Abstract Submitted
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Modeling of fractal intermediates in the self-assembly of silicatein filaments[1] MEREDITH MURR, UCSB, GUNJAN THAKUR, UCSB, IGOR MEZIC, UCSB, DANIEL MORSE, UCSB — Silicateins are proteins with catalytic, structure-directing activity that are responsible for silica biosynthesis in certain sponges, Self-assembly of the silicatein monomers and oligomers was previously shown experimentally (Murr and Morse 2005) to form fibrous structures through the formation of diffusion limited, fractally patterned aggregates on the path to filament formation. We present a diffusion-limited aggregation (DLA) based model that is capable of capturing the basic properties of this self-assembly process. The Silicatein oligomer is modeled with three sites of attachment. Rules of attachment are specified that allow for specific interaction between these sites when oligomers are in proximity. The process differs from a DLA process in the following: 1) The process of aggregation is continued dynamically, i.e. the growing structures are spatially distributed and keep diffusing as they are growing 2) The molecules are oriented. Thus rotational diffusion is important. 3) The attachment can happen at more than 1 site and the strength of the active sites can be varied. We show that the self-assembled structures have a good level of similarity with the in-vitro experimental results. We quantify this by comparing the fractal dimension of the experimental data and the model output.

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