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On the generation of intrinsic electric dipole fields as the basis for the understanding of the morphogenesis of fluoroapatite-gelatine nano-composites

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Systems of ordered fractal aggregates of fluoroapatite-gelatine composites were chosen to mimic the growth of the biosystem apatite-collagen, which plays an important role in the human body as functional material of teeth and bones. The morphogenesis of these particles starts with elongated hexagonal prismatic seeds, followed by fractal branching and the development of growing dump-bell states. In order to gain insight into structure formation a lot of experimental investigations were performed [1]. High resolution TEM micrograph of the [001] zone of a composite seed showed also the presence of triple-helical macromolecules oriented along the *c*-axis [2]. The general principles of the dramatic selforganization process are not yet understood. It is proposed that they should be manifested already in the structure of the seed. Molecular dynamics simulations on the basis of atomistic resolution models offer some ideas for the organisation principle. However, the effort is typically immense and unacceptable for systems with increasing size. The simulation scenario has to be drastically simplified. Our approach starts from the assumption of the formation of an intrinsic electric field - built by the permanent dipoles contained in each individual composite crystal [3] - which takes over control of the aggregate-growth. This assumption is consistent with the observation of the biological significance of electric fields (pyro- piezo electricity) during bones formation. The simulation strategy can be described as follows. Adopting a coarse grained model, the first main task is the calculation of the electric field [4] (on the basis of given dipole arrangements). Each collagen molecule, is represented by two beads with opposite charges, in the hypothesis that all the C-termini and N-termini are completely deprotonated and protonated, respectively. All the beads are arranged in the seed according to the experimental geometrical parameters. A Monte Carlo simulation is performed in order to optimise the still missing geometrical parameters. According to the resulting force field lines, the orientation of the seeds belonging to the following generations can be predicted.

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