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ТЕЗИ ДОПОВІДЕЙ

VII Міжнародної науково-практичної конференції «Інформаційні технології в освіті, науці і техніці» (ІТОНТ-2024)

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Тези доповідей VII Міжнародної науково-практичної конференції «Інформаційні технології в освіті, науці і техніці» (ІТОНТ-2024), (Черкаси, 23-24 травня 2024 р.) [Електронний ресурс]. Черкаси : ЧДТУ, 2024. 349 с.

Матеріали конференції висвітлюють основні напрями розвитку інформаційних технологій і систем та їх використання в освіті, науці, техніці, економіці, управлінні, медицині.

У матеріалах розглядаються питання, пов'язані з комп'ютерним моделюванням фізичних, хімічних і економічних процесів, інформаційною безпекою та застосуванням інформаційно-комунікаційних технологій у техніці, наукових дослідженнях і управлінні складними системами, з використанням інформаційно-комунікаційних технологій в освіті, зі створенням, впровадженням і використанням науково-освітніх ресурсів у закладах вищої освіти, а також з проблемами підготовки ІТ-фахівців у вищій школі.

Для наукових і педагогічних працівників, аспірантів і студентів закладів вищої освіти.

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Матеріали подані в авторській редакції. Автори опублікованих матеріалів несуть повну відповідальність за підбір, точність наведених фактів, цитат, даних, власних імен, посилань, грамотність, літературний стиль та інші відомості. Редколегія залишає за собою право скорочувати та редагувати подані матеріали. Рукописи не повертаються. Організатори конференції та члени редколегії не завжди поділяють думки авторів.

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КОРОТКИЙ ЗМІСТ

BRIEF CONTENTS

MODELING OF THE PHOTOSTRUCTURAL TRANSFORMATIONS IN BIOPOLYMERS

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Abstract. A comprehensive theoretical and experimental study of the photostructural transformations of acrylic epoxidized soybean oil under the action of ultraviolet light has been carried out. The photopolymerization process is controlled by a free radical mechanism that starts under the influence of light quanta and leads to heating of the material due to the formation of new bonds of the polymer network. In an electric field, a dielectric relaxation process is additionally observed, which is caused by orientational defects in the local structural components of the polymer. Their contribution is estimated by analyzing the entropy of the dielectric constant time series, and the energy and structural properties are modeled using modern tools of computer materials science –machine learning interatomic potentials.

Keywords: acrylated epoxidized soybean oil, photopolymerization, dielectric relaxation, Shannon entropy, correlation integral, machine learning potentials, machine learning interatomic potentials.

Presentation of the main material. Polymers, being intricate macromolecules, embody the essence of complex systems, exhibiting hierarchical organization and emergent behaviors. In the realm of polymer science, photopolymerization stands as a quintessential process demonstrating such complexity. During photopolymerization, monomer molecules undergo radical polymerization upon exposure to light, resulting in the formation of polymer chains with distinct properties. Under the influence of an electric field, the structure changes dielectric properties, the characteristic dynamics of which contains extremely interesting and valuable information [1, 2]. Structural (electronic and atomic) changes in the polymer are manifested in the form of so-called dynamic time series (fluctuations in temperature, dielectric constant, etc.), the analysis of which by the theory of complex systems allows us to identify and predict specific states of the system [3, 4, 7].

The goal of this study. In this work, the dynamics of dielectric relaxation of the AESO:VDM photopolymerization process with and without a photoinitiator was first studied under a protocol containing intermittent on/off light with variable periods of both on and off. A feature of this protocol is the ability to simultaneously study the relatively fast photopolymerization process (tens of seconds) and the relatively slow dielectric relaxation processes.

Experimental samples of acrylated epoxidized soybean oil (AESO), sealer (vanillin dimethacrylate), and reaction accelerator – photoinitiator (2,2-dimethoxy-2-phenylacetophenone) [5]. The AESO fragment is shown in Fig. 1, along with the key factors of relaxation properties: acrylate, epoxy, and hydroxy.

