Dynamical Model of Elastic-plastic Hysteresis in Fullerens Film

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Abstract— In this paper the model of the unusual elastic-plastic hysteresis is presented and discussed in connection with the recent progress in investigation of fulleren films. The constructive model is based on the operator technique for hysteretic nonlinearities, namely, in order to describe the input-output conformity we use the Ishlinkii operator together with the probability model based on the Kolmogorov-Chapman equation.

1. INTRODUCTION

The hysteretic effects take place in various areas of material science (both in macro and micro levels). Depending on the purposes of investigation both the phenomenological and constructive models can be used and there are many literature sources on this subject (see, e.g., [1] and related references). As a rule in the constructive models which are described by the relations "input-state" "state-output" [2, 3] the dynamical properties of the hysteresis carrier have no taken into account. It is a well-known fact that the mechanical properties almost all the materials (these properties the elastic-plastic hysteresis) remain unchanched (hysteretic dependence of elastic-plastic materials does not depend on the speed of mechanical affection). However, the results of experiments with the fulleren nanofilms [4] show that the hysteretic curve in the coordinates "force-displacement" depends on the speed of force application.

In this work we propose the dynamical probability model of hysteresis for description of elastic-plastic properties of nanoscale fulleren film taking into account the electromagnetic nature of fulleren clusters binding. This model is based on the fact that the decay law for fulleren supercluster $[C_{60}]_n$ (especially for $n = 2$) depends on the external conditions (temperature, pressure, etc.) as well as has a probability nature. The description of the decay law in the macroscopic level can be made using the theory of random processes (Kolmogorov-Chapman equation).

2. HYSTERESIS IN NANOSCALE FILMS

In recent years the self-regenerating covers are intensively investigated [4–6]. Such covers regenerate when on its surface a little injury takes place. Usually, such covers contain the capsules with the "regenereting agent". When the damage takes place the capsules break and as a result there are chemical reactions that lead to vanishing of injury. In this work we consider the covers that have a self-regenerating properties, but such an effect provides by the hysteretic properties of the cover's material. This cover is coated by two beams of buckyball, namely the molecular (PVD technology) and ion (magnetron technology). In the base of the regeneration effect lies the abnormal elastic-plastic hysteresis which is caused by the depolymerization of fulleren. As was shown in [4] on the surface of nanofilm there are some "liftings" at small mechanical affection by the probe with the diameter less than 200 nm. It is also shown that the relief changing does not connect with the adhesion of the film to the probe.

As is known the elastic-plastic hysteresis manifests in macro level in such a way that the hysteresis loop get over the clockwise. Herewith, as a rule, the form and other characteristics of the loop do not depend on the speed of mechanical affections. However for the material under consideration such a dependence takes place (namely, the form of the hysteretic loop depends on the speed of force affection).

3. MODEL

In this section we present the model of the observable effect. The dependence of the loop's form on time means that the presented model should be non-stationary.

It is well known that the physical properties of nanofilms depend on the structure of the materials. Main processes in such nanocovers occure due to the polymerization and depolymerization.

These processes can be initialized by the temperature, light or mechanical affections. It should also be pointed out that the polymerization together with the depolymerization are caused by the probability laws. The main assumption of this model consists in the fact that the depolymerization process is turning on when the cover is under temporal excess pressure.

The state of the cover can be described by the pair of parameters $(\omega_1(t); \omega_2(t))$ that are the fraction of the domains under polymerization and depolimerization respectively. The dynamics of these parameters can be described by the Kolmogorov-Chapman equation (here dot displays the time derivative):

$$\begin{cases} \dot{\omega}_1 = -\lambda_1\omega_1 + \lambda_2\omega_2, \\ \omega_1 + \omega_2 = 1, \end{cases} \tag{1}$$

with the initial conditions

$$\begin{cases} \omega_1(0) = \omega_{01}, \\ \omega_2(0) = \omega_{02}. \end{cases}$$

With each of these states is connected the linear volume, namely x_1 and x_2 respectively. At the same time the dependence on the external force u we can define as:

$$x_1 = x_1(u), \quad x_2 = x_2(u) \tag{2}$$

using the Ishlinskii operator which will be described below. Finally, the dependence of the displacement on the force can be determined by the relation:

$$l = \omega_1 x_1 + \omega_2 x_2. \tag{3}$$

The Equations (1)–(3) are the base of the proposed model.

At the same time the intensities of the transitions λ_1 and λ_2 are driven by the relations

$$\lambda_1 = \lambda_1(u), \quad \lambda_2 = \lambda_2(u).$$

Identification of these dependencies from the known experimental data is a complicated problem. Namely, there are certain facts which indicate that these functions are monotonically increasing. In this work we choose these functions in the form

$$\lambda_1(u) = \lambda_{01} + c_1 u, \quad \lambda_2(u) = \lambda_{02} + c_2 u \tag{4}$$

with positive parameters.

3.1. Ishlinskii Operator

Let us introduce the necessary definitions.

