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Determination of the Synergetic Effect of the Damage Accumulation Process in Polymer Materials using Catastrophe Theory

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Abstract—In this paper, synergistic principles and the mathematical apparatus of the catastrophe theory have been used to simulate the processes of the destruction of polymer materials. In polymer materials, the accumulation of damages at different scale levels is proposed to consider through a synergistic effect, which has been calculated here using the mathematical apparatus of the catastrophe theory. It has been shown that the transition of the system from one stable state to another occurs through the bifurcation point, the value of which is determined using a fold-type catastrophe.

Keywords: polymer materials, dynamical systems, synergetics, self-organization, bifurcation point, catastrophe theory, degradation

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INTRODUCTION

Reduced performance of polymeric materials is the result of many dynamic processes, which description is associated with a number of difficulties; the main difficulty is the ambiguity of the relationship between the state of the system and the quantitative value of parameters. It is obvious that various polymeric materials greatly differ from each other not only in their properties, but also in the mechanics of the destruction process. At first glance, it may seem that there is nothing in common between the destruction of the polymeric materials containing encapsulated (Fig. 1) or fibrous fillers (Fig. 2). However, the destruction of any polymeric materials and, especially, the fatigue failure does not occur abruptly, but is a result of a number of reasons. Despite the variety of polymeric materials, scenarios of their transition from a workable to inoperative state are uniform for all polymeric materials.

It is known that damage accumulates gradually in polymeric materials, but under certain conditions, failures occur abruptly [1–5]. Thus, the system makes an abrupt transition from one state to another during a continuous changing of external conditions. Therefore, it is quite possible to use the principles of synergetics and the mathematical apparatus of the catastrophe theory, which is widely used to analyze a variety of objects ranging from studies of human heart beat to the theory of elementary particles to explain the sudden failure of this system [6, 7].

In the technical literature, the term *disaster* implies an abrupt change in a parameter that occurs as a sudden response in the system to smooth changes in external conditions [1, 8].

Some authors determine synergetics as the theory of dissipative structures, the theory of reversible dynamic chaos, the theory of the formation of new qualities [1, 9, 10], etc. The term *synergetics* (cooperation) can be interpreted in different ways, but most commonly this term refers to the phenomenon of self-organizing of systems that acquire new properties during the operation processes, and none of the components of this system possesses the properties; i.e., the values of indicators of the properties of the resulting system is more than just the sum of all parameter items.

THEORETICAL ANALYSIS

The accumulation of damages is a dynamic system in which the future is uniquely determined by the past; this relationship is called *heredity* [1]. Small causes may have large effects referred to in mathematics as "sensitive to the initial conditions."

In this paper, a theoretical approach is proposed that makes it possible to find universal trends in the behavior of complex dynamic systems. The essence of this approach is to build a synergistic model of the accumulation of damages in the polymer material based on so-called soft modeling that uses plausible hypotheses and value regularities rather than rigorous mathematical models.

The process of the destruction of the polymer material in this approach is considered to be a catas-

