REGULAR ARTICLE



Static and Dynamical Elastic Modules of Nanocomposites Polypropylene, Teflon and Multiwalled Carbon Nanotubes

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The mechanical properties of nanocomposites based on polypropylene and Teflon with multi-walled carbon nanotubes (MWCNTs) were investigated. In this study, the absolute value of the elastic modulus (E), elasticity limit (σ_E), anelasticity limit ($\sigma_{0.2}$), and ultimate stress limit (σ_S) of nanocomposites based on polypropylene (PP) with 5 %, 0.5 %, and 0.1 % MWCNTs were determined. The influence of ultrasonic deformation (EUS) on the mechanical properties of nanocomposites based on polypropylene, teflon, and MWCNTs was also examined. A key factor in the modification of composite polymeric materials is the degree of adhesion at the interface, which is determined by the interaction of macromolecules with multi-walled carbon nanotubes. Since aromatic groups in various families of free monomers act as effective radical traps, they enable interaction with MWCNTs. This interaction, due to covalent bonding, leads to the fixation of polymer chains on nanotubes and the migration of radicals to the traps. The correlation between the crystalline and amorphous components of polymer macromolecules interacting with rigid MWCNTs influences the elastic and inelastic characteristics of the nanocomposites. Multi-walled carbon nanotubes have a highly disordered structure, whereas strictly ordered crystals are idealized objects. One of the methods to deliberately modify the properties of MWCNTs for nanoelectronics applications is the introduction of foreign element impurities. An increase in the crystalline degree of nanocomposites with rising MWCNT concentration, along with nanotube filling of the polymer matrix, results in a reduction of the well-organized phase content. The results of this work are important for understanding and predicting the properties of composite materials based on polymer matrices with carbon fillers.

Keywords: Elastic modulus, Elasticity limit, Anelasticity limit, Nanocomposite, Ultrasonic deformation.

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1. INTRODUCTION

The mechanical characteristics of nanocomposites based on polypropylene and Teflon with multi-walled carbon nanotubes (MWCNTs), in which the number of atoms on the surface is comparable to the total number of atoms, and whose dimensions in at least one direction range from several to hundreds of nanometers, fundamentally differ from those of macroscopically homogeneous systems.

Quantum-size effects, which are absent in macroscopically homogeneous systems, play a significant role in such nanocomposites. Examples of such nanostructures include MWCNTs, materials with quantum wires, quantum wells, and quantum dots. Depending on chirality (i.e., the orientation of the roll axis relative to the graphene layer), MWCNTs can have a band gap $\varepsilon_g = 0 \div 1.2$ eV, changing their properties from metallic to semiconducting [1-3]. Impurities significantly impact the vibrational spectrum of the crystal lattice, the energy spectrum of electrons, and the mechanical properties of MWCNTs.

The characteristics of polymer nanocomposites, whose dimensions in at least one direction are

comparable to the De Broglie wavelength for electrons (i.e., from several to hundreds of nanometers, $\lambda_{DB} = 10 \div 100$ nm, fundamentally differ from those of macroscopically homogeneous systems. In such polymer nanocomposites, quantum-size effects, which are absent in macroscopically homogeneous systems, play an important role [4].

The total deformation of the nanocomposite based on polypropylene and multi-walled carbon nanotubes consists of elastic and anelastic components: $\varepsilon_{\Sigma} = \varepsilon_{E} + \varepsilon_{AE}$ [5]. Elastic deformation ε_{E} occurs "instantly." A key factor in polymeric matrix formation is the creation of molecular structures, with MWCNTs serving as nucleation centers for the crystalline phase.

The influence of ultrasonic (US) deformation ϵ on the elastic and anelastic characteristics of a nanocomposite based on polypropylene, Teflon, and MWCNTs was studied. Even relatively small strains can accumulate in non-ideal crystals, altering their anelastic and elastic characteristics [6-8]. One of the ways to purposefully modify the properties of MWCNTs for applications in nanoelectronics is the introduction of impurity atoms of other elements.

