Catastrophic models of materials destruction

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Abstract. The effect of concentration and type of fillers on mechanical properties of composite material based on polyimide were studied. Polyethylene terephthalate (PET, polyester), polycarbonate (PCAR) and montmorillonite (MM) were used as the fillers. The samples were prepared by mechanically blending the polyimide-based lacquer solutions with different concentrations of the second component. The concentration of filler and its class, especially their internal structure and technology of synthesis determine features of physical and mechanical properties of obtained materials. Models of catastrophic failure of material satisfactorily describe the main features depending on tension $\sigma$ from deformation $\varepsilon$.

1. Introduction

Currently, modern industrial production is characterized by different image types of used raw materials, methods of processing and an extremely wide assortment it as-received production [1, 2]. Modern technology puts new challenges to material science. When creating new materials one of the main objectives is to improve the complex of technological and operational properties. Obtaining composite materials (CM) is solution of problem. One of the main ways to create CM is injection of fillers [3]. The optimal choice of polymers for mixing provides obtain material with properties that do not possess any of the used components. Moreover, the main goal is directed on material strength, change in a wide range of physical-mechanical, chemical, and optical properties, and etc. Reaction of polymer (matrix) with the filler particles at the interface characterizes compositional modification of material properties. In this regard, significant attention is paid to thermoplastic matrix. Type of filler and its concentration significantly affects to properties of polymer composites [4, 5]. As it is known, physical and mechanical properties of material are significantly determined by contained amount of defects in it and probability of occurrence of various rearrangements with their participation. Deformation of solid body while subjected various loads (mechanical, thermal, electrical, radiation, etc.), leads to an electron-stimulated processes, causing internal (local and extended) tension. It is divided to an elastic, wherein shape and dimensions of the body substantially reduced and plastic in which the material does not return to its original state. In general, fairly complicated processes are occurred during long-term operation and high mechanical and thermal loads in solids. Elongations, commensurate with length of sample are observed in the polymers, and even exceed it.

There has not yet created general theory describing laws and mechanisms of processes in polymers under influence of ionizing radiation so far. Study of changes in physical and mechanical properties of
polymer composites under influence of high-energy particles, causing significant changes in the structure, has scientific and practical interest [6]. The effect of different fillers on physical and mechanical properties of a series of composite films was studied and models of destruction were suggested in this paper.

2. The experimental procedure
Polyethylene terephthalate (PET, polyester), polycarbonate (PCAR) and montmorillonite (MM) were used as the fillers. The samples were prepared by mechanically blending the polyimide-based lacquer solutions with different concentrations of the second component. Composites were previously irradiated, and then subjected to mechanical testing. The samples were irradiated on electronic linear accelerator ELU-6 in the air at 25 °C with energy of 4 MeV. The average current density of beam on the sample was 0.5 mA/cm². Pulse width corresponds to 5 ms with a frequency of 200 Hz. The irradiation dose was calculated according to standard procedure [7]. The absorbed dose was 250 kGy.

Studies of strength characteristics of these materials is carried out by mechanical tensile testing on tensile testing machine type RMU-0.05-1 with the speed of clips 36.09 ± 0.05 mm/min. Moving capture associated with the measurer does not exceed 0.1 mm. Uniaxial tension was measured in a constant load and temperature (20 ± 2) °C, relative humidity (45 ± 5)%. Computerized installation had appropriate software in standard Windows - applications [8]. The dependence of the elongation ε on the tension σ (up to the limit of material strength) are measured.

Workspace samples in the form of films were 50 mm (length) 5 mm (width). The thicknesses of the materials were equal: from polyimide – 35 microns, from composite materials – (70 ÷ 140) mm.

3. Results
Table 1 show the relative elongation and tension unirradiated polymer compositions based on PI. It can be seen that the introduction of the filler PET 5 wt.% leads to improved mechanical properties of the material.

| Table 1. Dependence of the elongation from tension for the non-irradiated composites |
|---------------------------------|-----------------|----------------|----------------|----------------|----------------|
|                                 | PI              | PIₐᵣ + 1 wt. % MM | PIₐᵣ + 2 wt. % PCAR | PIₐᵣ + 5 wt. % PET |
| ε (%)                           | σ (MPa)         | ε (%)           | σ (MPa)        | ε (%)           | σ (MPa)        |
| 36                              | 51.7            | 45.8            | 36.7           | 59.5            | 34.2           | 229.2          | 72              |

The table 1 shows that the CM with MM filler has characteristic σ drop by 29% as compared with polyimide and increase plasticity by 27%.

Introduction concentration of 2 wt.% polycarbonate reduces the strength by 34% and to increase the plasticity by 65% compared with the pure polyimide (table 1).

The strength increases by 37% in samples with concentration of 0.5 wt. % PET; further increasing concentration (up to 5 wt.%) does not cause any significant changes in the strength, but causes a monotonic increase in elongation 6.7 times in comparison with the pure polyimide.

Changing strength and plastic properties of composite material based on montmorillonite due to the fact that the filler comprises interlayer water. In preparation technology of CM mixing polyimide with montmorillonite is carried out at 170 °C, promoting release of -HOH- radical from filler to the matrix, which does not completely react with the polyimide macromolecules. As a result, water accumulates in the matrix and causes destruction [9]. Changes associated with the introduction of polycarbonate determined by the characteristics of mesh matrix of polyimide on the one hand and with high rigidity chain polycarbonates on the other.

