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Centric diatom morphogenesis: a model based on a DLA algorithm investigating the potential role of microtubules

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Abstract

Diatoms are single-celled algae which possess characteristic rigid cell walls (frustules) composed of amorphous silica. Frustule formation occurs within a specialised organelle termed the silica deposition vesicle (SDV). During diatom morphogenesis, silica particles are transported to the SDV by silica transport vesicles. Once released within the SDV, the particles are then thought to diffuse until they encounter part of the growing aggregate upon which they adhere. The particles may then undergo a further period of surface relocalisation (sintering) which leads to a smoothing of the surface. A number of computer simulations based on a modified diffusion-limited aggregation (DLA) algorithm, have been undertaken to investigate the potential role of microtubules (which are known to be associated with the periphery of the SDV) in localising deposition of new siliceous material. Based on our findings, we present a new model of diatom morphogenesis which is able to account for many morphological features of diatoms including the influence of environmental effects such as changes in pH and salinity, and the formation of a regular branched pattern. © 1999 Elsevier Science B.V. All rights reserved.

Keywords: Diatom; Morphogenesis; Diffusion-limited aggregation; Computer simulation; Microtubule

1. Introduction

Diatoms are single-celled eukaryotic algae responsible for about 25% of the world's net primary pro-

duction [1]. They possess a characteristically rigid cell wall (termed a frustule) composed of silica. Diatom frustules consist of two usually nearly identical halves (valves) which fit together like the bottom and cover of a petri-dish, enclosing the cell. There are currently estimated to be over 100 000 different species classified by their unique frustule morphologies [2]. Diatoms may be split into two main groups depending upon the symmetry of their frustules. Centric diatoms tend to be radially symmetric whilst pennate diatoms tend to be elongated and generally have parallel striae (furrows or rows of holes in the silica) arranged normal to the long axis.

Abbreviations: SDV, silica deposition vesicle; STV, silica transport vesicle; DLA, diffusion-limited aggregation; K , a tunable parameter used to represent surface tension; T , a tunable parameter relating to temperature; X , a tunable parameter used to represent surface mobility; R_{\max} , distance of the furthest point of the growing aggregate from its centre

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al, DLA algorithms cannot model the morphological stability of these structures with respect to subsequent ageing. Phenomena such as the sintering observed during diatom morphogenesis, require an investigation into the subsequent diffusion of accreted particles over the surface of the aggregate after adsorption. To account for this surface diffusion, the DLA algorithm must be modified to include terms that describe the behaviour of accreted particles. In this paper we describe a modified version of the basic DLA algorithm which includes these terms and focus on the qualitative consequences on the morphology. The results are displayed using morphology maps which can be readily interpreted in terms of experimental parameters and may therefore be used to predict the consequences of changes in growth conditions for diatom morphogenesis. In addition, the influence of microtubules postulated to be responsible for the localised deposition of new material [3] was also explored. Due to the relative flatness of the SDV (the initial thickness of the SDV is comparable to the diameter of the silica particles diffusing within it [3,18]), the model was simulated in two dimensions.

2. Materials and methods

All simulations were undertaken on a SGI Impact 10000 workstation running IRIX 6.5.3. Programs were written in the C programming language. The model was based on a 2000×2000 hexagonal lattice [19]. An initial nucleus consisting of 61 accreted particles arranged as a solid hexagon was placed at the centre of the lattice. During the growth of the aggregate, new particles were placed on a circular release template of radius $R_{max} + L$ (where R_{max} is the distance of the furthest point of the growing aggregate from its centre and L was a constant defined at the beginning of the simulation as a number ranging from 1 to 100). Although the initial placement of particles on the release template was random the perimeter, in some simulations, particles were placed at defined release sites (representing the termini of microtubules). After their initial placement, particles were allowed to move at random (diffuse) on the lattice. Note that we are assuming that particles involved in sintering are the same size as precipitating

The process of frustule formation is not well understood but is thought to involve the diffusion-limited precipitation of silica within a specialised or-ganelle termed the silica deposition vesicle (SDV) [3]. Amorphous silica particles of relatively low molecular mass (approximately 1–10 nm in diameter) are thought to be transported to the periphery of the SDV by silica transport vesicles (STVs) [4]. Once released inside the SDV, the particles presumably diffuse until they encounter part of the growing aggregate upon which they adhere. The surface of the particles is thought to consist mainly of silanol groups [5] ($=Si(OH)_2$ or $\equiv Si-OH$) which enable them to diffuse over the surface of the aggregate in a process termed sintering [3]. This surface migration allows the molecules to re-organise their positions towards a thermodynamic equilibrium, usually resulting in a smoothing of the aggregate surface. Growth of the frustule then proceeds by the further release of new material. Sintering is linked with the phenomenon of Oswald ripening [6] and appears to be dependent upon both pH and salt concentration [7,8] (for an explanation of Oswald ripening see Section 2). This may explain the changes in frustule morphologies observed when a single diatom species is grown under varying conditions [9–11]. After deposition and a period of surface relocalisation, the silica morphology becomes stabilised in a process which may involve a surface inorganic cation such as aluminium. Although little is known about how the silica is transported to the SDV, microtubules have been found to be associated with the lateral margins of the SDV and remain in association as the SDV increases in size (due to accumulation of STVs) [12]. The aim of this study was to attempt to simulate the process of frustule formation in order to further understand the roles of surface diffusion and microtubules in the generation of diatom morphology.

Previous attempts at modelling frustule formation have involved the use of computer simulation of diffusion-limited aggregation (DLA) [3,13]. DLA has been used in a number of studies to model a range of diverse growth phenomena including snowflake formation [14,15], electrolytic deposition [16] and the creation of drainage networks [17]. The complex shapes obtained from these models are typical of out-of-equilibrium growth processes. However, in gener-

