



UvA-DARE (Digital Academic Repository)

A Particle-Based Model for Aggregate Formation in Biomineralization

Javaheri, N.; Cronemberger, C.M.; Kaandorp, J.

Publication date

2011

Document Version

Final published version

Published in

Molecular iomineralization in marine organisms: Nanobiotechnology and biomedical application

[Link to publication](#)

Citation for published version (APA):

Javaheri, N., Cronemberger, C. M., & Kaandorp, J. (2011). A Particle-Based Model for Aggregate Formation in Biomineralization. In V. Matranga (Ed.), *Molecular iomineralization in marine organisms: Nanobiotechnology and biomedical application: Biomintec International Workshop, 2011 Palermo : abstracts* (pp. 23). IBIM-CNR.
http://biomintec.ibim.cnr.it/images/stories/book_abstracts.pdf

General rights

It is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), other than for strictly personal, individual use, unless the work is under an open content license (like Creative Commons).

Disclaimer/Complaints regulations

If you believe that digital publication of certain material infringes any of your rights or (privacy) interests, please let the Library know, stating your reasons. In case of a legitimate complaint, the Library will make the material inaccessible and/or remove it from the website. Please Ask the Library: <https://uba.uva.nl/en/contact>, or a letter to: Library of the University of Amsterdam, Secretariat, Singel 425, 1012 WP Amsterdam, The Netherlands. You will be contacted as soon as possible.

A particle-based model for aggregate formation in biomineralization

N. Javaheri, C. M. Cronemberger, J. Kaandorp

Section Computational Science, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands (N.Javaheri@uva.nl)

Biosilicification is a process in which meaningful behaviors happen in different temporal and spatial scales. Hence, one might consider different approaches depending which part of the dynamics is under scrutiny. In the kind of simulation that we are currently dealing with, the growth of spicules in sponges has been modeled from the beginning of the intracellular nucleation process. It simulates the interaction of inorganic-organic materials with the view of forming an aggregate of mineral nanoparticles on an organic matrix. It is based on DLA (Diffusion Limited Aggregation) in the first step and then a modification by adding a Poisson equation to describe the interaction of acidic sites of proteins with charged particles. The boundaries of the 3D simulation box have cylindrical symmetry, which has been chosen based on the simplified geometry of the organic matrix. This approach describes the general behavior of silica deposition, but could contain more parameters, both physical and protein-based, in order to produce more realistic results in comparison with growth of real spicules.