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1. EXPERIMENTAL METHODS

For measuring the stress-strain diagram (σ - ε) and the static elastic modulus (E), the IMASH-20-75 device was used [9]. To measure the dynamic elastic modulus (E), the impulse-phase method was applied at frequencies $f \approx 1.67$ and 5 MHz under deformation $\varepsilon \approx 10^{-7}$. The measurement error of the relative change in the dynamic elastic modulus was $\Delta E/E \approx 0.5\%$ [10]. To determine the elastic modulus (E) and internal friction (IF) (Q^{-1}), the complete piezoelectric oscillator method was used at a frequency of $f \approx 118$ kHz under deformation $\varepsilon \approx 10^{-6}$ in vacuum conditions ($P \approx 10^{-3}$ Pa).

Atomic force microscopy (AFM) and optical observation of the microstructure using the "LOMO MVT" microscope were performed. A shallowly dispersed smooth surface was observed, where small islands coalesce and their shape becomes rounded. The sites exhibited a highly fragmented structure consisting of slightly misoriented islands with a size of $H = 400 \pm 80$ nm.

The US impulse-phase method using the computerized "KERN-4" system at frequencies $f_{\perp} \approx 0.7$ MHz and $f_{\parallel} \approx 1$ MHz was employed [11-14]. The measured velocity error was $\Delta V/V \approx 1.5$ %.

To analyze the experimental data obtained, we also conducted computer modeling of the mechanical behavior of individual components of the studied composites. In particular, the mechanical response of a multi-walled carbon nanotube was investigated using molecular dynamics simulations. The model structure consisted of three coaxial nanotubes of different diameters, created with the Atomsk software package. The interactions between carbon atoms in the nanotube were described by the Tersoff potential [15]. All calculations were performed using the LAMMPS molecular dynamics package.

The generated structure was first subjected to an energy minimization procedure using the conjugate gradient method. Next, the system was equilibrated in the NPT ensemble for 500 ps. Finally, the nanotubes were uniaxially stretched at a constant rate, during which the relative strain and internal mechanical stresses in the structure were calculated. The obtained dependencies were used to determine the elastic modulus of the nanotubes by linear approximation of the elastic deformation region. The obtained values of the elastic modulus in different computer experiments ranged from 700 to 900 GPa.

2. RESULTS AND DISCUSSION

The total deformation of a nanocomposite based on a polymer and MWCNTs consists of elastic and anelastic components: $\varepsilon_{\Sigma} = \varepsilon_{E} + \varepsilon_{AE}$. Anelastic deformation (ε_{AE}) is caused by the motion of dislocations, while the elastic deformation (ε_{E}) occurs instantaneously.

During the recording of the stress-strain $(\sigma - \varepsilon)$ curves, two loading-unloading cycles were performed. The absolute values of static elastic modulus (E), yield stress (σ_E) , anelastic limit $(\sigma_{0.2})$, and ultimate tensile strength (σ_S) were determined based on the mean slope angle (tga) of the linear sections of the unloaded and reloaded curves. The stress-strain diagram $(\sigma - \varepsilon)$ of the

nanocomposite based on polypropylene with 5 % MWCNTs is shown in Fig. 1.

Under mechanical loading, the total deformation of a real crystal consists of both elastic and anelastic components: $\varepsilon_{\Sigma} = \varepsilon_E + \varepsilon_{AE}$. Anelastic deformation (ε_{AE}) is caused by the motion of dislocations, while the elastic deformation (ε_E) occurs instantaneously. Anelastic deformation also exhibits a temperature dependence $\varepsilon_{AE}(T)$, which is associated with the presence of relaxation times (τ) characterizing the motion of crystalline structure defects.

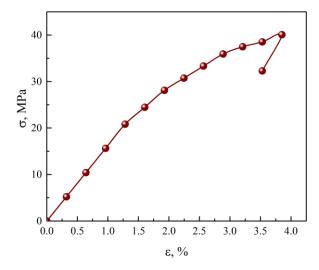


Fig. 1 – Stress-strain (σ - ε) diagram of the nanocomposite based on polypropylene and 5 % MWCNTs

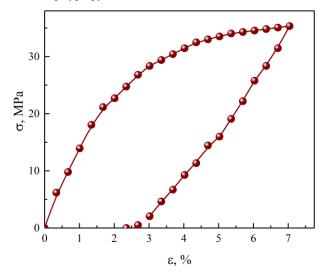


Fig. 2 – Stress-strain (σ – ε) diagram of the nanocomposite based on polypropylene and 0.5 % MWCNTs

For the nanocomposite based on polypropylene with 5 % MWCNTs, static elastic modulus was determined to be approximately $E \approx 1.623$ GPa, elasticity limit $\sigma_E \approx 20.83$ MPa, anelastic limit $\sigma_{0.2} \approx 30.72$ MPa, and ultimate tensile strength $\sigma_S \approx 40.09$ MPa.

