ISOMORPHIC SUBSTITUTIONS IN THE TETRAHEDRAL POSITION OF APATITES AND THEIR INFLUENCE ON PHYSICOCHEMICAL PROPERTIES

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Structural modification by isomorphic replacements in tetrahedral sublattice results in essential changes of physical properties of apatites. In this work influence of anharmonicity vibration in a lattice of apatites mixed structure $Ca_{10}(PO_4)_{6-x}(VO_4)_x(M)_2$, where $M=OH^-$, F^-, Cl^-, x=0, 1, 3, 5, 6 on its physical and chemical characteristics is investigated.

It was established, that for chlorine-containing apatites of any level doping of topotetrahedral matrix significant decrease of tetrahedrons absorption band - from ~ 400 sm^{-1} up to ~ 90 sm^{-1} for boundary concentration is observed. Similar effects are observed for fluor- and hydroxylapatites too however theirs are less expressed. Decrease of width occurs from ~ 200 sm^{-1} up to ~ 95 sm^{-1}. High sensitivity of a chloroapatites matrix to changes of fluctuations of tetrahedral sublattice after doping should have an effect on the thermal stability, as it was revealed after thermogravimetric analysis. The fusion temperature of compound shifts as the decrease with VO_4 ions fraction increase in calcium fluor- and chloroapatites.

Thus, decrease IR absorption band half-width describing XO_4 tetrahedrons, is related to decrease of interaction between tetrahedrons of one type, and, as a consequence, to anharmonicity vibrations suppression in quasi-free tetrahedrons.

It was established, that vibration anharmonicity in the lattice of apatite may change depending on the concentration of tetrahedron that type in crystal structure. These changes are local and by means of various replacements it is possible to create necessary spatial distribution of anharmonic component in the crystal that opens the prospect of controllable change of heat conductivity, factor of temperature expansion and other parameters in the crystal which depend on the vibration anharmonicity of the lattice.