_{2c}}{Z_{2S}}\right)^r, \tag{3}$$

where $\dot{W}^P$, $\dot{W}^P = \boldsymbol{\sigma} : (\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}^e) = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^{in}$, is the inelastic work rate and the associated rise of temperature is neglected, $\dot{\boldsymbol{\varepsilon}}^{in} = \dot{\boldsymbol{\varepsilon}}^{vp} + \dot{\boldsymbol{\varepsilon}}^{ve}$ is referred to as inelastic strain; Z_{10} is the initial value of Z_1 introduced to represent the onset of the plasticity, Z_{2S} is the saturation value of Z_2, m and h are the hardening and softening rate parameters, respectively, α is a parameter controlling the onset of the re-hardening; A, Z_{2c} and r are three parameters introduced in the model equations to simulate the static recovery. It should be emphasized that nonlinearity is also included in the viscoelastic part. In order to determine the viscoelastic response of the polymer, the unmodified Bodner–Partom model [4], used to describe the nonlinear pre-peak viscoelastic behavior, can be expressed as:

$$\dot{\boldsymbol{\varepsilon}}^{vp} = \sqrt{3}D_0 \exp\left(-\frac{1}{2}\left(\frac{Z_3}{\sigma_e}\right)\right)^{2n}\frac{\boldsymbol{\sigma}'}{\sigma_e}, \tag{4}$$

where Z_3 is an added internal state variable and the remaining terms are as defined earlier. The parameter Z_3 is governed by the following differential equation:

$$\dot{Z}_3 = q(Z_{3s} - Z_3)\dot{W}^P, \tag{5}$$

where q is the pre-yield hardening rate parameter, Z_{3s} is the saturation value of Z_3 and the initial value of Z_3 is defined by the parameter Z_{30}.

3. Procedure of complex moduli derivation

Harmonic loading is one of the most widely used and important types of loadings imposed upon a mechanical structure. In this investigation, approximate model of inelastic behavior developed in [1,7] for the case of proportional harmonic loading has been used. In this case, the cyclic properties of the material are described in terms of complex moduli. It is important to notice that the inelastic deformation is considered to be incompressible and thermal expansion is dilatational, it may be more convenient in some applications to separate the isotropic stress-strain relations into deviatoric and dilatational components that can be shown by equations as:

$$\boldsymbol{\sigma}' = 2G(\boldsymbol{e} - \boldsymbol{\varepsilon}^{vp} - \boldsymbol{\varepsilon}^{ve}),\ \sigma_{kk} = 3K_V(\varepsilon_{kk} - \varepsilon^{\theta}), \tag{6}$$

where G is the shear modulus, K_V is the bulk modulus, i,j,k = 1,2,3 and repeated index implies a summation over. Due to incompressibility of plastic deformation, $\dot{\varepsilon}^{in}_{kk} = 0$, i.e. the plastic strain rate is deviatoric: $\dot{\boldsymbol{\varepsilon}}^{in} = \dot{\boldsymbol{e}}^{in}$.

According to this model, if a body as a system subjected to harmonic deformation or loading, then its response is also close to harmonic law:

$$\begin{aligned} \boldsymbol{e}(t) &= \boldsymbol{e}'\cos\omega t - \boldsymbol{e}''\sin\omega t, \\ \boldsymbol{\sigma}(t) &= \boldsymbol{\sigma}'\cos\omega t - \boldsymbol{\sigma}''\sin\omega t. \end{aligned} \tag{7}$$

The complex amplitudes of the deviator of total strain, $\tilde{\boldsymbol{e}}$, inelastic strain, $\tilde{\boldsymbol{e}}^{in}$, and the stress deviator, $\tilde{\boldsymbol{\sigma}}'$, are related in the N^{th} cycle by the complex shear modulus, $\tilde{G}_N$, and plasticity factor, $\tilde{\lambda}_N$, as shown below:

$$\tilde{\boldsymbol{\sigma}}' = 2\tilde{G}\tilde{\boldsymbol{e}}, \quad \tilde{\boldsymbol{e}}^{in} = \tilde{\lambda}\tilde{\boldsymbol{e}}, \quad N = 1,2,3,\ldots, \tag{8}$$

where

$$\begin{aligned} \tilde{\boldsymbol{e}} = \boldsymbol{e}' + i\boldsymbol{e}'',\ \tilde{\boldsymbol{\sigma}} = \boldsymbol{\sigma}' + i\boldsymbol{\sigma}'',\ \tilde{\boldsymbol{e}}^{in} = \boldsymbol{e}'^{in} + i\boldsymbol{e}''^{in}, \\ \tilde{G} = G'_N + iG''_N,\ \tilde{\lambda}_N = \lambda'_N + i\lambda''_N, \end{aligned} \tag{9}$$

where N is the cycle number and $(\cdot)'$ and $(\cdot)''$ denote the real and imaginary parts of complex quantities.

