Characterization and Modeling of Local Electronic Properties of Native Bone Tissue in Intact and Damaged Areas

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Abstract:

Hierarchical organization in life science is extended from atoms to ecological spheres. This organization is regarded as a platform for application of various physical and chemical models to scientific research in diseases and body functions [1]. Applying quantum mechanics to study chronobiological and osteochondral processes as well as for diagnosis of native bone in subcellular levels we encounter with great difficulties because the major morphological models are mainly developed for qualitative description of structure-functional organization of the skeleton whereas quantitative characterizations of bone tissue in nanoscale are poorly investigated. Development at the beginning of ex- and then in-vivo quantitative approaches to hierarchical nanostructures in combination with the novel 3D superlattice of "black-nanoboxes-in-muddy-waters" (3DSL) model [2] is a pathway in medical, material and life sciences. In addition to changes in elemental composition the 3DSL model takes into account both the structure-functional organization of the skeleton and the peculiarities of electron wave propagation through the 3D superlattice assembled from nanocrystallites of hydroxyapatite (HAP) $Ca_{10}(PO_4)_6(OH)_2$ (see, Figure 1).

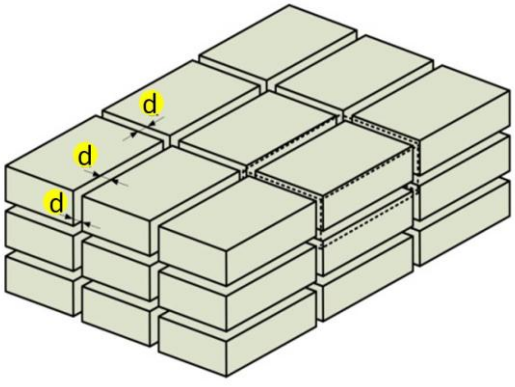

Figure 1: Figure illustrating the coplanar assembling of HAP-nanocrystallites separated by the hydrated nanolayers with the thickness ***d***.

Distinct HAP-to-bone spectral changes in core-to-valence transitions are predicted and confirmed by the recent X-ray absorption spectroscopic measurements of young, adult and mature bone and HAP [2]. The 3DSL approach is applied to model the thermal and age related changes in electronic and atomic structure of mineralized bone.

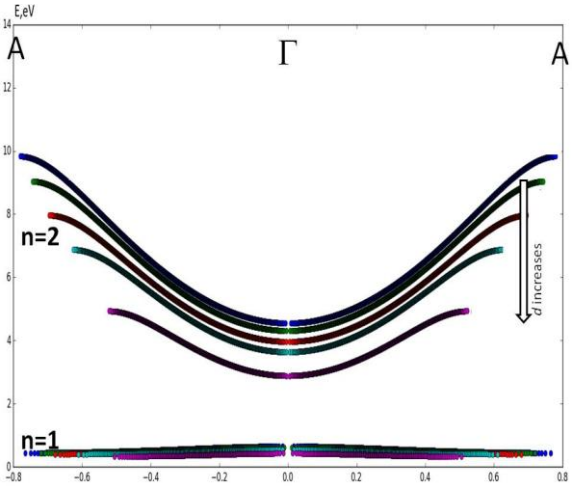

Figure 2: Figure presents model changes in dispersion $E(k)$ of band energy in the superlattice as a function of ***d***. Heine equation:

$$e^{2ikr} - 2Re[T^{-1}(E, \langle d \rangle, \langle L \rangle)]e^{2ikr} + 1 = 0$$

is used to model the band dispersion and to assign the certain energy E with the electron wave number k. T is the amplitude of electron transmission through the cell of the superlattice and $\langle d \rangle$ and $\langle L \rangle$ are the mean sizes of the hydrated nanolayers and nanocrystallites.

Keywords: hierarchical organization, bone tissue, superlattice, electronic and atomic structure

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