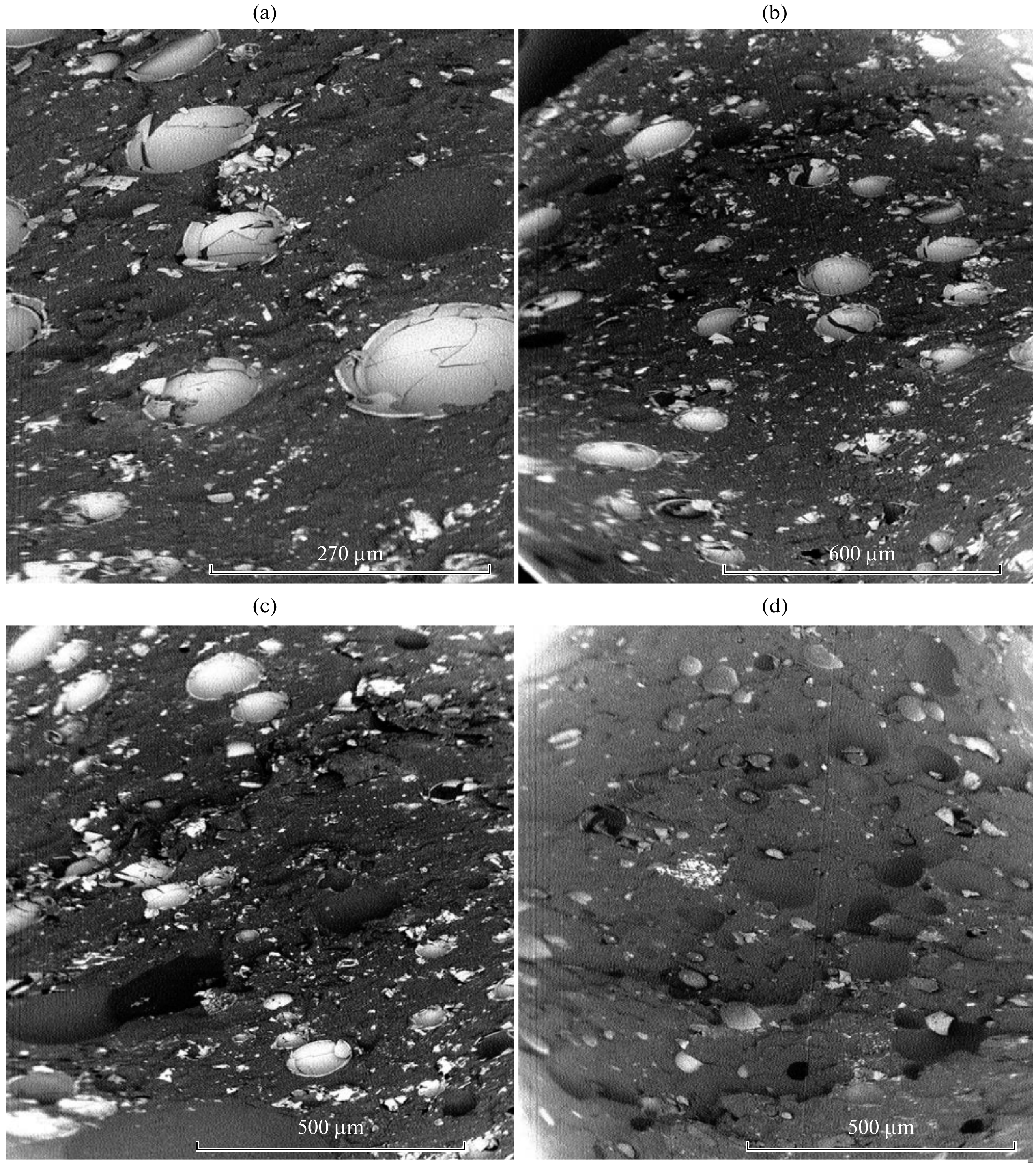
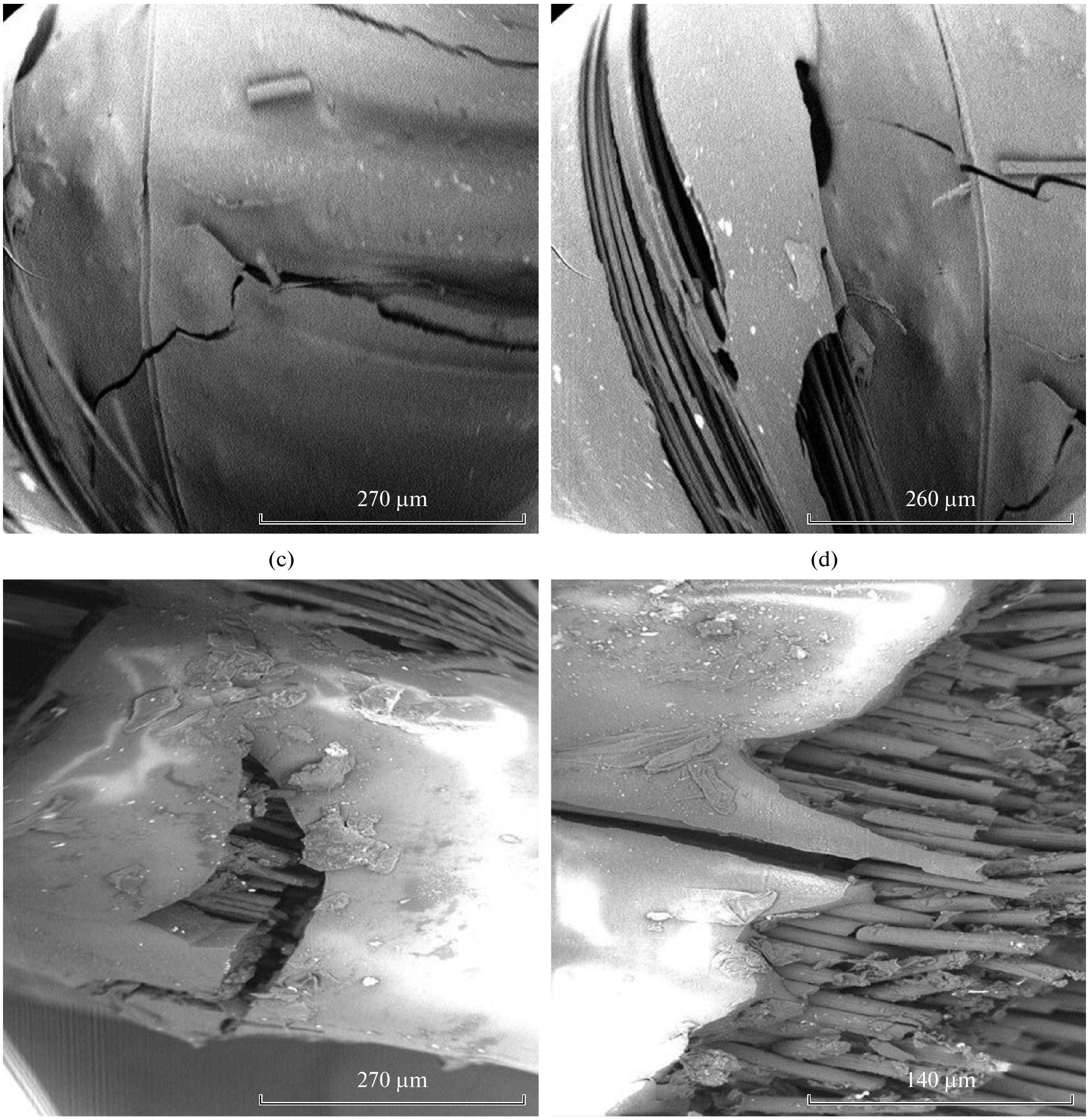