The concentration of PI used was 3 mol%, determined based on the total molar amount of all monomers involved. AESO and DMPA were from Sigma-Aldrich, while VDM was obtained from Specific Polymers. The incorporation of VDM into AESO resulted in an elevation of the mixture's viscosity [5]. Photo-polymerization of the AESO/VDM samples was carried out using a Jaxman U1 LED light source emitting in the UV region at 365 nm. The dielectric relaxation properties were investigated by measuring the real (Re ε) and imaginary (Im ε) parts of the dielectric constant at frequencies of 500-5000 Hz at room temperature. Dielectric relaxation spectroscopy (DRS) is the most suitable tool for characterizing the microscopic behavior of polymer systems [1] and is one of

the most important methods for studying the structure and dynamics of polymer systems [2]. The time series of Re ε and Im ε were analyzed using entropy analysis.

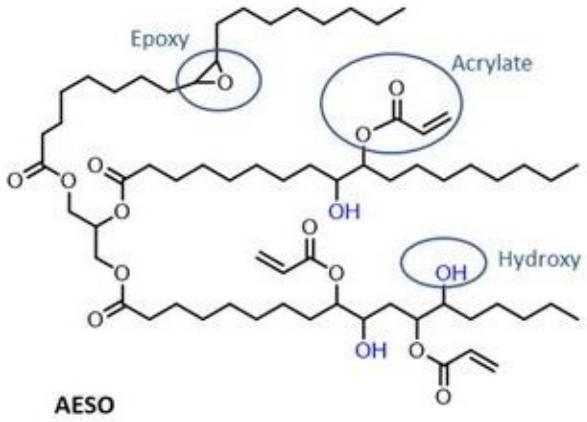

Fig. 1. Fragment of acrylated epoxy soybean oil, including main chains and side chains of acrylate, hydroxyl and epoxy groups

Entropy and correlation analysis of dielectric relaxation processes. The idea of entropy analysis is to define the average amount of information that a process transmits with each symbol [8]. Let $X = \{x_1, x_2, \dots, x_N\}$ be a stationary random process associated with a probability distribution $p(\cdot)$. Information (Shannon) entropy (ShEn) for such process is defined as

$$H(X) = -\sum_{x \in X} p(x) \log p(x). \tag{1}$$

The ShEn of an information source is a measure of the uncertainty associated with this source. If there is high uncertainty in the studied signal, ShEn of the source is maximal. If there is high regularity in the studied signal's structure, then ShEn goes towards zero.

In order to construct an appropriate model of the underlying photopolymerization process, it is necessary to obtain an information about the correlation characteristics of the underlying attractor of the system. Besides the entropy approach, it is possible to study via the correlation integral introduced by Grassberger and Procaccia [9]. The correlation integral of a signal in a pseudo-phase space can be defined as

$$C(r) = \lim_{N \to \infty} \frac{1}{N^2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} H\left(r - \left\|\vec{x}_i - \vec{x}_j\right\|\right), \tag{2}$$

where N is the number of considered phase space vectors $\vec{x}$, $H(\cdot)$ is the Heaviside unit step function, r is the radius of a hypersphere in a pseudo-phase space. The higher the value of $C(r)$, the more densely the pseudo-phase space vectors adjoin each other in the boundaries of the sphere with radius r, and thus the higher is the self-organization of the studied processes.

Fig. 2 shows a typical picture of the analysis of the real part of the dielectric constant.

Discussion of the research results. The analysis of dielectric relaxation processes shows the complexity of the latter. There are several competing temperature-activated processes, which are commonly referred to as α, β...-relaxation. The α-relaxation process is the primary relaxation process that results from the reorientation of segmental chains (main chains) in the polymer, covers a significant group of atoms, and has a clearly expressed collective character. β, γ,...-relaxations are secondary relaxations that result from the fluctuating motion of side groups attached to polymer chains. The low-frequency α-relaxation corresponds to the rotation of the AESO side groups around the axis of the main chain, i.e., segmental or crank motion. β-relaxation is caused by the rotation of the acrylate functional group around the C-O bond that connects them to the main chain. It appears

mainly in the intermediate frequency region and has a large contribution to the dielectric loss. In addition to these main relaxation processes, AESO can also have γ-relaxation and others at higher frequencies, which are related to the rotation of the hydroxyl and epoxy groups bonded to the main chain of the AESO monomer unit.

