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Controllability of brushite structural parameters using an applied magnetic field

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ABSTRACT

The paper studies the influence of low intensity static magnetic field on brushite structural and microstructural parameters using the X-ray diffraction and the transmission electron microscopy. This effect was shown to have various influences on DCPD (Dicalcium Phosphate Dihydrate) structure depending on a magnetic field configuration or time of synthesis, which allows achieving controllability of the main properties of an obtained material. The influence of the magnetic field leads mostly to the decrease of crystallite sizes with no impact on the crystal lattice parameters. In (0 2 0) and (1 5 0) planes the growth of crystallite sizes is observed after 2 and 3 days of crystallization, respectively. The analysis of different contributions to peak broadening in [0 b 0] direction showed a similar trend for the crystallite sizes with the lower lattice microstrains after 2 days of synthesis. The effect similar to the preferred orientation was observed and classified with the Harris method.

1. Introduction

The number of calcium phosphate materials used in medicine increases every year. One of such promising materials is Dicalcium Phosphate Dihydrate (DCPD), also named brushite, with chemical formula $CaHPO_4 \cdot 2H_2O$. DCPD can be crystallized from aqueous solutions at ~2.0 < pH < ~6.5 [1]. Brushite is metastable under physiological conditions [2]. In vivo, it tends to convert into hydroxyapatite (HA) [3–5]. DCPD has monoclinic lattice (Fig. 1) with parameters $a = 5.812 \pm 0.002$, $b = 15.18 \pm 0.003$, $c = 6.239 \pm 0.002$ Å and $\beta = 116.417 \pm 0.033°$, a space group *Ia* [6].

Brushite was tested in vitro, in vivo and clinically for a wide variety of uses in orthopedics, dentistry and other biotechnological applications including drug delivery, cancer therapy and the development of biosensors [4,8–12]. DCPD is also employed in toothpastes for caries protection and as an abrasive as well, which does not damage an enamel [1,9]. Generally, brushite is used as a calcium phosphate cement basis [4,5,8,11–19]. Such cements are applied for bone defects restoration and have a much higher resorption rate as compared to that of the apatite ones [4,5,8,11,12,19].

The influence of various crystallization conditions (e.g., calcium-phosphorus ratio [9], synthesis temperature [20], solution pH [9]) on calcium phosphates structure is a very important study due to its significant effect on the main properties of the obtained biomaterials including bioactivity, biocompatibility and mechanical strength [9,10,12–14,21]. DCPD materials with appropriate parameters show osteointegration, osteoconduction and osteoinduction qualities [8].

The influence of the magnetic field (MF) during crystallization from the solution is one of such factors. Some researchers indicate that it might lead to visible effects like accelerated crystallization [22]. The influence of MF promotes both the dissolution of metastable precursor phases and the nucleation of more stable phases with overall transformation sequence ACP (amorphous calcium phosphate) → DCPD → OCP (octacalcium phosphate) → HA [22].

The orientations of crystallites could be changed under the influence of MF, but several conditions must be met: the materials must have a magnetic anisotropy in their unit crystal cells; the magnetization energy should be larger than thermal energy; the materials should exist in the weak constraint medium enough to be rotated by such a feeble magnetization force [23,24]. The changes in crystallite sizes and their numbers are also observed [25–28], as well as in surface values of obtained agglomerates [25].

This paper continues our previous researches started in [29,30]. For a more precise qualification of the influence of different factors on DCPD structure, synthesis was carried out without magnesium allowing a more complex structural and microstructural analysis. The experimental setup was also extended. The current study is aimed at the investigation of changes in a crystal structure of brushite synthesized under the influence of static magnetic field applied in various configurations. It allows obtaining materials with controllable structural and microstructural parameters thus their biomedical properties.

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