Fig. 1. Sequence of the destruction of the epoxy adhesive material containing encapsulated filler upon application of (a) 50, (b) 60, (c) 70, and (d) 80% from degradation.

trophe, and the processes that precede the destruction are divided into a large number of scale levels. At each of the levels, original smooth changes in the coefficient take place that characterize the losses of strength in the polymer, followed by a sharp increase. An abrupt change in a parameter causes the system to transition from one scale level to another.

In the literature, four scale levels are usually distinguished, i.e., nano, submicro, micro, and macro levels, which are characterized by significant features

(a) (b)



(c) (d)

Fig. 2. Sequence of fracture of the epoxy adhesive material containing a fibrous filler (carbon fiber) at different magnifications (a–d).

related to their heterophase structure [2–5] as applied to the polymeric and composite materials. In fact, this division is rather conditional and, in real systems, the number of scale levels is greater. Each scale level is characterized by its dimension, which in turn determines the number of parameters to be determined in order to describe and predict the behavior of the system [4]. In the present work, we do not attempt to classify strictly scale levels. Our task was to find a causal relationship in order to simplify the real situation and, at the same time, to see the picture of damage accumulation in general.

In this paper, we take the time of the beginning of main crack formation, which leads to an irreversible change in the properties of the polymer material, for the catastrophe (Figs. 1a, 2a). The description of changes in the state of the system is performed using the mathematical apparatus of the catastrophe theory.

Table 1. Classification of forms of catastrophes

Nos.	Type of the form	Formula
1	Fold	$V = x^3 + u_1x$
2	Cusp	$V = x^4 + u_2x^2 + u_1x$
3	Swallowtail	$V = x^5 + u_3x^3 + u_2x^2 + u_1x$
4	Butterfly	$V = x^6 + u_4x^4 + u_3x^3 + u_2x^2 + u_1x$
5	Wigwam	$V = x^7 + u_5x^5 + u_4x^4 + u_3x^3 + u_2x^2 + u_1x$

In the classification of V.I. Arnold and I. Prigozhin [8, 9], the loss of the efficiency is proposed to describe using five equations that have received the appropriate names (Table 1). All functions listed in Table 1 belong to the class of cusp catastrophes. A distinctive feature of the catastrophe theory is the versatility of the proposed models and their geometric graphic representation.

