Disaccharides mediate the interplay between collagen and carbonate ions in biomineralization processes

Patrick Duchstein[1], Rüdiger Kniep[2], Dirk Zahn[1]

[1]*Computer Chemie Centrum, Friedrich Alexander Universität Erlangen-Nürnberg*

[2]*Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden*

Biominerals, such as bone, teeth, otoconia, and mollusc shells are composite materials, composed of an inorganic mineral, closely interacting with organic tissue, in many cases collagen. Otoconia in particular consist of calcite and collagenous proteins, enamel comprises a calcium hydrogen phosphate matrix with embedded collagen fibers[1]

We investigated crystal nucleation of calcium carbonate and of carbonated calcium hydrogen phosphate along various types of collagen. Our method of choice consisted in the Kawska-Zahn approach [2,3] which allows for the simulation of crystal growth ion by ion along a triple helical collagenous strand. By analyzing various collagen types with different degrees of glycosylated lysine residues we found out that a very high degree of glycosylated amino acids is necessary to ensure calcification along a collagenous triple helix, and thus embedding of the collagen fiber.

Simulations with biological, i.e. carbonated, calcium hydrogen phosphate yielded similar results. We therefore conclude that glycosated lysine residues are crucial to allow carbonate ion association to collagen fibers without compromising the protein structure.

[1] E. Bäuerle, P. Behrens, M. Epple (eds.), Handbook of Biomineralization, **2007**

[2] A. Kawska, J. Brickmann, R. Kniep, O. Hochrein, D. Zahn, *J Chem Phys*, **2006**, *124*, 024513

[3] A. Kawska, O. Hochrein, J. Brickmann, R. Kniep, D. Zahn, *Angew Chem Int Ed*, **2008**, 47, 4982-4985