Nanocomposites and nanomaterials

On the PAL testing of light-curing nanostructurization processes in dimethacrylate-based dental restorative composites

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The characterization possibilities of positron annihilation lifetime (PAL) spectroscopy is analyzed in application to commercially available dimethacrylate-based dental restorative composites Charisma (Heraeus Kulzer GmbH, Germany), Dipol (Oksomat-AN Ltd, Ukraine) and ESTA-3 (Kiev, Ukraine), all based on monomer matrix consisted of bisphenol A-diglycidyl dimethacrylate (BisGMA) and triethyleneglycol dimethacrylate (TEGDMA) modified with multisized filler particles having highly dispersive phase of silica glass. The nanocomposites were studied in initial and deeply light-cured states using conventional fast-fast coincidence PAL spectrometer equipped with ORTEC® electronics. The PAL spectra were reconstructed from unconstrained x3-term and partially-constrained x4-term fitting assuming shortest lifetime fixed at theoretical value of intrinsic para-Ps self-annihilation lifetime ($_1$=0.125 ns).

In respect to the data parameterized within constraint-free x3-term analysis, the annihilation processes in the studied nanocomposites are identified as conversion from "purely" positron trapping to positronium (Ps) decaying, where ortho-Ps component is caused entirely by free-volume holes in the polymer matrix, and positron-trapping component is defined preferentially by interfacial free-volume holes between filler particles and surrounding polymer matrix. It is shown that most adequate model-independent estimation of polymerization volumetric shrinkage in the studied nanocomposites can be performed in terms of average positron lifetime. The meaningful phenomenological description of photoinduced ortho-Ps transferring in positron-trapping sites (which occurs more efficient in the Charisma nanocomposite), can be developed at the basis of semi-empirical model exploring a so-called x3-x2-coupling decomposition algorithm [1,2].

1. *Shpotyuk O., Filipecki J., Ingram A., Golovchak R., Vakiv M., Klym H., Balitska V., Shpotyuk M., Kozdras A.* Positronics of subnanometer atomistic imperfections in solids as high-informative structure characterization tool // Nanoscale Res Letters-2015.-**10**.-P. 77-1-77-5.

2. *Shpotyuk O., Ingram A., Filipecki J., Bujňáková Z., Baláž P.* Positron annihilation lifetime study of atomic imperfections in nanostructurized solids: On the parameterized trapping in wet-milled arsenic sulfides As_4S_4 // Phys Stat Sol B.-2016.-**6**.-P. 1054-1059.