In [6, 7], the procedure for finding the values of the bifurcation point using the mathematical apparatus of the catastrophe theory is described using the adhesive material as an example and residual stresses as the output parameter. In this paper, we propose a more general solution, since various physical parameters that define the behavior of the material under the influence of external factors can be used as the output parameters.

The sequence for determining the accumulation of damage in polymeric materials is shown in Fig. 3. The feature of the proposed algorithm for determining the coefficient of strength loss of a polymer material is that the material structure is divided into *n* levels differing by the scale. The traditional division into three structural levels, namely, the macrostructure, microstructure, and nanostructure, is not obvious, since this approach does not include supramolecular and atomic levels. The processes that take place at the atomic level are described by methods of quantum mechanics, including those that take place on the supramolecular level, using methods of molecular and physical chemistry, and those that take place on the levels of macro-, micro-, and nanostructures using solid mechanics. The transition from one scale level to another occurs abruptly, while inside of each level there is a gradual increase in function *V*.

The object under discussion, the role of which can be played by not only a polymeric material but also any composite material, is presented as a complex hierarchical system with multiple scales. Despite that this approach further increases the uncertainty and complexity of the situation, it accurately quantifies the point of time at which there is an abrupt change in the determining parameter.

In order to mathematically describe the process of accumulating damage in polymeric materials, we propose to use a small number of variables called channels [8–10] that adequately reflect the kinetics of the processes that occurs in the destruction of polymeric materials.

EXPERIMENTAL

A number of authors describe the processes of damage accumulation in polymeric materials propose various models, which are second-order differential equations [1–4]. In the present study, in order to evaluate coefficient *V*, which characterizes the strength loss of a polymeric material, we propose to use the equation of the fold catastrophe (Table 1) in the form reported in shown below [9]:

$$V = \frac{1}{3}x^3 + ux, \tag{1}$$

where *x* is the coefficient that characterizes the crack size (length, radius at the apex, and others) and *u* is the coefficient that characterizes the rate of growth (positive values) or the braking (negative values) of the crack.

The model used for the numerical description of the behavior of polymeric materials on the example of the catastrophe theory consists of a number of *n* (when using the theory of the fold catastrophe, $n = 2$) interacting elements differing by quantitative characteristics of internal parameters. Consequently, the simplified system under study may be presented in the form of a number of interacting units, and each link is characterized by its own set of parameters. The studied system is characterized by the presence of elements between horizontal and vertical bonds. Vertical communications characterize the dynamics of changes in coefficient *x*. Horizontal bonds characterize properties of the system at one scale level, and their change depends on the values of the numerical coefficient *u*.

Equation (1) provides quantitative estimation of the output parameter *V* using very simple numerical examples. This model is highly parametrically sensitive and describes the behavior of polymeric materials under loading, taking into account processes of the relaxation and destruction. This model also allows one to take into account the violations of the reversibility of the structure of the material accumulated at various loading conditions.

The basis for the proposed synergetic model of the damage accumulation process is the assumptions that processes of the plastic flow of the material are followed by the formation of the new surface. Between the two poles, fragile and elastic behavior of the material, there is an infinite number of intermediate states. The dynamics of the accumulation of damage on the example of the simplest model of the fold catastrophe is considered by coefficients *u* and *x*.