There are two characteristic values of the elastic modulus: the anrelaxation elastic modulus (E_{R}) and the relaxation elastic modulus (E_{R}). Under an externally applied periodic stress $\sigma(\omega)$ with frequency ω , the experimental elastic modulus takes an intermediate

value within the range $E_R < E < E_{AR}$. The stress-strain diagram (σ - ε) of the nanocomposite based on polypropylene with 0.5 % MWCNTs is shown in Fig. 2.

The relative change $\Delta E/E$ is given by: $\Delta E/E = (E-E_R)/E_R = \Delta/(1+\omega^2\tau^2)$, where the maximal defect of the modulus $\Delta = (E_{AR}-E_R)/E_{AR}$, E_{AR} — anrelaxation, E_R — relaxation elastic modulus. E_{AR} was measured in time of appendix of tension σ , when a anelastic contribution is to deformation $\varepsilon_{AE} = 0$; E_R measured after a time $\Delta t >> \tau$, when anelastic deformation maximal $\varepsilon_{AE} = \max$. For polypropylene + 0.5 % MCNTs static elastic modulus $E \approx 1.262$ GPa, elasticity limit $\sigma_{E} \approx 21.15$ MPa, anelasticity limit $\sigma_{0.2} \approx 28.37$ MPa were. The diagram of strain — deformation $(\sigma - \varepsilon)$ of nanocomposite based on polypropylene and 0.1 % MCNTs is represented in Fig. 3.

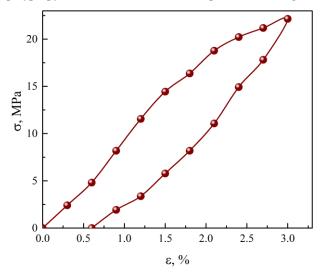


Fig. 3 – Stress-strain (σ - ε) diagram of the nanocomposite based on polypropylene and 0.1 % MWCNTs

For the nanocomposite based on 0.1 % MWCNTs and polypropylene, elastic modulus was determined as $E \approx 0.8942$ GPa, elasticity limit as $\sigma_E \approx 18.78$ MPa, and anelasticity limit as $\sigma_{0.2} \approx 21.19$ MPa. The value of Δ is determined by the number of microrelaxations of different types and their individual contributions to anelastic deformation ε_{AE} at temperature T. The contributions of different microrelaxations summed. At temperatures where the defect of the elastic modulus $\Delta E/E$ increases sharply, relaxation maxima IF $Q_{\mathrm{M}^{-1}}$ appear in the temperature dependences. The considerable width of the $\Delta E/E$ relaxation peak over temperature indicates a broad distribution of activation parameters H for the corresponding relaxation processes. The stress-strain $(\sigma - \varepsilon)$ diagram of polypropylene is shown in Fig. 4.

The absolute values of the longitudinal velocity V_{\parallel} and shear velocity $V_{\perp} = 617 \pm 10$ m/sec for the nanocomposite based on Teflon-4 and MWCNTs were determined. After irradiation, the decrease in velocity of longitudinal ultrasonic elastic waves V_{\parallel} , velocity of transverse ultrasonic elastic waves V_{\perp} , elastic modulus E, and shear modulus G of the specimen was observed. Absolute values of longitudinal velocity V_{\parallel} and shear velocity $V_{\perp} = 893 \pm 10$ m/sec for the nanocomposite based on modified Teflon-3M and MWCNTs were also

determined. The correlation between the crystalline and amorphous components of polymer macromolecules, which interact with rigid MWCNTs, influences anelastic and elastic characteristics of nanocomposites. For polypropylene + 0.5 % MWCNTs, static elastic modulus $E \approx 1.262$ GPa, elasticity limit $\sigma_E \approx 21.15$ MPa, and anelasticity limit $\sigma_{0.2} \approx 28.37 \,\mathrm{MPa}$. For polypropylene + 0.1 % MWCNTs, static elastic modulus $E \approx 0.8942$ GPa, elasticity limit $\sigma_E \approx 18.78$ MPa, and anelasticity limit $\sigma_{0.2} \approx 21.19$ MPa. Electronic irradiation results in an increased degree of crystallinity and growth of elastic modulus E, shear modulus G, and microhardness $H \approx E/10$ of nanocomposites. This occurs due to the formation of additional bonds that enhance interfacial adhesion at the boundary and the cross-linking of internal layers of MWCNTs.

