Synthesis and research of polymer composites reinforced with carbon nanotubes using computer models

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Abstract. Nanocomposites are a new type of material that differs from conventional composite materials in the size of the hardening phase. One of the most promising fillers for nanocomposites is carbon nanotubes. The paper studied structural and functional properties of polymer composite materials based on epoxy resins reinforced with carbon nanotubes. Impact resistance at high speed effects of multilayer composites, which are multilayer structures made of glass fabric and basalt fabric impregnated with polymer on the basis of epoxy resins, has been studied.

1. Introduction
One of the urgent tasks in material science is the creation of materials resistant to high-speed particles. At present, the most promising structural materials are polymer-fabric composites that combine the properties of different components and effectively withstand shock loads. Nanocomposites are a new type of material that differs from conventional composite materials in the size of the hardening phase. Nanocomposites are capable of realizing a high level of both special properties of materials (electrical conductivity, magnetic permeability, thermal conductivity) and mechanical properties (strength, impact toughness, hardness). One of the most promising fillers for nanocomposites is carbon nanotubes. The paper studies the change in properties of composite materials when CNT is introduced into a polymer matrix.

This work is a natural continuation of previous work, where the low speed impact on multi-layer composites reinforced with nanocarbons was studied, and the properties of such structures when exposed to speeds of about several meters per second were investigated [1]. Here, the range of speeds is extended to hundreds of meters per second.

2. Objective and object of study
The object of investigation in this work are polymer composite materials synthesized in laboratory conditions. In the course of the work two types of samples were produced for testing:
1) Entirely polymeric samples with different content of carbon nanotubes in the polymer matrix;
2) Layered structures of glass fabric and basalt fabric impregnated with epoxy resin-based polymer reinforced with nanocarbons.

Objective: Study of structural and functional properties of polymer composite materials based on epoxy resins with the addition of carbon nanotubes. Investigation of impact resistance of multilayer composites.

The set goal requires solving the following tasks:
Development of methods for synthesis of samples;
• Selection of the main evaluation parameter of the quality of the obtained samples (in this work the impact toughness is selected as a quantitative parameter);
• Study of the effect of MNT introduction into the polymer matrix on impact toughness of samples;
• Carrying out a series of experiments to study the impact toughness of multilayer composites reinforced with nanocarbons.

3. Synthesis of composites
Two methods for the synthesis of samples for research have been developed:
1) Entirely polymeric samples with different content of carbon nanotubes in the polymer matrix (Type 1);
2) Layered structures of glass fabric and basalt fabric impregnated with polymer based on epoxy resins (Type 2).

For production of the first kind of images we used a polymer binder from L epoxy resin and hardener 285. Pre-treated carbon nanotubes of "Taunit" brand were used in the polymer matrix. As already mentioned in the Introduction, carbon nanotubes perform reinforcing functions in the polymer matrix of the composite. The main difficulty in synthesizing samples with disperse CNTs is to ensure an even distribution of nanotubes in the matrix. Analysis of literature sources has shown that the optimal parameters for polymer processing, for uniform distribution of nanotubes in the matrix, is to process the solution with ultrasound at 30°C for 10 minutes [2, 3, 4].

The polymer binder with the implanted CNT is formed in thin disks of a given diameter and thickness. The manufactured samples are polymerized within 24 hours at room temperature. The synthesis process allows controlled variation of the CNT content in the polymer matrix. Figure 1 shows the manufactured samples with the percentage of CNT by mass: 0%, 1%, 3%, 5%.

![Figure 1. Samples type 1 with a percentage of CNT by mass: 0%, 1%, 3%, 5% (left to right).](image)

For the production of the second type of samples (layered structures of glass fabric and basalt fabric reinforced with nanocarbons) a method was developed that includes several steps illustrated in Figure 2:
• Preparation of fiberglass sheets;
• Preparation of the substrate for synthesis of composites;
• Preparation of polymer matrix from L epoxy resin and hardener 285;
• Preparation of CNT to mix with the polymer matrix;
- Application of polymer binder to fiberglass sheets.

![Figure 2](image1.png)

**Figure 2.** Photos of the steps of the process of synthesis of composites with CNT Taunit: 1. Basalt tissue preparation. 2. Synthesis substrate. 3. Preparation of polymer. 4. CNT "Taunit". 5. Preparation of CNT. 6. Mixing of polymer and CNT. 7. Ready polymer. 8. Applying the polymer to the fabric. 9. Ready sample before polymer curing.

4. Impact Toughness Measurement Machine
A specially designed unit is used to determine the impact toughness of the synthesized samples.

