SYNTHESIS, PROPERTIES AND STRUCTURE OF INORGANIC COMPOUNDS

Mathematical modeling of the process of hydroxyapatite synthesis

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Trauma, lesions and diseases of the joints are a global medical and social problem. The most effective way to treat and restore the integrity of bone tissue is endoprosthetics. At present, hydroxyapatite (HA), obtained by roasting bones of cattle with subsequent grinding, is used as the bioactive material for endoprosthetic coatings [1, 2]. Powders with a wide dispersion spectrum are obtained, and particles comprising up to 50–100 μm in size are produced. Synthesis of artificial HA is carried out by precipitation from aqueous solutions of calcium salts with ammonium hydrophosphate [2]. Therefore, the urgent task is the research and development of new methods for the synthesis of fine crystalline HA by inexpensive and technological way for the formation of bioactive coatings. The aim of our research was the synthesis of hydroxyapatite powder suitable for applying biocompatible coatings onto medical implants. Samples of HA were synthesized by chemical precipitation. Optimization of the synthesis parameters was carried out by mathematical modeling method. Based on the results, the influence of the time of synthesis of the precipitate, pH, temperature, the concentration of calcium nitrate, the concentration of ammonium hydrophosphate was studied. The optimal parameters of synthesis of the HA sample were determined as follows: the time of synthesis – 60 min; the aging time of the precipitate – 16 hours; the pH – 9; the temperature – 50 °C, the power of the ultrasonic generator – 60 %, the concentration of calcium nitrate – 1 mol/l; the concentration of ammonium hydrophosphate – 0.6 mol/l; the calcination temperature of synthesized HA – 800 °C. The derived mathematical models of the process optimization made it possible to calculate the conditions for carrying out the synthesis by changing at least one of the variable factors in the studied ranges in order to obtain HA with a controlled stoichiometric composition, particle size, and solubility.The prototypes of HA coatings on substrates made of titanium medical alloys have been obtained.

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References

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Synthesis and physico-chemical properties of spinel compounds with general formula $Zn_{1-x}Mn_xCr_2Se_4$

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The $ZnCr_2Se_4$compound crystallizes in cubic spinel structure (space group *Fd*-3*m*), with lattice parameter a = 10.4970 Å. It is a semiconductor with magnetic helical structure below the Néel temperature $T_N \approx 20$ K [1, 2]. The normal cations distribution occurs in this spinel: zinc ions are located at the tetrahedral sites and chromium ions are in octahedral sites. It is known that elements substitution can strongly influence on the parent compound properties [3–6].

The compounds based on the $Zn_{1-x}Mn_xCr_2Se_4$ system, x = 0.1–0.5, were synthesized by ceramic method, according to the following reaction:

$$(1-x)ZnSe + xMnSe + Cr_2Se_3 = Zn_{1-x}Mn_xCr_2Se_4$$

Chemical compositions of the obtained samples were determined using ICP-AES method. XRD and Rietveld refinement analysis were used in order to obtain structural parameters (anion and lattice parameters).

Fig. 1 shows that the structural parameters increase with the growth of Mn amount, according to the assumption, because the ionic radius of Mn^{2+} (0.66Å) is larger than that of Zn^{2+} (0.60Å).

The magnetization of manganese doped compounds has been studied and magnetic isotherms were measured within a temperature range of 4.2÷300 K in high magnetic stationary fields (up to 14 T) using an induction magnetometer. The magnetic susceptibility was determined in the temperature range of 1.8–300 K using a Quantum Design SQUID-based MPMSXL–5-type magnetometer.