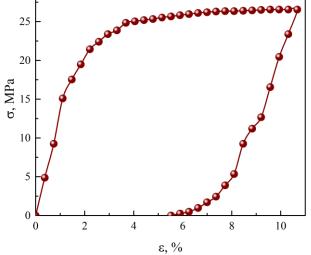


Fig. 4 – Stress-strain (σ – ε) diagram of polypropylene

For polypropylene in Fig. 4 static elastic modulus $E \approx 1.367$ GPa, elasticity limit $\sigma_E \approx 15.10$ MPa, anelasticity limit $\sigma_{0.2} \approx 22.41$ MPa.

The concentration dependence of static elastic modulus E(C) for the nanocomposite based on polypropylene and MWCNTs is shown in Fig. 5.

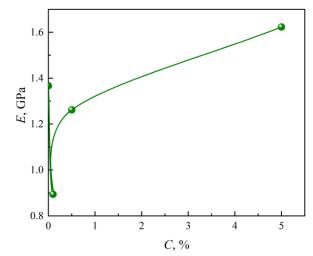
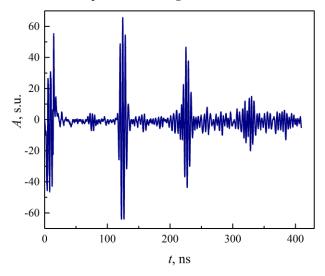


Fig. 5 — Concentration dependence of the static elastic modulus E(C) of the nanocomposite based on polypropylene and MWCNTs

The presence of interaction, even at a negligible quantity of reinforcing nanotubes, contributes to a substantial increase in many functional properties of polymers. During the irradiation of composites, with an increasing irradiation $_{
m dose}$ and nanotube concentration, processes of macromolecule cross-linking occur, improving the specimen structure. At lower doses, this is accompanied by the formation of nanostrains σ_i , which relax as the irradiation time increases. The formation of additional bonds, stimulated by radiation-induced defects, can also result from the cross-linking of internal MWCNTs layers. As the absorbed dose increases, leading to a rise in the number of internal carbon atoms C_i , both mechanisms of additional bond formation contribute to the enhancement of mechanical properties. This is accompanied by an increase in elastic modulus E and microhardness $H \approx E/10$ of nanocomposites as the irradiation dose D increases. The oscillogram of impulses with transversal polarization, which are reflected in nanocomposite based on Teflon-4 and MWCNTs is represented in Fig. 6.



 $\begin{array}{lll} \textbf{Fig. 6} - Oscillogram \ of \ impulses \ with \ transverse \ polarization \\ reflected \ in \ the \ nanocomposite \ based \ on \ Teflon-4 \ and \\ MWCNTs \end{array}$

The threshold radiation dose D is determined by the need to generate a sufficient number of electron carriers (e). The electrical resistance R and total conductivity σ of nanotubes with a quasi-ballistic scattering mechanism [16]:

$$R = \frac{L}{\sigma^c},\tag{1}$$

$$\sigma = \frac{e^2 n \tau(E_F)}{m^*}.$$
 (2)

To determine the temperature position of the relaxation of the elastic modulus $\Delta E/E$, the temperature dependence of E was measured simultaneously with IF measurements. Annealing of structural defects distorts the shape of the IF temperature spectrum. During annealing, impurities and vacancies V are released. The absolute values of the longitudinal velocity V_{\parallel} and shear velocity V_{\perp} = 617 ± 10 m/sec for nanocomposites based on Teflon-4 and MWCNTs were determined. The

Poisson's ratio was calculated using the formula: $\mu = \frac{\frac{1}{2} V_{\parallel}^2 - V_{\perp}^2}{V_{\parallel}^2 - V_{\perp}^2} \quad [17\text{-}18]. \quad \text{The values obtained were} \\ \mu_{0.5\%\text{MWCNT+T}} \approx 0.332 \quad \text{and} \quad \mu_{2\%\text{MWCNT+3}MT} \approx 0.358. \quad \text{After irradiation, the decrease of velocity of longitudinal ultrasonic elastic waves V_{\parallel}, velocity of transverse ultrasonic elastic waves V_{\perp}, elastic modulus E and shear modulus G of the specimen was observed. The concentration dependence of dynamic elastic modulus $E(C)$ for the nanocomposite based on modified Teflon-4 and MWCNTs is shown in Fig. 7.$