![Figure 3](image2.png)

**Figure 3.** Block diagram of the experimental installation

Figure 3 shows the block diagram of the installation. The accelerator device accelerates the projectile to speeds of 90-110 m/sec. The projectile is a copper ball with a radius of r=(2.00±0.05) mm and weight m=(0.355±0.005) g. The projectile velocity is measured before and after interaction with the sample using chronographs. Chronograph is a device designed to measure the projectile velocity. It uses optical chronographs to record any of body that has passed through the sensitive area of the instrument.

The initial velocity of the bullet determines the energy reserve $K_0$ (initial kinetic energy $K_0=(mv_0)^2/2$).

After the impact and the energy consumption for deformation and destruction of the sample, the energy of the projectile $K_1=(mv_1)^2/2$ decreases. The chronographs record the change of projectile velocity, and
thus the values of $K_0$ and $K_1$ can be calculated. The projectile work on deformation and destruction of the sample is defined as $A = K_0 - K_1$.

The value of impact toughness $a$ [J/mm$^2$] is calculated as the ratio of fracture operation per projectile cross-section area.

$$a = \frac{A}{\pi \cdot r^2}, \left[ \frac{J}{\text{mm}^2} \right],$$

where $r$ is the projectile radius, mm.

Thus, the final formula for calculating impact toughness:

$$a = \frac{m \cdot (v_0 - v_1)^2}{2 \pi \cdot r^2}, \left[ \frac{J}{\text{mm}^2} \right],$$

where $a$ - impact toughness, J/mm$^2$; $m$ - mass of the projectile, d; $v_0,1$ - projectile velocity before and after the destruction of the sample, m/s; $r$ - projectile radius, mm.

5. Impact toughness tests of type 1 specimens

Samples of polymer composite material reinforced with nanotubes with concentrations of 0%, 1%, 3%, 5%, 7% and 10% CNT by mass were produced for testing. The tests were carried out on a specialized unit. During the tests, the experiments were video recorded at a rate of 120 frames per second. The qualitative results of the experiment are shown in Figure 4.

![Figure 4](image-url)

**Figure 4.** Pilot samples of the first type (from left to right from top to bottom: 0%, 1%, 3%, 5%, 7%, 10%) after the impact of an accelerated projectile.

Quantitative analysis of the results of the experiments is presented in the table 1. Recall that work $A$, spent by the projectile on the destruction of the sample is defined as

$$A = \frac{m}{2} \cdot (v_0 - v_1)^2,$$
where \( m \) is the mass of the projectile, \( d \); \( v_{0,1} \) - projectile velocity before and after the destruction of the sample, m/s

**Table 1.** Dependence of projectile energy loss on the concentration of CNT in the polymer matrix.

| \( V_0, \text{m/s} \) | \( V_1, \text{m/s} \) | \( M, \text{d} \) | \( a, \text{J} \) | \( A \) \( \text{(average), J} \) |
|----------------|----------------|-------------|---------|----------------|
| **0\%**          |                  |             |         |                |
| 1                | 111.4            | 94.5        | 0.355   | 0.050          | 0.051          |
| 2                | 111.7            | 95.6        | 0.355   | 0.046          |                |
| 3                | 110.9            | 93.3        | 0.355   | 0.054          |                |
| **1\%**          |                  |             |         |                |
| 1                | 110.1            | 88.8        | 0.355   | 0.080          | 0.055          |
| 2                | 106.2            | 94.3        | 0.355   | 0.025          |                |
| 3                | 104.5            | 86.2        | 0.355   | 0.059          |                |
| **3\%**          |                  |             |         |                |
| 1                | 102.2            | 80.7        | 0.355   | 0.082          | 0.077          |
| 2                | 93.2             | 74.1        | 0.355   | 0.064          |                |
| 3                | 104.1            | 82.5        | 0.355   | 0.082          |                |
| **5\%**          |                  |             |         |                |
| 1                | 101.4            | 70.2        | 0.355   | 0.172          | 0.181          |
| 2                | 103.2            | 69.7        | 0.355   | 0.199          |                |
| 3                | 102.1            | 71          | 0.355   | 0.171          |                |
| **7\%**          |                  |             |         |                |
| 1                | 125.4            | 72.8        | 0.355   | 0.491          | 0.510          |
| 2                | 127.3            | 72.3        | 0.355   | 0.536          |                |
| 3                | 126.4            | 73.3        | 0.355   | 0.500          |                |
| **10\%**         |                  |             |         |                |
| 1                | 125.3            | 99.1        | 0.355   | 0.121          | 0.095          |
| 2                | 119.2            | 97.4        | 0.355   | 0.084          |                |
| 3                | 121.3            | 100.1       | 0.355   | 0.079          |                |

Based on the results of the experiments, a schedule on Figure 5 was drawn.

