XANES and USXES investigations of the hydroxyapatites

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In spite of increasing importance of materials based on apatites the data concerning their electron structure remains rather limited. We performed the investigations of the electron states energy distribution in the valence and conduction bands, determined the width of the band gap using USXES and XANES techniques for a set of hydroxyapatites (HAPs) in the form of powders, nanopowders including those ones doped with Ni, Fe, Mg as well as dental enamel HAP.

Interpretation of the experimental spectra was performed in the dipole approximation with the use of theoretical calculations of the total and partial densities of states for HAP within the frames of the band and cluster models.

USXES P L_{2,3}-spectra allowed us to determine the width of the valence band as ~ 10 eV, the influence of OH group on redistribution of elector density between P-O bonds in HAP as compared with Ca_3(PO_4)_2.

XANES Ca Lα spectra allow to estimate the value of spin-orbit splitting of Ca 2p_{1/2,3/2} ~ 3.2 eV, the value of the crystal field splitting of ~ 1 eV for Ca 3d band in the conduction band of stoichiometric Ca-HAP Ca_{10}(PO_4)_6OH. By matching XANES P L_{2,3} with USXES P L_{2,3} in the common energy scale we have determined the value of the band gap in this compound as ~ 8 eV.

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