The shear modulus and plasticity factor are functions of the intensity of the strain-range tensor, frequency and temperature

$$\tilde{G} = \tilde{G}_N(e_0,\omega,\theta), \quad \tilde{\lambda}_N = \tilde{\lambda}_N(e_0,\omega,\theta), \tag{10}$$

where the square of the intensity of strain-range tensor is calculated as $e_0^2 = \boldsymbol{e}' : \boldsymbol{e}' + \boldsymbol{e}'' : \boldsymbol{e}''$.

The imaginary parts of the complex moduli are determined from the condition of equality of the energies dissipated over a period and are calculated according to the formula

$$G''_N = \frac{\langle D' \rangle_N}{\omega\, e_0^2}, \quad \lambda''_N = \frac{G''_N}{G_0}, \qquad \langle (\cdot) \rangle_N = \frac{1}{T} \int_{T(N-1)}^{TN} (\cdot)\, dt, \quad T = \frac{2\pi}{\omega}, \tag{11}$$

where D' is the rate of dissipation of mechanical energy, G_0 is the elastic shear modulus.

The real parts are found with making use of the condition that generalized cyclic diagrams $\sigma'_{aN} = \sigma'_{aN}(e_0, \omega)$ and $e_{paN} = e_{paN}(e_0, \omega)$, which relate the ranges of the stress and plastic-strain intensities in the N^{th} cycle, coincide in the frame of the complete and approximate approaches

$$G'_N(e_0,\omega) = \left[\frac{\sigma'^{\,2}_{aN}(e_0,\omega)}{4e_0^2} - G''^{2}_N(e_0,\omega) \right]^{1/2}, \qquad \lambda'_N(e_0,\omega) = \left[\frac{\sigma'^{\,2}_{aN}(e_0,\omega)}{4e_0^2} - \lambda''^{2}_N(e_0,\omega) \right]^{1/2}, \tag{12}$$

where G' and λ' are the sought-for real part of shear modulus and plasticity factor.

4. Problem statement and numerical integration procedure

Due to significant nonlinearity of the stiff type, the numerical integration of Zaïri equations was adopted. Three step scheme of attacking the problem of complex moduli determination was designed. At the first step, the elastic-viscoplastic response of the material to harmonic deformation was calculated by direct application of standard MATLAB solver ODE45 to constitutive equations for different amplitudes of loading strain. At the second step, the stabilized cyclic stress–strain and inelastic-strain–strain diagrams were obtained for the whole set of calculated data. At the final step, the complex moduli were calculated by the averaging over the period of vibration of the results of direct integration and making use of cyclic diagrams and formulae (11) and (12).

The system of nonlinear ordinary differential equations that describes the polymer response to harmonic loading in the case of pure shear consists of the one-dimensional equations of Zaïri model comprising equations (2), (3), (5) and evolutionary equations

$$\dot{\varepsilon}^{vp} = D_0 \left(\frac{3\sigma^2}{(Z_1 + Z_2)^2} \right)^n \frac{\sigma}{|\sigma|}, \tag{15}$$

$$\dot{\varepsilon}^{ve} = D_0 \exp\left(-\frac{1}{2} \left(\frac{Z_3^{\,2}}{3\sigma^2} \right) \right)^n \frac{\sigma}{|\sigma|}. \tag{16}$$

The law of strain deviator variation $e = e_0 \sin \omega t$, as well as Hooke law for shear stress

$$\sigma = 2G\left(e - \varepsilon^{vp} - \varepsilon^{ve}\right) = 2G\left(e - \varepsilon^{in}\right), \tag{14}$$

should be added to the system.

The values of material constants for PC, which were used for calculations, has been taken from [5]. The list of the values is given below
$E = 2000$ MPa, $D_0 = 10^4$ 1/sec, $n = 10.3$, $q = 2.5$, $Z_{10} = 176.5$ MPa, $Z_{2c} = 20$ MPa, $Z_{2s} = -60$ MPa, $Z_{30} = 50$ MPa, $Z_{3s} = 100$ MPa, $\alpha = 0.9$, $a = 0.0035$, $h = 1.25$, $m = 6.5$, $r = 2.0$.

