Poster Presentation

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Growth and structure of K2CoxNi(1-x)(SO4)2•6H2O mixed single crystals

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To date, crystals of Tutton salts with the general formula (M+)2M2+(SO4)2*6H2O (where M+- alkali metal or ammonium, M2+ bivalent metal - Co2+, Ni2+) are used as a materials for ultraviolet (UV) filters. Only in recent year effort of ternary crystal growth has been taken. The main problem of mixed crystal growth from liquid solution is high level of the crystal inhomogeneity, which leads to generation of the elastic stress, inclusion trapping and micro- and macrocrack formation in the bulk crystal. For the first time the optically homogeneous mixed K2CoxNi(1 – x)(SO4)2 · 6H2O (KCNSH) large single crystals have been grown from solutions of different compositions by the temperature-reduction technique. Precise X-ray experiment of three mixed crystals was carried out by four-circle diffractometer CAD-4F and XcaliburS diffractometer with two-dimensional CCD detector at the room temperature. KCNSH crystals belong to the monoclinic space group P2(1)/c. Each Co2+ or Ni2+ ion is coordinated with six H2O molecules, forming a distorted octahedral (Co(H2O)6)2+ and (Ni(H2O)6)2+ unit. With increasing content of nickel ions in the crystal, the octahedral unit is narrowed and the unit cell volume is decreased. Chemical formulas refined using diffraction data are K2Co0.657Ni0.343(SO4)2•6H2O, K2Co0.226Ni0.774(SO4)2•6H2O and K2Co0.216Ni0.784(SO4)2•6H2O. Ratios of isomorphic cobalt and nickel components in the mixed crystals are conformed to data obtained by atomic emission spectroscopy. Effect of the Co2+ and Ni2+ ion ratio in KCNSH single crystal to crystal quality is considered.

Keywords: mixed crystal, crystal growth, structure