Oxygen Deficiency and Crystallinity as Determinants of Charge Trapping in Hydroxyapatite Thin Films

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Abstract. Hydroxyapatite is a dielectric ceramic and a major constituent of human bone, exhibiting piezoelectric properties that are believed to play an important role in physiological bone healing and remodelling by electrostatically influencing calcification and bone cell activity [1]. Consequently, hydroxyapatite bulk samples have been extensively studied in relation to artificial charge induction and its impact on bone-like layer formation and cell attachment *in vitro* [2]. According to simulations, excess charge injected into the material is trapped in electron traps associated with oxygen-related defects [3]. To investigate this further, we prepared hydroxyapatite thin films using Pulsed Laser Deposition followed by various post-deposition treatments aimed at inducing different levels of oxygen deficiency. The films were deposited by irradiating a pure microcrystalline hydroxyapatite target with either 10 000 or 50 000 laser pulses. The evaporated material was deposited onto sapphire and silicon substrates. X-ray diffraction confirmed that the as-deposited thin films were amorphous. X-ray Photoelectron Spectroscopy and Energy Dispersive X-ray Spectroscopy revealed Ca and O deficiency at the surface and enrichment in the bulk. The development of crystallinity and chemical composition was investigated as a function of temperature in different environments: atmospheric air, O_2 at atmospheric pressure, and high vaccum (3.5×10^{-5} Pa or better). The films were subsequently irradiated with a 30 keV electron beam in a Scanning Electron Microscope, and the value of the trapped charge was quantified using an innovative application of the pendant drop method in an electric field [4]. The results were correlated with structural and chemical characteristics of the films, highlighting the critical role of crystallinity in electron trapping efficiency. This study was supported by Comenius University grants no. UK/158/2022 and UK/288/2023 and by Horizon project COLOSSE no. 101158464.

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