5. Results of calculation

In this section, we present the results of transient response simulation and the complex moduli calculations performed in the frame of modified technique described in Sec. 3. In Fig. 1, the stress–strain curve was obtained for PC polymer under monotonic loading in pure shear. In this figure, the numerical predictions of the model are generated for strain rate $1.0 \cdot 10^{-2}$ sec^{-1} at room temperature. As can be seen, this figure demonstrates a very good with the results presented in [5].

Evolution of stress and inelastic strain for PC polymer under harmonic loading in pure shear with strain amplitude $e_0 = 7.0 \cdot 10^{-2}$ are shown in Fig. 2 and Fig. 3 respectively for frequency 1 Hz. The material demonstrates cyclically stable response over the whole interval of loading amplitudes and frequencies investigated. As a result, stabilization of the response amplitude occurs after several initial cycles. Relatively slow stabilization is observed only in the vicinity of yield point.

Fig. 4 illustrates the mechanical hysteresis phenomenon under cyclic loading that enable one to measure the phase shift between stress and total strain. The energy dissipation capacity for PC polymeric material under harmonic loading in the maximum dissipation condition ($e_0 = 7.0 \cdot 10^{-2}$) at the frequency 1 Hz is quite high. Calculated value of the normalized loss modulus is about 0.34.

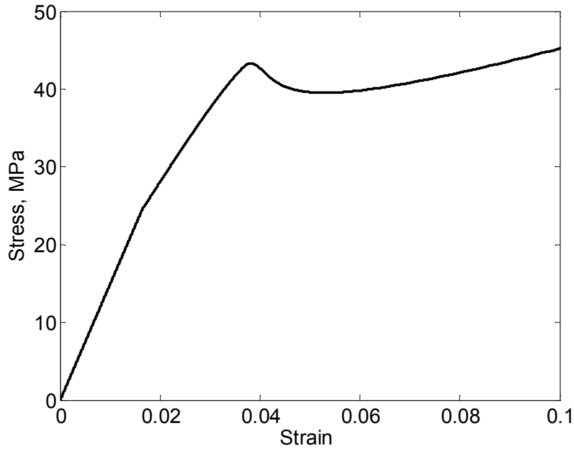

Fig. 1. The stress–strain curve under pure shear monotonic loading.

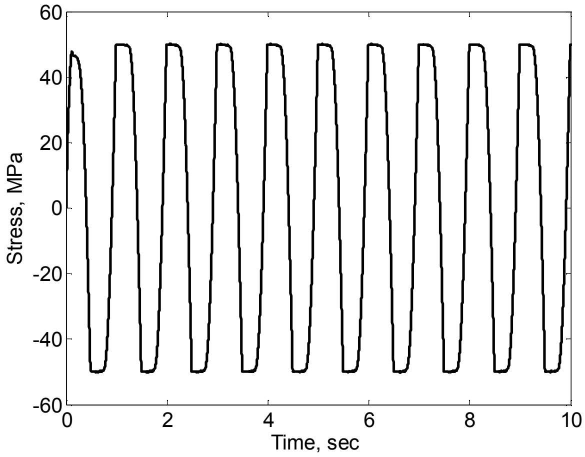

Fig. 2. Stress evolution under harmonic loading.

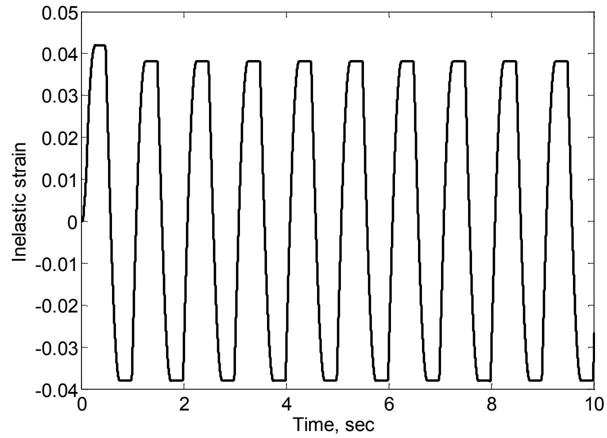

Fig. 3. Inelastic strain evolution under harmonic loading.