![Figure 5. Dependence of projectile energy loss on the UNT concentration in the polymer matrix.](image-url)
Qualitative and quantitative analysis of the results of the experiment shows that increasing the concentration of nanotubes in the polymer matrix leads to improved crack resistance of the composite material. In addition, samples with 7% concentration of carbon nanotubes show peak values of projectile energy absorption under high-speed exposure. Thus, the best configuration for Type 1 samples is the 7% CNT content in the polymer matrix.

6. **Type 2 impact toughness tests of specimens**

Several variants of layered polymer composites based on L resin and hardener 285 were produced as samples of the second type:
- Fabric 1. Fiberglass fabric, density: 220 g/m², weave: linen, fiber: 1.6 mm;
- Fabric 2. Glass fabric, density: 105 g/m², weave: satin, fibers: 1 mm;
- Fabric 3. Basalt fabric, density: 200 g/m², weave: linen, fibers: 1 mm.

Quantitative analysis of the results of the experiments is presented in the Table 2.

### Table 2. Impact toughness dependence for samples from all types of fabric, for L resin polymer and hardener 285.

| V₀, m/s | V₁, m/s | m, d | breakdown | Ah, J. | a, J/mm² |
|--------|---------|------|-----------|--------|----------|
| 1 fabric 1 layer |
| 1 | 108.7 | 90 | 0.355 | 0.062 | 0.079 |
| 2 | 99.9 | 86.8 | 0.355 | 0.030 | 0.039 |
| 1 fabric 2 layers |
| 1 | 97.4 | 71.6 | 0.355 | 0.118 | 0.151 |
| 2 | 106.9 | 69.9 | 0.355 | 0.243 | 0.310 |
| 1 fabric 3 layers |
| 1 | 91.1 | no data | 0.355 | punctured | no data | no data |
| 2 | 93.7 | no data | 0.355 | punctured | no data | no data |
| 2 fabric 1 layer |
| 1 | 114.3 | 103.3 | 0.355 | 0.021 | 0.027 |
| 2 | 111.3 | 98.9 | 0.355 | 0.027 | 0.035 |
| 2 fabric 2 layers |
| 1 | 107.8 | 92.1 | 0.355 | 0.044 | 0.056 |
| 2 | 101 | no data | 0.355 | punctured | no data | no data |
| 2 fabric 3 layers |
| 1 | 100.5 | 81.5 | 0.355 | 0.064 | 0.082 |
| 2 | 94.8 | 76.4 | 0.355 | 0.060 | 0.077 |
| 3 fabric 1 layer |
| 1 | 127.1 | 85.6 | 0.355 | 0.306 | 0.389 |
| 2 | 124.4 | 81.6 | 0.355 | 0.325 | 0.414 |
| 3 fabric 2 layers |
| 1 | 119.1 | 70.3 | 0.355 | 0.423 | 0.538 |
| 2 | 105.8 | no data | 0.355 | no data | no data |
| 3 fabric 3 layers |
| 1 | 111.7 | no data | 0.355 | punctured | no data | no data |
| 2 | 105.1 | no data | 0.355 | punctured | no data | no data |

A "no data" mark on the table indicates that either the sample was not punctured by the projectile or the chronograph was unable to capture the projectile after exposure to the sample.
Experimental results show the highest impact toughness value for fabric-based samples 3. At breakdown in the samples there were observed a rupture of fibers, significant stratification and pulling of threads. The weak connection between the matrix and the fibers allowed pulling out the threads that were in direct contact with the projectile. Images of the fiber break are shown in Figure 6.

The composite based on fabric 2 had a "loose" structure despite the minimal degree of fiber curvature (satin weave). A small projectile tore only a few central fibers, while the rest of the fibers were pulled apart without compromising their integrity. In addition, the slightly curved structure resulted in low resistance to pulling the fibers. It should also be noted that the weave structures in tissues 1 and 3 were identical, and it was expected that for samples from tissue 2 the impact toughness would be higher. During the tests, the situation was reversed. This suggests that only on the basis of real impact tests can the final conclusion about the effectiveness of a particular material be made [6,7,8].

7. Conclusion
The structural and functional properties of polymer composite materials based on epoxy resins reinforced with carbon nanotubes have been studied.

For samples of the first type based on L epoxy and 285 hardener the increase of impact resistance (increase of impact toughness, localization of deformation area, improvement of resistance to crack formation) at the value of 7% by weight of CNT content in polymer matrix was found.

Impact resistance at high speed effects of multilayer composites, which are multilayer structures of glass and basalt fabric impregnated with polymer on the basis of epoxy resins, has been studied. The best configuration of the composite is a combination of basalt fabric and polymer based on L epoxy resin with hardener 285.

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