ROLE OF LOCALIZED STATES DUE TO NANOPARTICLE INCLUSION IN FORMATION OF ELECTRICAL CONDUCTIVE PROPERTIES OF NANOCOMPOSITE MATERIALS

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РОЛЬ ЛОКАЛИЗОВАННЫХ СОСТОЯНИЙ, ОБУСЛОВЛЕННЫХ ВКЛЮЧЕНИЕМ НАНОЧАСТИЦ, В ФОРМИРОВАНИИ ПРОВОДЯЩИХ СВОЙСТВ НАНОКОМПОЗИЦИОННЫХ МАТЕРИАЛОВ

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Аннотация. *В рамках модели Роуза-Фаулера исследована роль локализованных состояний в проводящих свойствах нанокомпозиционных материалов при радиационном воздействии. На примере нанокомпозитов с дырочной (полиметилметакрилат (ПММА) + CdS) и электронной (α-Al2O3+SrO) проводимостями, а также чистых ПММА и α-Al2O3, было показано, что мелкие ловушки влияют на скорость релаксации к равновесному значению радиационной электропроводности, а доля глубоких ловушек, глубина которых много больше kT, на чувствительность к поглощенной дозе ионизирующего облучения. Показано, что наиболее перспективными для дозиметрии являются нанокомпозиты на основе оксида алюминия, в которых концентрация примесных центров, обусловленных наночастицами, не превышает концентрацию собственных локализованных состояний, а размер наночастиц не превышает ~ 2 нм.*

Introduction. Electrophysical properties of dielectrics and semiconductors are determined by kinetics of charge carriers, which depends on the spectrum of localized states specified by different structural defects. For example, polymethylmethacrilate (PMMA) has an exponential spectrum of localized states for holes [1, 2], while the spectrum of localized centers of aluminum oxide includes only deep traps for electrons, that makes possible the usage of this material in dosimetry [3, 4].

The introduction of nanoparticles into dielectric matrix material leads to an appearance of additional localized states, which stem from the formation of the potential well due to a difference in Fermi levels of materials at the nanoparticle-matrix interface (impurity traps). In contrast to intrinsic localized traps in the matrix, the concentration and energy spectrum of impurity traps can be changed by varying the concentration and size of nanoparticles. As a result, the nanocomposite materials with new properties can be created.

Based on PMMA+CdS nanocomposite material different photogalvanic and optoelectronic devices are created [5]. Since high-radiation conditions should not affect the instrumental data of these devices, the question about radiation resistance of PMMA+CdS arises. On the other hand, corundum and nanocomposite materials on its basis are sensitive to radiation and able to register and save information about absorption dose for a long time, until the sample is exposed to external effects, for example, by heating.

In connection with above-mentioned, the task about electrophysical properties of nanocomposite materials under radiation exposure appears.

Rouse-Fowler equation system describes the kinetics of charge carriers in the band gap and allows us to describe different electrophysical properties of a dielectric material. In the frame of Rouse-Fouler model, the radiation electrical conductivity of polymer materials [1, 6] and the dose dependence of thermostimulated luminescence of the pure aluminum oxide under radiation effect with low dose rates [3, 4] were investigated. The existing solutions of Rouse–Fowler equation system consider only pure materials, where energy spectrum of traps has one or two energy levels [3, 4], or the case, where trap energy distribution follows the exponential law [1, 6]. To describe the electrophysical properties of nanocomposite materials we need to solve Rous–Fowler equation system for a random spectrum of localized states [7, 8].

This work aims to investigate physical processes, which determine the role of localized states of the pure PMMA and aluminum oxide, as well as nanocomposite materials made of them, in formation its electrical properties under gamma-rays exposure with low and big dose rates. By knowing these physical processes, we could evaluate the possibility of application of these materials in dosimetry.

Mathematical model. Properties of polymer materials are well understood. In polymer the distribution of intrinsic localized states, which stem from defects of the matrix materials, follows the exponential law [1]. To calculate the energy spectrum of localized states originated from the spherical nanoparticle introduction into the matrix material, we solved the Schrodinger equation with the potential of quantum dot [7, 8].

The kinetics of charge carriers in nanocomposite materials is described in the frame of Rose-Fowler model, which including following processes: the charge carrier generation, the capture of charge carrier by localized states and the thermal release of charge carrier from them.

It is important to note, that we consider only low values of absorbed energy (below 103 J/kg), so the heating does not exceed a few Kelvin degrees. It allows us to neglect the temperature effects. Radiation damages are not considered, so the concentration of localized centers is constant.

Results and conclusion. The nanocomposites are promising materials because of the possibility of controlling the energy spectrum of impurity localized states, which due to the nanoparticle inclusion.

The large relaxation time to equilibrium state makes PMMA unsuitable for dosimetry. PMMA+CdS nanocomposite material returns to the equilibrium state fast, but this nanocomposite material is not able to accumulate the information about the absorbed radiation energy.

From the dosimetry point of view, aluminum oxide has the most suitable energy spectrum of localized states. In case of the introduction of SrO nanoparticles with concentration of less than 1 vol. %, the basic role in the accumulation of charge carriers is played by the intrinsic trap with the energy of 1,3 eV (this trap is partially filled after annealing). After irradiation even with the absorbed energy of 20 J/kg (prolonged irradiation with the low absorbed dose rate) the trap is almost completely filled, which makes it difficult to accumulate charge carriers in case of longer irradiation. In the case of pulsed irradiation, when the basic process of relaxation to equilibrium state is the charge carrier recombination, the population of the intrinsic trap with the energy of 1,3 eV does not exceed 30 % even with the absorbed dose rate 105 J/kg.

Taking into account all the above mentioned, the creation of the nanocomposite materials should meet the following requirement: the concentration of the impurity localized states, which stems from the nanoparticle introduction, should not exceed the concentration of the intrinsic localized states of the matrix material. The nanoparticle dimensions should not exceed ~2–5 nm. The large size of nanoparticles leads to the formation of the large proportion of small traps in the energy spectrum of impurity localized stated, that makes the relaxation time long, so the material will not be sensitive to the absorbed radiation energy.

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