m12.p01

Structural characterization of bioactive glasses

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Keywords: bioactive glasses, GIWAXS, drug delivery

Several bioactive materials have been studied in the last decades for many applications in medicine [1,2]. We will focus our attention on bioactive glasses, which represent the first class of inorganic materials, which showed the peculiar surface property of bonding to living bone. When a bioactive glass is soaked in a fluid mimicking the inorganic composition of human plasma (simulated body fluid, SBF) several surface reactions can occur, leading, by a complex mechanism including ion leaching, silica gel formation, Ca^{++} and PO_4^{3-} diffusion, to the precipitation of hydroxy-carbonate apatite (HCA) with composition and structure close to the mineral phase of bone. The precipitation of HCA on bioactive glasses has been extensively investigated [2], but information on the structural features of the HCA film, especially in the early stages of deposition, is still lacking. Bioactive glasses can be massive or porous to host drugs to be delivered after prosthesis insertion. We present here the characterization of different kinds of glasses (both massive and porous) for applications in orthopedic and dental devices, to shed some light on the growth mechanism of: *i)* HCA on massive SCK (silica, Ca and K) bioactive glass plates and *ii)* an ordered mesoporous SBA phase inside porous SCK bioactive glass scaffolds.
Synchrotron radiation GIWAXS measurements were carried out on plates of massive SCK glass, soaked in SBF for increasing times. Initially the scattering curves only show the presence of an amorphous phase, due to the glass itself, but the presence of a new crystalline phase is already evident after 15 h soaking. This diffraction profile due to a crystalline phase increases with the soaking time and after 15 days it is possible to identify the full pattern of HCA present on the surface of the SCK bioactive glass.
The deposition of an ordered silica mesophase inside the macroporous structure of a SCK bioactive glass scaffold allows to combine the bioactivity of the latter with the drug delivery properties of the ordered mesoporous systems [3]. The X-ray diffraction patterns of the SCK (scaffold)-SBA composite materials clearly indicate the presence of peaks with d-spacings consistent with the presence of a hexagonal SBA material. The collected diffraction patterns show that the crystallinity of the SBA phase depends on the aging conditions and our data suggest that the ageing at 60 °C for 72 h is more efficient in obtaining an ordered SBA layer.

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m12.p02

X-Ray Line Profile Analysis of Nanostructured Oxytocin

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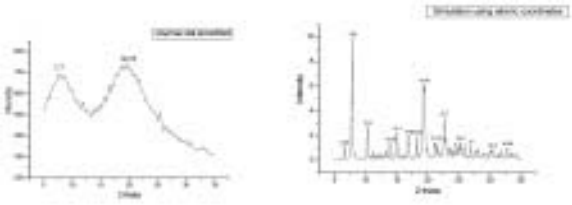
Keywords: profile analysis, nanocrystallites, drug molecules

Oxytocin is a synthetic peptide hormone having the property of causing the contraction of uterine smooth muscle. Oxytocin has been always considered as amorphous powder and is able to ''suck in'' humidity up to 10%. The aim of this work was to explain the water binding mechanism of oxytocin substance. By means of X-ray line profile modeling it was shown that the origin of higroscopicity of oxytocin substance in air is related to formation of nanosized oxytocin crystallites in the form of heptahydrates. The figures below show experimental (left) and theoretical (right) X-ray diffraction patterns of oxytocin. The existence of two broad diffraction maxima at 2(angles 7.7(and 19.7(respectively undoubtedly indicates the presence of crystalline phase. Moreover experimental peaks are just smeared out (broadened) the strongest peaks of the theoretical diffraction pattern. To evaluate the dimensions of crystallites in the oxytocin sample two different diffraction profile modeling techniques were used. 1. Langford distribution modeling [1]. In this method crystallites are assumed to be spherical, no microstrain effects are considered. Application of this method to oxytocin diffraction data produced the values of crystallite diameter dimensions in the range of 25-30 Å. 2. Modeling using Debye formula [2]. This method allows to calculate theoretical diffraction pattern for crystallites of a given size and shape when crystal structure is known. Crystallites were constructed from different number of oxytocin unit cells (ranging from 1 to 150) and the diffraction patterns were calculated and compared with experimental ones. The best agreement was achieved for crystallites containing 15-18 unit cells with dimensions 20x60x80 Å approximately.



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