This comparative in silico study highlights the utility of computational screening tools like G4–QuadScreen for generating new hypotheses about drug mechanisms and identifying potential polypharmacology that may contribute to both therapeutic and adverse effects [7, 2, 1].

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УДК 547:691.175.5/8

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PHYSICO-CHEMICAL AND MECHANICAL CHARACTERISTICS OF FULLERENE-CONTAINING POLYMERIC MATERIALS

Introduction

Existing publications confirm that the use of ultrafine materials as fillers, among which carbon clusters – fullerenes – are increasingly playing a prominent role, can be considered as a basis for producing new high-tech materials and drugs for engineering and medicine [1, 2]. The introduction of fullerenes into the polymer matrix provides composites with new properties, such as antiviral and anticancer activity. Fullerenes also possess high magnetic and sorption properties.

Goal

To study the physico-chemical interaction of ultra-high molecular weight polyethylene (UHMWPE) and fullerene filler and evaluate the deformation and strength characteristics of the composites.

Material and methods of research

Polymer composite materials based on Hostalen GUR 4120 UHMWPE and a fullerene filler (UDDD-SF ultrafine detonation diamonds) were selected as the study objects.

Experimental composite material samples were manufactured using process equipment from a powder mixture of UHMWPE and a molecular filler at various component percentages (from 0.01 to 10% by weight of UDDD-SF). Samples were formed by thermal pressing on a hydraulic press with electrically heated plates at a temperature of 170 °C and maintained at a pressure of 10–12 MPa until the samples cooled completely to room temperature, followed by mandatory degreasing with ethyl alcohol.

The size and shape of the samples (films, sectors, etc.) were determined depending on the subsequent composite material testing method.

The results pf the research and their discussion

According to the literature [3], the formation of a fullerene-polymer composite involves the diffusion of fullerene molecules and the dissolution of fullerene clusters in polymer matrices. More intense fullerene dissolution in the polymer binder is observed when using UHMWPE as the polymer matrix. This fact indicates good thermodynamic compatibility of the components we selected. The physico-chemical interaction of UHMWPE and the fullerene filler is accompanied by the formation of chemical bonds between the binder macromolecules and the surface of the filler particles. The interfacial surface layer differs in a few characteristics from the binder. During the formation of adhesive joints, contact oxidation of UHMWPE macromolecules and fullerene particles occurs. The formation of interfacial layers causes electrical polarization of the composite via the Maxwell-Wagner mechanism, which affects the physico-chemical characteristics of the polymer composites.

The physical and mechanical properties of the experimental specimens were assessed using a ZP 40 tensile testing machine (Germany). The tensile testing machine and the experimental specimen shapes are shown in Figure 1.

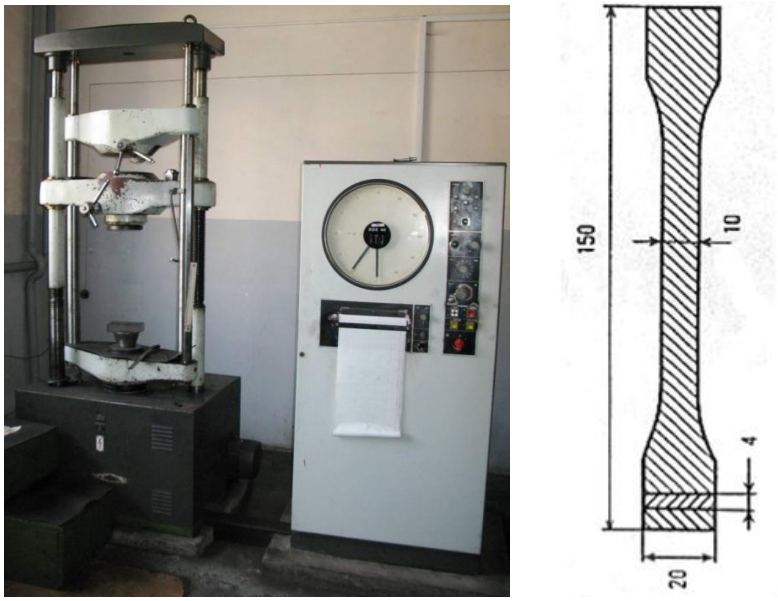


Figure 1 – Tensile testing machine ZP 40 and the shape of experimental samples

Blade-shaped specimens, in accordance with GOST 112262, were used, with an initial cross-section of 10 mm. The tensile testing machine's loading clamp travelled at 50 mm/min. The average value of five repeated measurements was taken as the result. The results of the physical and mechanical properties assessment for the experimental specimens are presented in Table 1.

Table 1 – Deformation and strength parameters of samples

Concentration of UDDD-SF in the sample, %	0	0,01	0,03	0,05	0,1	0,5	1,0	5,0	10,0
Tensile strength at break, MPa	22,2	78,0	54,0	67,2	44,7	74,0	54,3	53,9	49,0

The best result was obtained when testing samples containing 0.01% of the filler by weight: the tensile strength σ_p=78 MPa, which significantly exceeds the strength of unfilled UHMWPE and samples containing high concentrations of UDDD-SF (1–10% by weight).

Conclusions

Depending on their nature and degree of dispersion, carbon filler particles actively interact with the composite matrix, dramatically altering its physical and chemical properties. The deformation and strength characteristics of the composites were studied.

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УДК 616.36-003.826-07+616.36-002.2

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THE CLINICAL POWER OF DE RITIS RATIO IN ALCOHOLIC LIVER DISEASE AND NON-ALCOHOLIC FATTY LIVER DISEASE

Introduction

The aspartate aminotransferase to alanine aminotransferase ratio, commonly known as the De Ritis ratio (DRR), acts as an important indicator in the clinical differentiation of Alcoholic Liver disease (ALD) and Non-Alcoholic Fatty Liver disease (NAFLD). This ratio is an also a non-invasive biomarker of damage to liver functions, and can be utilized to assess the causes and mechanisms of both these conditions. The term non-alcoholic fatty liver disease (NAFLD) refers to the entire spectrum of liver diseases that result from the presence of steatosis in more than 5% of the hepatocytes in the absence of alcohol use. NAFLD has a broad spectrum of severity and progression, ranging from mild steatosis to the more inflammatory condition known as non-alcoholic steatohepatitis, which may progress to the development of cirrhosis and finally hepatocellular carcinoma. ALD refers to liver injuries due to excessive usage of alcohol, that stimulates a redox imbalance and acetaldehyde toxicity. Despite these distinguishable etiologies, both conditions converge on hepatic steatosis as a common pathological starting point [1–3].

Goal

To showcase the significance of De Ritis ratio as a diagnostic marker in patients of non-alcoholic fatty liver disease and alcoholic liver disease, and to evaluate its prognostic value in assessing disease severity and progression.