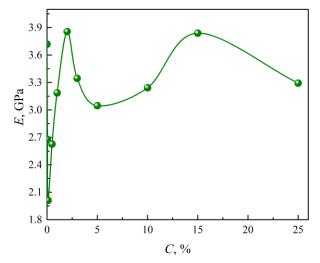
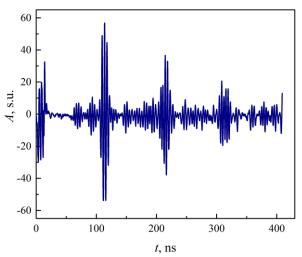


Fig. 7 – Concentration dependence of the dynamic elastic modulus E(C) of the nanocomposite based on Teflon-4 and MWCNTs

The oscilloscope trace of pulses with transverse polarization, reflected in the nanocomposite based on modified Teflon-3M and MWCNTs, is shown in Fig. 8.



 $\begin{tabular}{ll} Fig.~8-Oscillogram~of~impulses~with~transverse~polarization~reflected~in~the~nanocomposite~based~on~modified~Teflon-3M~and~MWCNTs\\ \end{tabular}$

The absolute values of longitudinal velocity V_{\parallel} and transverse velocity $V_{\perp} = 893 \pm 10$ m/sec for nanocomposites based on modified Teflon-3M and MWCNTs were determined. Concentration dependence of the dynamic elastic modulus E(C) of nanocomposite based on modified Teflon-3M and MWCNTs is shown in Fig. 9.

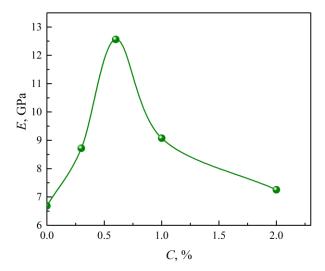


Fig. 9 – Concentration dependence of the dynamic elastic modulus E(C) of the nanocomposite based on modified Teflon-3M and MWCNTs

Under the application of external periodic stress $\sigma(\omega)$ with frequency ω , the experimental elastic modulus takes an intermediate value $E_R < E < E_{AR}$. $\Delta E/E = (E - E_{AR})$ E_R)/ $E_R = \Delta I(1 + \omega^2 \tau^2)$ where the maximal defect of the modulus Δ is given by: $\Delta = (E_{AR} - E_R)/E_{IR}$. Here, E_R is the relaxation elastic modulus, and E_{AR} is the anelastic modulus. E_{AR} was measured at the moment of stress application σ , when the anelastic contribution to deformation $\varepsilon_{AE} = 0$. E_R was measured after a time interval $\Delta t >> \tau$, when the anelastic deformation reaches its maximum $\varepsilon_{AE} = \text{max}$. Electronic irradiation leads to an increase in the degree of crystallinity and the growth of the elastic modulus E, shear modulus G, and microhardness $H \approx E/10$ of nanocomposites. This occurs due to the formation of additional bonds, which enhance the interface at the phase boundary and result in the cross-linking of internal layers of MWCNT. The concentration dependence of the elasticity limit $\sigma_E(C)$ for the nanocomposite based on polypropylene and MWCNTs is shown in Fig. 10.

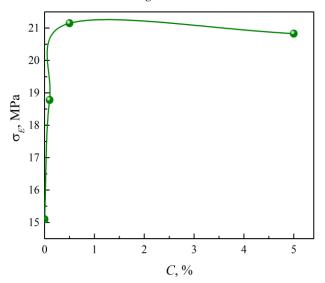


Fig. 10 – Concentration dependence of the elasticity limit $\sigma E(C)$ of the nanocomposite based on polypropylene and MWCNTs

The presence of cooperation, even at a negligible amount of reinforcing nanotubes, contributes to a substantial increase in many functional properties of polymers. Concentration dependence of the anelasticity limit $\sigma_{0.2}C$) of the nanocomposite based on polypropylene and MWCNTs is shown in Fig. 11.

