Structural Conditionality of Physical Properties in Nb or Sb Doped KTP Crystals

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$KTiOPO_4$ (KTP) crystals and their solid solutions attract researches attention by nonlinear optical characteristics. High ionic conductivity and ferroelectric phase transition of these crystals are also of great interest. All of these properties are susceptible to the changing of the crystals composition and can be regulated within certain limits by means of isomorphic replacements. Two series of KTP single crystals (sp.gr. $Pna2_1$) doped with Nb and Sb were grown. Features of physical properties and atomic structure of five crystals doped with Nb and three crystals doped with Sb were studied. For single crystals $K_{1-x}Ti_{1-x}Nb_xOPO_4$ (KTP:Nb) и $K_{1-x}Ti_{1-x}Sb_xOPO_4$ (KTP:Sb) the maximal x values are 0.11 and 0.23 correspondingly. New additional positions of K cations and a lot of potassium vacations were found in the structure of KTP:Nb and KTP:Sb crystals. X-ray structural study of $K_{0.93}Ti_{0.93}Nb_{0.07}OPO_4$ crystal at 30K was done in order to localize safely the additional K positions with low occupancy. Results of this structural study confirmed the model received at room temperature and allowed establishing of presence of the potassium positions removal along c axis, which depends on temperature. Decreasing of the temperature of ferroelectric phase transition and strengthening of relaxation effect in the doped crystals are concerned with displacement and splitting of potassium positions. Disorder in the potassium sub-lattice leads to the increase of conductivity.

Keywords: structure-physical properties relationships, superionic conductivity, nonlinear optical materials