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Матеріали
V Всеукраїнської науково-практичної
інтернет-конференції з міжнародною участю

# НАНОТЕХНОЛОГІЇ І НАНОМАТЕРІАЛИ У ФАРМАЦІЇ ТА МЕДИЦИНІ

(23 квітня 2021 року)

Materials of
V Ukrainian Scientific-Practical Internet Conference
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# NANO-TECHNOLOGY AND NANOMATERIALS IN PHARMACY AND MEDICINE

(April 23, 2021)

Материалы
V Всеукраинской научно-практической интернет-
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Для широкого кола наукових та практичних фахівців у галузі фармації та медицини, магістрантів, аспірантів, докторантів, співробітників фармацевтичних підприємств, викладачів вищих навчальних закладів.



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# INVESTIGATION OF DIELECTRIC PROPERTIES OF BOUND WATER IN ACTIVE NANOCOMPOUNDS DEPENDING ON TEMPERATURE

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One of the main goals of nanotechnology is the creation of nanoparticle-based drug delivery systems, which is vital in the event of infectious diseases, in particular, the spread of viral pandemics such as COVID19 [1,2]. Nanoparticles, known as ultrafine nanodiamonds (UDD), with characteristic sizes from 4 to 6 nm, high specific surface area (250-280 $m^2/g$), a labile functional cover and a chemically inert crystalline core make it possible to increase the bioavailability of a drug and reduce its toxicity, making UDD a promising carrier for creating systems for the delivery of biologically active of medicinal substances, luminescent markers for studying cellular interactions [2,3]. UDD have a "coat" of oxygen-containing, nitrogen-containing, sulfur-containing and other functional groups, and have a large sorption capacity. The sorption properties of UDD depend on the presence of charges on the surface of aggregates of particles, which is due to the presence of oxygen-containing groups with acidic properties on the surface of UDD. When working with UDD, the effect of the chemical state of the particle surface on many of its physicochemical properties is most pronounced. In particular, because of the narrow pores in the reticuloendothelial system, the circulation time of UDD aggregates in the blood increases by an order of magnitude, which leads to the maintenance of the required concentration level of the immobilized drug substance inside the target, for example, in a tumor. It was also found that the sorption of small amounts of water on the surface of detonation diamond powders causes a strong increase in its dielectric constant. Oxidation of the UDD surface is used to create carboxyl or hydroxyl groups on it, suitable for further covalent grafting of medicinal and biologically active substances. Information on the frequency dependence of the UDD dielectric permittivity $\varepsilon^* = \varepsilon' - i\varepsilon''$ (1) is necessary to understand the relationship between cells and nanoparticles in the study of blood erythrocytes in the microwave range [3].

In this paper, we consider a mathematical model of the dependence of the dielectric permittivity of water in active UDD on frequency which had include the frequency range from 0.3 to 10 GHz, taking into account the obtained practical data at a frequency of 9.2GHz, in the temperature range from 0 °C to 45°C. An aqueous suspension of UDD was considered, with an initial concentration of nanodiamonds of 0.1–0.3% by weight (0.05-0.15 g). To convert the volume of bound water to the amount of bound water in grams, the density of bound water was considered to be 1 $g/cm^3$. By the water, whose molecules, due to the asymmetric distribution of charges, have a significant electric dipole moment, the decisive role is played by orientational polarization. This circumstance determines its high relative dielectric constant ($\varepsilon \approx 80$ at 20 ºC). Thus, it is quite obvious that the value of the dielectric constant of UDD is determined, first of all, by the moisture content in them. Commercial UDDs, in contrast to conventional diamonds, are hydrophilic after the oxidative chemical purification step, but this property naturally prevents the formation of stable UDD suspensions in non-polar media. By modifying the

surface of hydroxylated UDD with alkyl chains of different lengths by the reaction of formation of esters from carboxylic acid chlorides and surface hydroxyl groups, it is possible to obtain on the nanodiamond grafted layers of different degrees of hydrophilicity. The obtained temperature dependences of the real ($\varepsilon'$) and imaginary ($\varepsilon''$) parts of the complex permittivity ($\varepsilon^*$) for UDD are linear. In experimental modeling, it was obtained that at a water saturation coefficient of 166.6%, water forms a film with a thickness of one monomolecular layer on the surface of UDD particles. With a further increase in humidity, the increase in the actual and imaginary parts of the permittivity index slows down. Thus, we can conclude that are appear on the surface nanoparticles a monotonic continuous films of bound water change the slopes of its dependences ($\varepsilon'$) and ($\varepsilon''$). The frequency dependence of the complex permittivity of bound water was described by the Debye and Cole-Cole relaxation models:

$$\varepsilon^* = \varepsilon_\infty + \frac{\varepsilon_{S1} - \varepsilon_\infty}{1 + i\omega\tau_1} + \frac{\Delta\varepsilon_{S2}}{(1 + i\omega\tau_2)^{1+\alpha_2}} + \frac{\Delta\varepsilon_{S3}}{(1 + i\omega\tau_3)^{1-\alpha_3}} \quad (2)$$

where $\varepsilon_\infty$ - high-frequency dielectric permittivity, is equal to 4.9; $\varepsilon_{S1}$ - low-frequency dielectric permittivity of the 1st relaxation region; $\Delta\varepsilon_{S2}$, $\Delta\varepsilon_{S3}$ - the differences between the low-frequency and high-frequency limits of the dielectric permittivity; $\tau_1$, $\tau_2$, $\tau_3$ - relaxation times for the 1st, 2nd, 3rd relaxation areas, respectively; $\alpha_2$ и $\alpha_3$ - relaxation time distribution coefficients; $\omega$ - cyclic frequency; $i$ - imaginary unit. These dependences change when the water saturation coefficient changes (the volume fraction of water which are exceeding the value of 0.999), are exceeding the value of 166.6%, which confirms the difference between the dielectric properties of bound water in the form of monomolecular layers and in the form of "clusters" of molecules grouped at adsorption centers. As the volume fraction of water in the sample increases, there will be groups of water molecules that are in varying degrees of contact with the surface of the UDD and have different degrees of "participation" in polarization processes. The dielectric constant values of bound water found in (1) and (2) will be some "effective" values describing the properties of the whole volume of water as a whole. Obtained, as the temperature increases, the values tend to one limit, which can be explained by the evaporation of bound water molecules upon heating, which practically ceases when the film thickness decreases to one monomolecular layer.

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