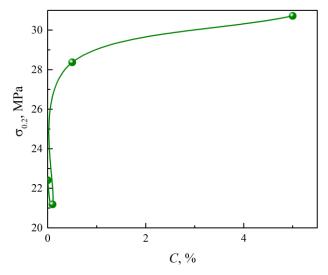


Fig. 11 – Concentration dependence of the anelasticity limit $\sigma_{0,2}(C)$ of the nanocomposite based on polypropylene and MWCNTs

The relationship between stress $\delta = F/S$ and strain $\varepsilon = l/l_0$ for polymers is given by [19]:

$$\delta = \frac{\rho RT}{Mc} \left(\varepsilon - \frac{1}{c^2} \right), \tag{3}$$

where l_0 is the initial polymer length, l is the stretched polymer length, M_c is the average molecular weight of the unit contained between the cross-links, and ρ is the specific polymer density. For elastic modulus:

$$E = \frac{\delta}{\varepsilon} = \frac{3\rho RT}{Mc} = \frac{3\rho RTq}{Mo},\tag{4}$$

where q – cross-links density. The relationship between elastic modulus E, the cross-linking quantum yield F_x , and the radiation dose D is:

$$E = \frac{6\rho RTDFx}{Mo}.$$
 (5)

Equation (5) is valid only for small deformations ε , when the "entanglement" of polymer molecules can be neglected. Relation (5) predicts that elastic modulus E should increase with the increasing radiation dose D at a rate proportional to the cross-linking quantum yield F_x .

During electron e^- irradiation, vacancies V and internodal atoms J_i appear. Point defects introduced by irradiation cannot exist in a free, isolated state but combine into double V-V, J_i - J_i and triple V-V-V complexes.

Radiation treatment allows, through the directed effect on the defective and crystalline structure of MWCNTs, as well as through physical and chemical transformations, to achieve mechanical properties that cannot be obtained by other methods.

For relativistic electrons e^- of low energies, anelastic collisions with atomic electrons are the main source of energy loss W. Collisions occur quite frequently, and the

mean free path λ_e^- relative to an elastic collisions in Si is of the order of the crystal lattice constant $\lambda_e \approx a$; the energy loss W in each collision event is small (scattering is neglected). Therefore, the discrete nature of energy losses can be neglected. In this approximation, to describe the transfer processes, it is sufficient to know the average energy losses per unit path λ_e^- [20].

The Poisson's coefficient μ in Fig. 12 is equal to the ratio of relative transversal compression ε_{\perp} to relative longitudinal elongation ε_{\parallel} and is given by [21, 22]:

$$\mu = \frac{\varepsilon_{\perp}}{\varepsilon_{\parallel}} = \frac{1}{2} \left[1 + \frac{1}{1 - \left(\frac{V_{\parallel}}{V_{\perp}}\right)^2} \right], \tag{6}$$

where V_{\parallel} – quasilongitudinal US velocity, V_{\perp} – quasitransversal US velocity.

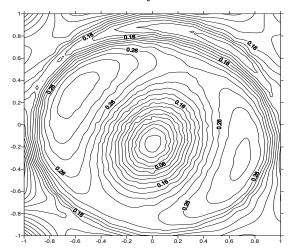


Fig. 12 – Stereoprojection of Poisson's ratio μ isolines of SiO₂

Dynamical elastic modulus $E = \rho V_{\parallel}^2$ of SiO_2 is shown in Fig. 13. Poisson's coefficient μ is the elastic constant, which is equal to the ratio of relative transversal ε_{\perp} compression to relative longitudinal elongation ε_{\parallel} , and is given by [23]:

$$\mu = -\frac{\varepsilon_{\perp}}{\varepsilon_{\parallel}} = -\frac{\frac{\Delta X}{X}}{\frac{\Delta l}{l}} = -\frac{\Delta X}{\Delta l} * \frac{l}{X}, \tag{7}$$

$$\mu = -\frac{\varepsilon_{\perp}}{\varepsilon_{\parallel}} = \frac{\frac{1}{2}V_{\parallel}^{2} - V_{\perp}^{2}}{V_{\parallel}^{2} - V_{\perp}^{2}} = \frac{1}{2} \left[1 + \frac{1}{1 - \left(\frac{V_{\parallel}}{V_{\perp}}\right)^{2}} \right]. \tag{8}$$

One oscillator produces three waves: one longitudinal and two transversals. Debye temperature θ_0 was determined using the formula [24]:

$$\theta_D = \frac{h}{k_B} * \left(\frac{9N_A \rho}{4\pi A}\right)^{\frac{1}{3}} * \left(\frac{1}{V_{\parallel}^3} + \frac{2}{V_{\perp}^3}\right)^{\frac{1}{3}}, \tag{9}$$

where k_B – Boltzmann constant, h – Plank constant, N_A – Avogadro number, A – middle gram-molecular mass.