The stop is an operator $W[t_0, x_0, E, h]$ that connects every continuous input $u(t)$ $(t \geqslant 0)$ with the output $x(t)$ by the following rule (on the monotonic inputs):

$$x(t) = \begin{cases} \min\left\{h, E\left[u(t) - u(t_0)\right] + x(t)\right\}, & \text{if} \quad u(t) \quad \text{increase}, \\ \max\left\{-h, E\left[u(t) - u(t_0)\right] + x(t)\right\}, & \text{if} \quad u(t) \quad \text{decrease}. \end{cases}$$

Here E is the elastic modulus of the material (we understand $u(t)$ and $x(t)$ as a stress and deformation respectively).

On the piece-wise monotonic inputs the output can be determined using the semi-group identity

$$W[t_0, x_0, E, h]u(t) = W\left[t_1, W[t_0, x_0, E, h]u(t_1), E, h\right]u(t),$$

and then, using the special limit construction such an operator can be redefined on all continuous inputs. The detailed description of this operator as well as its properties are considered in the book of Krasnosel'skii and Pokrovskii [7].

Let $U(h) = W[t_0, x_0, 1, h]$ is a single-parameter kind of stops with the elastic modulus equal 1 and the yeld stress $\pm h$. Let us define the nondecreasing continuous function $\Omega = \Omega(h)$ $(h \geqslant 0)$ which satisfies the following condition:

$$\int_0^\infty |\Omega(h)| \mathrm{d}h < \infty. \tag{5}$$

In the following consideration we will use the condition (5) in the form

$$\int_0^\infty h\mathrm{d}\Omega(h) < \infty. \tag{6}$$

Let us denote as Z the set of continuous functions $z(h)$ $(h \geqslant 0)$ that satisfy the inequality $|z(h)| \leqslant h$ $(0 \leqslant h < \infty)$. Then the pairs $\{u_0; z(h)\}$ form the set which determines the state space of the operator. And the dynamics of input-output relations is determined as:

$$x(t) = W\left[t_0, z_0(h), 1, \Omega(h)\right] u(t) = \int_0^\infty U\left[t_0, z_0(h), h\right] u(t)\mathrm{d}\Omega(h), (t \geqslant t_0)\,. \tag{7}$$

Here the integral is understood in the meaning of Riemann-Stieltjes. However it should be noted that this relation is uncomfortable for calculation of the output of Ishlinsky operator.

As follows from definition, the operator $U(h)$ describes the ideal-plastic fiber with the elastic modulus $E = \xi$ and the plastic limits $\pm\xi h$. Let us consider the so-called charge function

$$\chi_+(u, \xi, h) = \begin{cases} -\xi h, & \text{at} \quad u \leqslant -h, \\ \xi u, & \text{at} \quad -h < u < h, \\ \xi h, & \text{at} \quad u \geqslant h. \end{cases}$$

The analog of this function for the Ishlinsky operator is the function

$$\chi_+(u, \Omega) = \int_0^u |\Omega(|h|)|\mathrm{d}h, \quad (-\infty < u < \infty) \tag{8}$$

and the discharge function

$$\chi_-(u, \Omega) = 2\chi_+\left(\frac{u}{2}, \Omega\right), \quad (-\infty < u < \infty).$$

In this way, the Ishlinskii operator is the model of plastic body which is composed of the continual number of ideal-plastic fibers. As follows from definition, at monotonic input and uncharged state the alternating stress can be expressed in the terms of charge function, namely

$$x(t) = \chi_+(u(t) - u(t_0), \Omega).$$

On the piece-wise monotonic inputs the Ishlinskii operator (as previously) can be determined using the semi-group identity. Unfortunately, the relation (8) allows to determine the output using the charge function only at zero initial state. However in the considered case this condition is not restrictive because at initial moment the state of a nanomaterial is natural to assume uncharged.

Finally, the model which describes the dynamics of the system under consideration is based on the Equations (1)-(3) together with the relations:

$$x_1(t) = W\left[t_0, z_{01}(h), 1, \Omega_1(h)\right] u(t), \tag{9}$$

$$x_2(t) = W\left[t_0, z_{02}(h), 1, \Omega_2(h)\right] u(t), \tag{10}$$

where $u(t)$ is an external force applied to the sample, $z_{01}(h)$ and $z_{02}(h)$ correspond to initial uncharged states of polymerized and depolymerized fractions respectively.

In the experiments described in cite the external charge is determined as a pice-wise linear function, namely

$$u(t) = \begin{cases} at, & t \in \left[0, \frac{T}{2}\right], \\ -a(t - T), & t \in \left(\frac{T}{2}, T\right]. \end{cases}$$

4. CONCLUSIONS

The numerical experiments show that the qualitative behavior of the hysteretic curves significantly depends on the choice of the parameters c_1 and c_2 that determine the intensity of transitions from depolymerized state and back. Optimization of the model by these (and other) parameters allows to obtain the results that differ from the experimental results approximately within 3 percent.

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