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Structure and Properties of $Ca_{10.5-x}Pb_x(VO_4)_7$ Single Crystals

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The whitlockite-like compounds manifest multifunctional properties and have been under research recently [1,2]. These compounds are considered as new advanced materials with ferroelectric and antiferroelectric, piezo-electric, nonlinear optical, ionic-conductive, luminescence, nonlinear optical and laser properties. We have obtained by the Czochralski method and studied new whitlockite-like $Ca_{10.5-x}Pb_x(VO_4)_7$, x = 1.8; 3.5; 4.9 single crystals with record properties. According to the X-ray diffraction analysis, the compound crystallizes in *R*3*c* space group. Structures of $Ca_{10.5-x}Pb_x(VO_4)_7$ were refined by the Rietveld method and Pb^{2+} cations was occupied over the *M*1 - *M*2 and *M*3 sites in the β-$Ca_3(PO_4)_2$-type lattice. The crystals are ionic conductors. Conductivity measurements were carried out in the interval 500-1000 K and values are from 10^{-6} to 10^{-2} Sm/cm. Ca^{2+}-ion mobility in the solid solutions is manifold higher than in $Ca_3(VO_4)_2$ and other previously studied β-$Ca_3(PO_4)_2$-type compounds. Lead substitution for calcium in is investigated as a factor controlling ferroelectricity, ionic-conductivity and non-linear optical activity. Non-linear optical activity in the second harmonic generation effect strongly increases with x, in keeping with investigated $Ca_{10.5-x}Pb_x(VO_4)_7$ system in form of powders and ceramics in [3].

The combination of low temperature conductivity with high nonlinear optical activity and ferroelectricity extends ability of ion-exchange technology of integrated optical devices for a new class of materials. Based on the obtained data control of important properties in whitlockite-like phases aimed at creating multifunctional materials at their basis is possible.

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