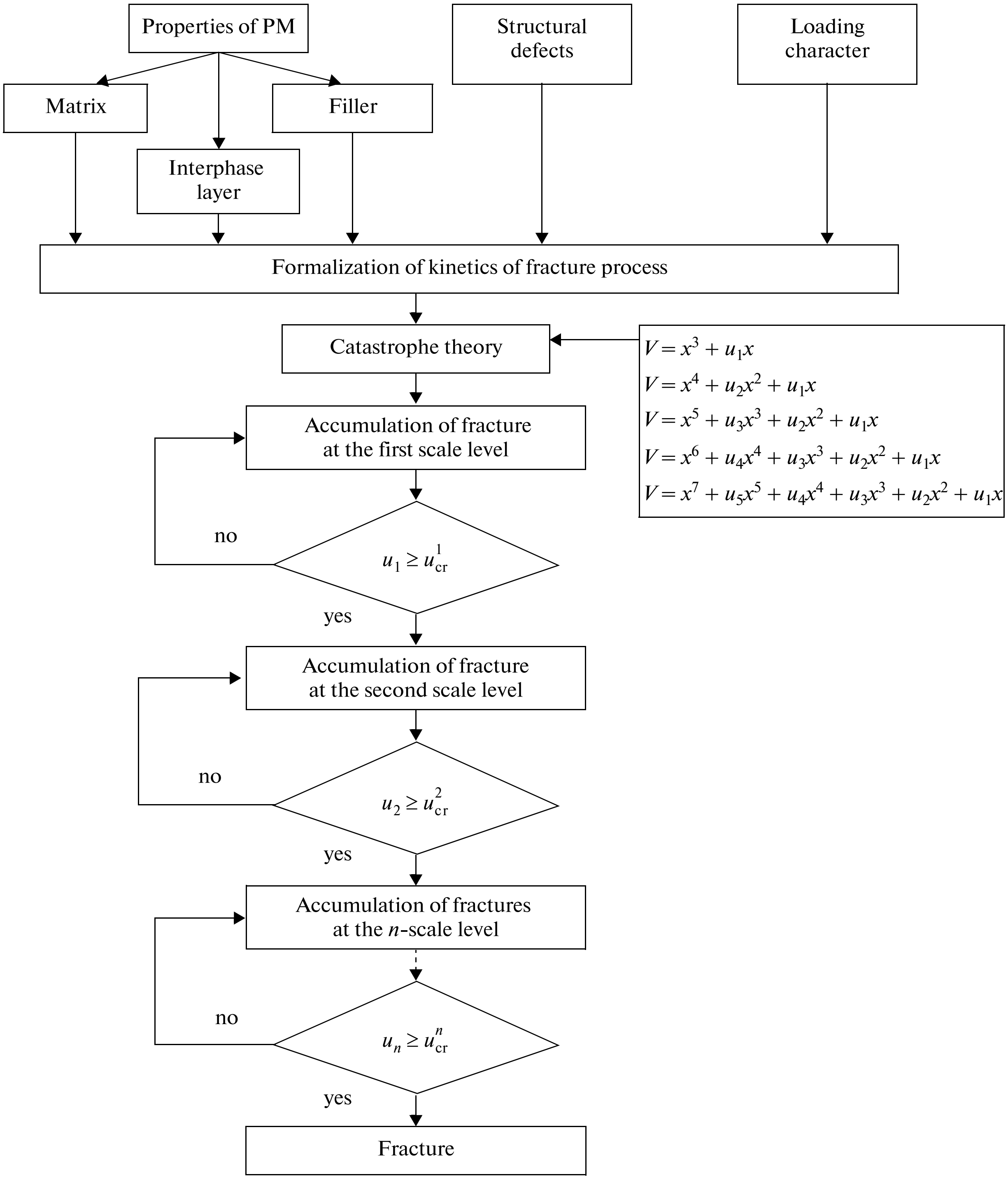


Fig. 3. General scheme of the study: PM is polymeric material.

Thus, it is necessary to decide on the extent of the destruction of the polymer material in order to unite all the characteristics that describe the processes of the accumulation of damage in materials into a single index. This allows one to construct the most reliable predictions about the durability of polymer materials.

RESULTS AND DISCUSSION

The numerical determination of coefficients x that describe the size of the crack (length, radius at the apex, and others) and coefficients u that characterize the rate of growth (or inhibition) of the crack (sometimes called channels) is a very complex and, in many

Table 2. Changes in parameter V that characterize the loss of strength in the polymer material

u \ x	1	3	6	9	12	15	18
−100	−99	−291	−528	−657	−624	−375	148
−50	−49.6	−141	−228	−207	−24	375	1044
−10	−9.6	−21	12	153	456	975	1764
0	0.3	9	72	243	576	1125	1944
10	10.3	39	132	333	696	1275	2124
50	50.3	159	372	693	1176	1875	2844
100	100.3	309	672	1143	1776	2525	3744

cases, unsolvable task. In this paper, it has been shown how the properties within the system change when changing coefficient u from −100 to +100 and stepwise changes in the values of coefficient x occur from 1 to 18 using the fold catastrophe as an example.

For the convenience of analyzing the obtained results, the negative values of the desired coefficient V, which characterizes the strength of losses of the polymer material, are shaded in gray. This allows one to demonstrate the nonlinearity of the process of changing the coefficient that characterizes the loss of strength of the polymeric material (Table 2).