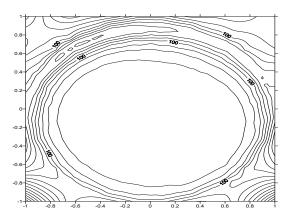


Fig. 13 – Stereoprojection of dynamic elastic modulus E of SiO₂

Radiation treatment, through its directed effect on the defective and crystalline structure of MWCNTs, as well as through physical and chemical transformations, allows for the attainment of mechanical properties that cannot be achieved by other methods.

3. CONCLUSIONS

- 1. The absolute values of elastic modulus E, elasticity limit σ_E , anelasticity limit $\sigma_{0.2}$, and ultimate stress limit σ_S of the composites with 5% carbon nanotubes + polypropylene, 0.5% carbon nanotubes + polypropylene, and 0.1% carbon nanotubes + polypropylene were determined.
- 2. The increase in the crystalline degree of the nanocomposite with the growth in the concentration of multiwalled carbon nanotubes (MWCNTs), filling the matrix with nanotubes, results in the decrease in the content of the well-organized phase.
- 3. The obtained results can be used in the development of practical recommendations regarding the use of nanocomposites based on polypropylene and teflon with MWCNTs as materials for nanoelectronics, for the creation of filters, diodes, transistors, and new devices for recording and processing information.
- 4. The spread of the internal friction ΔQ_{M}^{-1} maximum represents the relaxation process of new types of structural defects.
- 5. As a result of the mechanical study, the presence of a strong effect between polypropylene, Teflon, and MWCNTs was confirmed.
- 6. The obtained results can be used in the development of practical recommendations regarding the use of nanocomposites based on polypropylene and Teflon with MWCNTs as nanoelectronics materials for the creation of filters, diodes, transistors, and new devices for recording and processing information.

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Статичний і динамічний пружні модулі нанокомпозитів поліпропілена, тефлона та багатостінних вуглецевих нанотрубок

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Досліджено механічні характеристики нанокомпозитів на основі поліпропілену, тефлону з багатошаровими вуглецевими нанотрубками (БШВНТ). У роботі визначено абсолютне значення модуля пружності (E), межі пружності (σ_E) , межі непружності $(\sigma_{0.2})$, межі міцності (σ_S) нанокомпозитів на основі поліпропілену (ПП) + 5 % БШВНТ, ПП + 0,5 % БШВНТ, ПП + 0,1 % БШВНТ. Досліджено вплив ультразвукової деформації (єуз) на механічні властивості нанокомпозиту на основі поліпропілену, тефлону та БШВНТ. При модифікуванні композиційних полімерних матеріалів важливий ступінь адгезії на межі поділу, який визначається взаємодією макромолекул з БШВНТ. Оскільки ароматичні групи, що знаходяться в різних родинах вільних мономерів, є ефективними пастками радикалів, це дозволяє здійснювати їх взаємодію з БШВНТ. Така взаємодія за рахунок ковалентних сил зв'язку призводить до фіксації полімерних ланцюгів нанотрубок, а також до міграції радикалів на пастках. Співвідношення кристалічної та аморфної складової макромолекул полімерів, які взаємодіють із твердими БШВНТ, впливають на непружні та пружні характеристики нанокомпозитів. БШВНТ мають дуже невпорядковану структуру, і строго впорядковані кристали є ідеалізованими об'єктами. Одним із способів цілеспрямованої зміни властивостей БШВНТ з метою їх використання в наноелектроніці є введення домішок інших елементів. Збільшення ступеня кристалізації нанокомпозиту при вирощуванні БШВНТ, концентрації БШВНТ, заповнення нанотрубками матриці призводить до зниження вмісту добре організованої фази. Результати роботи мають значення для розуміння і прогнозування властивостей композитних матеріалів на основі полімерних матриць з вуглецевими наповнювачами.

Ключові слова: Пружний модуль, Межа пружності, Межа непружності, Нанокомпозит, Ультразвукова деформація.