Improved mechanical properties of composite materials with a filler of PET due to the fact that there is structuring circuits polyimide with plastic carcass of terephthalate. Further, dependency of elongation from the tension for irradiated materials was studied (Table 2).
Table 2. Dependence of the elongation from tension for the non-irradiated composites

|                | PI          | PI<sub>AB</sub> (D = 250 kGy) | PI<sub>AB</sub> + 1 wt.% MM (D = 250 kGy) | PI<sub>AB</sub> + 5 wt.% PЭТФ (D = 250 kGy) |
|----------------|-------------|-------------------------------|------------------------------------------|-------------------------------------------|
| ε (%)          | σ (MPa)     | ε (%)                         | σ (MPa)                                  | ε (%)                                     |
| 36             | 51.7        | 28.4                          | 39.6                                     | 37.3                                      |
| 36             | 51.7        | 28.4                          | 39.6                                     | 37.3                                      |
| 36             | 51.7        | 28.4                          | 39.6                                     | 37.3                                      |
| 36             | 51.7        | 28.4                          | 39.6                                     | 37.3                                      |

The electron irradiation dose of 250 kGy causes increase in plasticity for 1 wt. % MM by 3.6% and strength decreases by 27% from initial non-irradiated polyimide (Table 2). For compositions with 5 wt.% PET electron irradiation leads to increase in the plasticity of 3.8 times and increase in strength by 36%. The data show that samples of PCM following radiation exposure nature of interaction of structure of the matrix with the filler and between reaction products varies. The electron irradiation of the composite material with the filler of montmorillonite causes ionization of interlayer water contained in the structure of MM and its interaction with radicals of polyimide, which leads to hydrolytic degradation. Also, the irradiation results in the release of water from the matrix of polyimide. Ionized water reacts with dedicated -HOH- radicals of polyimide, forming accumulations of water in the matrix. This process also leads to degradation of polyimide and, as a consequence - in degradation in mechanical properties of CM. Increasing content of PET final structure of film becomes more porous with a pore size of 40 nm. Effects of electron irradiation lead to the predominance of cross linking process, which leads to structuring of polyimide chains to carcass of polyethylene terephthalate. This improves mechanical properties of composite material.

To describe physical and mechanical properties we proposed catastrophic models of materials destruction [10].

In terms of the physical meaning of the most correct it is to establish not depending on σ from ε, and ε from σ, as a function of deformation and the arguments - tension. The dependence of σ from ε has no physical meaning.

In this model, change in elongation is represented as:

\[ dl = l \ln \left( \frac{\sigma}{\sigma_0} \right)^{-1} \]

where \( l \) – length of sample, \( \sigma \) – tension, \( \sigma_0 \) – generalized module of strength.

Integrating the function \( l \) from \( l_0 \) to \( l \) and argument \( \sigma \) from 0 to \( \sigma \), and considering deformation \( \varepsilon = \frac{\Delta l}{l_0} \), we get:

\[ \varepsilon = e^{\frac{\sigma}{\sigma_0}} - 1 \]  \hspace{1cm} (1)

Or

\[ \sigma = \sigma_0 \ln(\varepsilon + 1) \]  \hspace{1cm} (2)

and \( \sigma_0 \) – is the tension at which the \( \varepsilon + 1 \) increases \( e \)-times.

Expanding the expression (1) in a row, we get

\[ \varepsilon = \frac{\sigma}{\sigma_0} + \frac{\sigma^2}{2\sigma_0^2} + \frac{\sigma^3}{3!\sigma_0^3} + ... \]  \hspace{1cm} (3)

When \( \sigma \ll \sigma_0 \) this ratio becomes classic Hooke’s law.

Hooke’s law describes a linear (elastic) of the curve of \( \sigma \) from \( \varepsilon \), but often does not cover whole course according to \( \sigma = \sigma(\varepsilon) \).

Similarly, we obtained the dependence of \( \varepsilon \) from \( \sigma \) for exponentially square, parabolic and other models:
\[ \varepsilon = e^{\frac{\sigma}{E_t}} - 1, \]

\( \varepsilon \) - strain, \( \sigma \) - stress, \( E_t \) - tensile modulus

(a) - PI\textsubscript{AB}; (b) - PI\textsubscript{AB} + 2 wt.% PCAR; (c) - PI\textsubscript{AB} + 1 wt.% MM; (d) - PI\textsubscript{AB} + 5 wt.% PET; (e) - PI\textsubscript{AB} + 1 wt.% MM irradiated (\( D = 250 \text{ kGy} \)); (f) - PI\textsubscript{AB} + 5 wt.% PET irradiated (\( D = 250 \text{ kGy} \))
1 – Hooke’s law, 2 – experiment, 3 – exponential model; 4 – parabolic model

**Figure 1.** Dependence of elongation from tension for composite materials.

\[ \varepsilon = \sigma^2 \cdot (E_2^2)^{-1} \]  \hspace{1cm} (6)

Figure 1 shows the experimental and calculated dependences of \( \varepsilon \) from \( \sigma \) for different models and composites.

Calculations based on \( \varepsilon \) from \( \sigma \) unirradiated composite materials (Figure 1) produced by the formulas (1), (3), taking into account only the first term (Hooke's law), and (6) for different concentrations of the second component.

Calculations show that, depending on \( \varepsilon \) from \( \sigma \) for non-irradiated and irradiated composite materials produced by different formulas for different concentrations of the second component, it is better to describe the experimental data exponential model.

4. Conclusions

Based on obtained results the following conclusions:

Study of effect of fillers allows creating a material with desired properties. The concentration of filler and its class, especially their internal structure and technology of synthesis determine features of physical and mechanical properties of obtained materials.

Various models are proposed under uniaxial loading materials. The best agreement with experiment gives the exponential model.

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