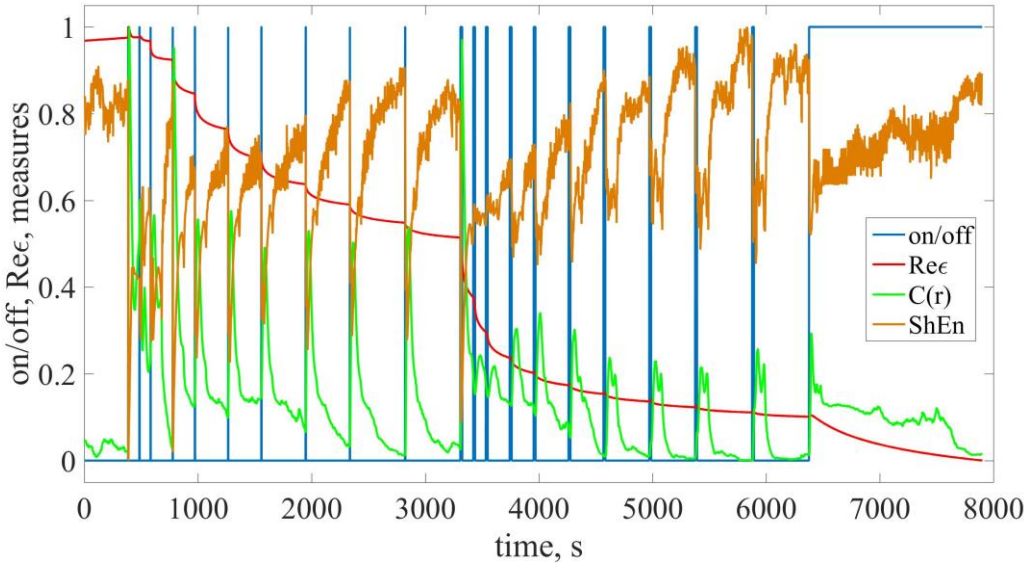

Fig. 2. Comparative dynamics of Re ε, the correlation integral $C(r)$, and ShEn calculated for a sliding window of 250 s with a step of 1 s. The experimental protocol includes turning on the light first for one second with increasing delays, then for 10 seconds with the same delay system. And finally, constant illumination until the end of the experiment

Fig. 2 shows that at the beginning of the experiment, when the light is turned on for a short time, highly correlated processes are observed that are inherent in the collective motion of a large number of atoms. The ShEn decreases markedly, which again indicates the collective self-organized motion of orientational defects. Each time the light is turned on, new free radical reactions occur, which stimulate both α-relaxation and other reactions, but over time, the influence of α-relaxation decreases and disappears even with the light constantly on. Only localized orientational defects remain active.

The processes of both primary and secondary relaxation are characterized by intrinsic activation energies, which are calculated by quantum mechanics. However, quantum mechanical calculations of energy and structural characteristics, for example, using the density functional theory (DFT) standard, require significant computer resources. Recent work in the field of artificial intelligence in materials science has made it possible to simplify this task and reduce it to finding the so-called interatomic machine learning potentials [6], which allow finding the range of required parameters with sufficient accuracy with limited resources. Preliminary results of such modeling of the key atomic and molecular structures of the polymer under study are presented and discussed.

Conclusions. In this study, we have experimentally modeled and analyzed the complex photo-stimulated polymerization phenomenon in an electric field for the first time. It has been shown that the tools of complex systems theory, in particular, entropy analysis, allow us to identify processes of structural transformations of varying degrees of collectivity and to separate them in time. The use of artificial intelligence technologies makes it possible to find interatomic potentials by building a neural network that finds the necessary information in the relevant special databases.

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APPLICATION OF THE NUMERICAL PHASE METHOD TO FIND THE ELECTRONIC ENERGY SPECTRUM IN A SPHERICAL QUANTUM DOT WITH ARBITRARY CONFINING POTENTIAL

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Abstract. This work explores the phase technique for addressing a second-order differential equation, specifically the equation for eigenfunctions and eigenvalues of the Hamiltonian operator, which is the Schrödinger equation. The conventional phase approach is adjusted to accommodate a scenario comprising two distinct domains with respective parameters. This technique is executed utilizing system of computer mathematics (like Wolfram Mathematica). The adapted approach is employed to calculate the electronic energy spectrum of an electron confined within a spherical quantum dot, under conditions of both rectangular and smooth potential. In instances of a rectangular potential, exact solutions of the corresponding Schrödinger equation are available, enabling a comparison with outcomes yielded by the proposed technique, demonstrating notable convergence accuracy. The method's strength and utility are rooted in its capability to address spherical quantum dots, be they single-layered or multi-layered, with arbitrary confining potentials.

Keywords: phase method, Schrödinger equation, quantum dot, system of computer mathematics.