As it was mentioned in Sec. 3, this actual loop can be approximated with making use of either standard or modified equivalent linearization scheme. In the same figure, the actual loop (line 1) is shown along with the loops calculated in the frame of standard (line 2) and modified (line 3) equivalent linearization techniques. The cyclic diagram at stabilized stage of the vibration $\sigma'_a = \sigma'_a(e_0)$ (i.e. concretization of general cyclic diagram $\sigma'_{aN} = \sigma'_{aN}(e_0, \omega)$ used in the formulae (12) for $N \to \infty$) is shown in Fig. 5. The curve is calculated for cyclic pure shear.

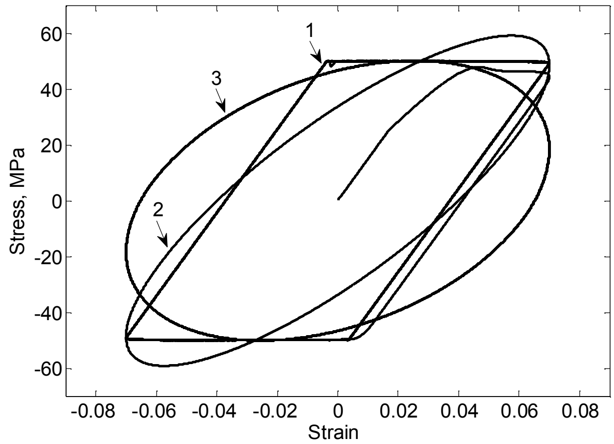

Fig. 4. Hysteresis loops.

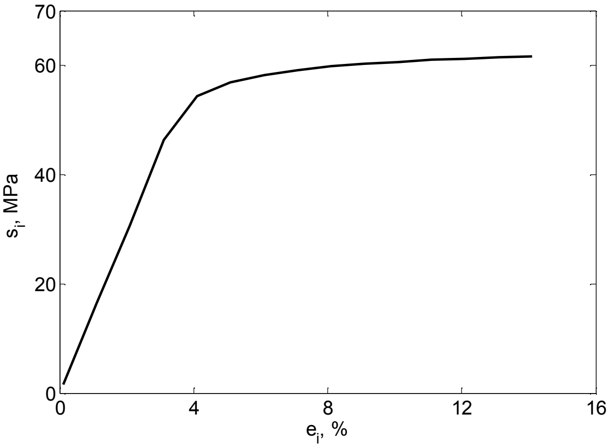

Fig. 5. Cyclic diagram for PC polymer at 1 Hz.

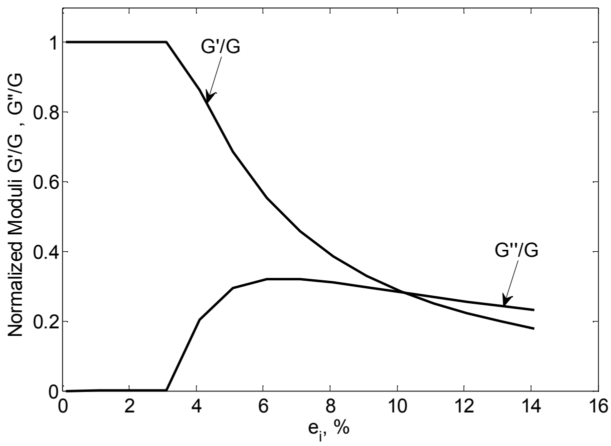

Fig. 6. Normalized values of the real and imaginary parts of complex shear modulus for PC polymer.

Having calculated the cyclic diagram and making use of formulae (12), it is easy to find the real parts of the complex moduli (storage moduli G' and λ') in the frame of modified equivalent linearization scheme. The imaginary parts of the complex moduli (the loss moduli G'' and λ'') are determined according to the formula (11). The normalized improved values of G'/G and G''/G found according to the modified scheme for frequency 1 Hz at steady-state cyclic regime and constant temperature are shown in Fig.6 for wide range of loading amplitudes. This diagram shows the highest losses occur at strain amplitude of about seven percent for this type of polymer.

6. Conclusions

The problem of characterization of material response to harmonic loading is addressed.

The approach that uses the complex-value amplitude relations is preferred rather than direct numerical integration of the complete set of constitutive equation for the material. The key point of the approach adopted lays in determination of complex moduli, i.e. storage and loss moduli under harmonic loading. It is usually done by making use of equivalent linearization technique. In this paper, Zaïri model was used simulate the time dependent response of PC polymer. Obtained histories of main field variables evolution were used to find the stress–strain cyclic diagram and real as well as imaginary parts of complex shear modulus with making use of both standard and modified equivalent linearization techniques. The prediction of stress amplitude obtained in the frame of the former scheme overestimates the actual value for more than 10% while the latter scheme gives it with desirable accuracy.

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