MS15-P35 Relationship between the composition, structural parameters and properties of single-crystal KDP with nano-titania

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Development perspectives for new nonlinear optical elements (NLO) based on combinations of inorganic matrix with various inorganic functional nanoparticles are discussed now. The presence of nano-TiO_2 in a crystalline matrix of KDP (KH_2PO_4) leads to increase the magnitude of cubic nonlinear susceptibility, changes the sign of the nonlinear refractive response and increases the efficiency of second harmonic generation of composite system KDP:TiO_2 (V.Ya. Gayvoronsky et al. 2013). The aim of this paper is to establish the relationship between composition, structural parameters and dielectric properties of composites KDP:TiO_2.

X-ray diffraction study of the initial samples with nano-TiO_2 (phase analysis, the sizes of coherent scattering regions - *D*) indicated the presence of anatase (sample 1; *D* = 50 (4) Å) and η-TiO_2 (sample 3; *D* = 38 (2) Å) (sulfate method) and anatase (sample 2; *D* = 150 (8) Å) (chloride method) at them. Pure KDP crystals and KDP:TiO_2 (composites I, II, III with incorporated TiO_2 nanoparticles from the samples 1,2 and 3, correspondingly) were grown by the temperature reduction method onto point seed. According to X-ray microanalysis, the sulfur content is greater in the sample 3 (4.37-7.58 wt %) and composite III (11.99 wt.%) as compared with sample 1 (2.17-3.73 wt %) and composite I (4.54 wt..%). The samples from growth sectors {100} and {101} of KDP and KDP:TiO_2 crystals were cut for the investigation.

Analysis of the results of X-ray single crystal study revealed the most significant structural changes in the composite III ({100}): a very small value of O-H distance and a short distance P-O compared with the same distances in the structures of KDP and composites I, II, vacancies in the K^{1+} sites and located ions Ti^{4+} in the vicinity of the K^{1+} positions. It was established that the general composition of the composite III ({100}) can be described as $(K_{0.950(1)}[\ ]_{0.050})(Ti_{0.052(2)i})(H^{1+}{}_{2-x}[\ ]_x)[(PO_4)^{3-}{}_y(SO_4{}^{2-})_{1-y}]$ ([ ]-vacancy).

It was established that the magnitude of dielectric permittivity (ε') for KDP and KDP:TiO_2 is different depending on the growth sectors (ε'{101}>ε'{100}). It is greater for composite II in comparison with composite I and composite III ({100}) has the smallest value of ε', which correlates with the interatomic distance O-H.

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Keywords: KDP: nano-TiO2, structure, dielectric properties

MS15-P36 Absolute structure of (E)-2,2'-[3-(2-Nitrophenyl)prop-2-ene-1,1-diyl] bis (3-hydroxy-5,5-dimethylcyclohex-2-en-1-one)

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Herewith we present the crystal structure of (E)-2,2'-[3-(2-nitrophenyl)prop-2-ene-1,1-diyl] bis(3-hydroxy-5,5-dimethylcyclohex-2-en-1-one) (**A**)[1], (E)-2,2'-[3-(4-nitrophenyl)prop-2-ene-1,1-diyl] bis(3-hydroxy-5,5-dimethylcyclohex-2-en-1-one) (**B**)[2]. In the compound (**A**), C25H29NO6, each of the cyclohexenone rings adopts a half-chair conformation. Each of the pairs of hydroxy and carbonyl O atoms are oriented to allow for the formation of intramolecular O—H---O hydrogen bonds, which are typical of xanthene derivatives. The nitro group is rotationally disordered over two orientations in a 0.544 (6):0.456 (6) ratio. In the crystal, weak intermolecular C—H---O hydrogen bonds link molecules into layers parallel to the *ab* plane. The compound (**B**), each of the cyclohexenone rings adopts a half-chair conformation. The hydroxy and carbonyl O atoms face each other and are oriented to allow for the formation of two intramolecular O—H---O hydrogen bonds. In the crystal, weak C—H---O hydrogen bonds are formed between molecules, generating a two-dimensional supramolecular structure.

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