Based on this simple numerical example, it was shown how the system moves abruptly from one point of the phase space to another one. Depending on the numerical values of coefficients u and x, all of the changes that occur within the system are divided into *fast* and *slow*. For example, for values $x = 1–6$, there are slow variations in coefficient V, whereas in the range of $x = 15–18$ (when $u = -100$), there is a very abrupt and significant change in the coefficient V that takes place with a change in sign (Table 2).

However, during the transition from one state to another, it is necessary to overcome the threshold effect. If the change that arises in the system is less than a certain critical value, the system returns to its original position. In the synergetics, this action is called *power switching* [1]. For the example considered in Table 2, this abrupt transition occurs at several points. For example, for values $u = -100$, these two points are at $x = 15$ and $x = 18$. At the first point (at $x = 15$ and $u = -100$), there is a first local minimum. At the second point (at $x = 18$ and $u = -100$), there is a second local minimum, and this critical point is the bifurcation point for this example. Similar points of local minima occur at values $u = -10$, and they are $x = 3$ and $x = 6$.

CONCLUSIONS

In this paper, based on the example of the fold type of catastrophe, it has been shown that the process of changing the properties of polymeric materials can be represented as a consequent transition from one stable state to another. The transition from one stable state to another proceeds through the point of bifurcation. Once the bifurcation point is passed, the new cycle of the existence of the system emerges on the next scale level. Thus, the use of the apparatus of the catastrophe theory provides the prediction of destruction processes in polymeric materials during the operation of constructions fabricated or reconstituted with their use.

NOTATION

u coefficient that characterizes the rate of growth (positive values) or braking (negative values) of the crack in the polymeric material

u_1, u_2, u_3, u_4, u_5, u_n coefficients that characterize the rate of growth (positive values) or braking (negative values) of the crack in the polymeric material on 1, 2, 3, 4, 5, and n scale level, respectively

u_{cr}^1, u_{cr}^2, u_{cr}^n critical values of the coefficient that characterize the rate of growth or braking of the crack in the polymeric material on 1, 2, and n scale level, respectively

V coefficient that characterizes the loss of strength of the polymeric material

x coefficient that characterizes the crack size (length, radius at the apex, and others) in the polymeric material

REFERENCES

1. Malinetskii, G.G., *Matematicheskie osnovy sinergetiki: Khaos, struktury, vychislitel'nyi eksperiment* (Mathematical Foundations of Synergetics: Chaos, Structures,

and Computational Experiments), Moscow: LIBROKOM, 2009, 6th ed.

2. Bazhenov, S.L., Berlin, A.A., Kul'kov, A.A., and Oshmyan, V.G., *Polimernye kompozitsionnye materialy* (Polymer Composite Materials), Dolgoprudny, Moscow oblast: Intellekt, 2010.
3. Aleksandrov, I.A., Muranov, A.N., and Malysheva, G.V., Effect of the strain properties of binders on the failure of carbon-fiber-reinforced polymers, *Vse Mater. Entsikl. Sprav.*, 2012, no. 7, pp. 40–45.
4. Baurova, N.I., Failure of composites under longitudinal loading in relation to their structural features at the microlevel, *Entsikl. Inzh. Khim.*, 2012, no. 11, pp. 35–41.
5. Malysheva, G.V., Predicting the endurance of adhesive joints, *Polymer Sci., Ser. D*, 2014, vol. 7, no. 2, pp. 145–147.
6. Baurova, N.I., Use of catastrophe theory for calculating the sudden failure of joints involving polymers, *Theor. Found. Chem. Eng.*, 2009, vol. 43, no. 3, pp. 345–348.
7. Zorin, V.A. and Baurova, N.I., Serviceability analysis of metalwork elements using catastrophe theory, *Vestn. Mosk. Avtom.-Dorozhn. Gos. Tekh. Univ.*, 2009, no. 1, pp. 7–10.
8. Arnol'd, V.I., *Teoriya katastrof* (Catastrophe Theory), Moscow: URSS, 1997, 5th ed.
9. Prigogine, I., *From Being to Becoming: Time and Complexity in the Physical Sciences*, New York: Freeman, 1981.
10. Ostreikovskii, V.A., *Analiz ustoichivosti i upravlyaemosti dinamicheskikh sistem metodami teorii katastrof* (Stability and Controllability Analysis of Dynamic Systems by Catastrophe Theory Methods), Moscow: Vysshaya Shkola, 2005.

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