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Zhao, Y., Billings, S.A. and Coca, D. (2008) A cellular automata modelling of dendritic crystal growth based on Moore and von Neumann neighbourhood. Research Report. ACSE Research Report no. 984 . Automatic Control and Systems Engineering, University of Sheffield

A Cellular Automata Modelling of Dendritic Crystal Growth based on Moore and von Neumann Neighbourhood

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Research Report No. 984

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August, 2008

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September 1, 2008

Abstract

An important step in understanding crystal growth patterns involves simulation of the growth processes using mathematical models. In this paper some commonly used models in this area are reviewed, and a new simulation model of dendritic crystal growth based on the *Moore* and *von Neumann* neighbourhoods in cellular automata models are introduced. Simulation examples are employed to find appropriate parameter configurations to generate dendritic crystal growth patterns. Based on these new modelling results the relationship between tip growth speed and the parameters of the model are investigated.

1 Introduction

Crystal growth, is one of the most fascinating natural phenomena in pattern formation, and has attracted considerable theoretical and experimental efforts in an attempt to develop a better understanding of the growth processes that are controlled by the environment conditions and the materials. Most studies aim to describe such complex patterns by extremely simple models, but it is always a challenge to determine mathematical representations directly from experimental data. Therefore, most investigations adopt an almost opposite approach, which involves simulation of crystal growth dynamics using postulated simple models. Components of such models may have no relationship

with the real system, but the acceptance criterion is that patterns from the model simulation and the real system have a high degree of similarity.

The results in this study focus on exploring the underlying relationship between the dynamic characteristics of crystal growth and the corresponding environmental conditions, particularly for dendritic crystals. For instance, it is well known that the cooling temperature plays an important role during crystal growth processes from a supersaturating solution, but few people know how to achieve a quantitive description of crystal shape and size by temperature. It is always a big challenge to generate a model relating physical variables and system outputs directly from real data, because it is often uncertain how many and which physical variables are involved. Moreover, any slight noise in one environmental variable may significantly affect the output of system. This can cause an *ill-posed* problem which makes identification very difficult. However, if such problems are solved, this will lead to important new insights into crystal growth processes. System identification of growth patterns is a potentially important tool for unravelling the complex relationships between these patterns and the system control variables. Ideally, it should be possible to predict the crystal form from a knowledge of the environment variables.

In this paper several commonly used simulation models for crystal growth are reviewed and their application, the advantages and disadvantages are discussed. A new model based on the *Moore* and *von Neumann* neighbourhoods in a cellular automata (CA) model is then introduced and several examples are discussed.

The paper is organized as follows. An overview of simulation models and discussion are presented in Sec. 2. Section 3 introduces the new CA model. Examples and an analysis of growth speed are discussed in Sec. 4. Finally, conclusions are given in Sec. 5.

2 Overviews of Current Models

A wide range of mathematical models have been developed to simulate the growth dynamics of crystals [P.Meakin, 2002]. This section describes some fundamental and important models, which have contributed to our understanding of problems in many areas of science and technology.

2.1 The Eden Model

The Eden Model, simulation of which can be carried out on almost all lattice types, was initially developed to investigate the growth of biological cell colonies [Eden, 1956a,b]. At the start of simulation of the basic Eden Model, one site or cell is selected and "filled". An occupied site on the perimeter of the cluster of filled sites is selected randomly, with equal probabilities, and one of its nearest-neighbour unoccupied perimeter sites is then selected randomly and filled to represent the growth process. This process can be repeated many times to generate a sufficiently large cluster. Many variations of the basic Eden growth model have been developed and investigated for application in physics, biomedical systems etc. [T.Williams and R.Rjerknes, 1972, P.Meakin, 1983, 1987, 1988].

2.2 The Diffusion-Limited Aggregation Model

The Diffusion-Limited Aggregation (DLA) Model [Witten and Sander, 1981, 1983] still attracts a high level interest even though it was presented 25 years ago, and is one of the most striking examples of pattern generation of fractals generated by a simple model and algorithm. The DLA model has been applied to a wide range of applications in both the physical and biological sciences as well as applications in other areas [M.Batty, 1991, Chang and Kan, 2007, Masters, 2004].

In the original DLA model, "particles", represented by lattice sites, are added, one at a time, to a growing cluster or aggregate of particles via random walk paths starting outside the region occupied by the cluster. Normally, a simulation is started by occupying a site in the center of a square or triangular lattice to represent the "seed". A site far from the cluster is then selected, and a random walk is started from the selected site. If the random walker moves too far from the growing cluster, it is terminated and a new random walk is started. If the random walker eventually reaches a site that is the nearest neighbour to a previously occupied site, the random walk is stopped and the unoccupied perimeter site is filled to represent the growth process. The process of launching random walkers from outside the region occupied by the growing cluster and terminating them when they wander too far from the cluster or "stick" to the growing cluster by reaching an unoccupied perimeter site is repeated many times to simulate the cluster growth process.

2.3 Phase Field Model

The model [R.Kobayashi, 1993] introduced here is a kind of phase field model in which the interface between the liquid and solid has a finite thickness although it is very thin and is expressed as a steep interval layer of a phase indicating function. The model includes two variables: one is a phase field $p(r,t)$ and the other is a temperature field $T(r,t)$. The variable $p(r,t)$ is an ordering parameter at the position r and time t, where $p=0$ indicates a liquid and $p=1$ indicates a solid.

The evolution rule of this model can be expressed as:

$$\tau\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}(\varepsilon\varepsilon'\frac{\partial p}{\partial y}) + \frac{\partial}{\partial y}(\varepsilon\varepsilon'\frac{\partial p}{\partial x}) + \nabla\cdot(\varepsilon^2\nabla p) + p(1-p)(p-\tfrac{1}{2}+m) \tag{1}$$

$$m(T) = (\alpha/\pi)tan^{-1}[\gamma(T_e - T)] \tag{2}$$

$$\frac{\partial T}{\partial t} = \nabla^2 T + K\frac{\partial p}{\partial t} \tag{3}$$

where ε is a small parameter which determines the thickness of the layer, T_e is an equilibrium temperature, and α, γ and K are constant variables. Various configurations of these parameters may produce significantly different dendritical crystals.

2.4 Boolean Model for Snowflake Growth

Wolfram proposed a Boolean model in cellular automata for snowflake growth [S.A.Wolfram, 2002] that evolves on a hexagonal lattice by the following rule. There are two states for each cell: ice or water. If the considered cell at time step t is ice, the state of this cell at time step $t+1$ remains ice. If the considered cell at time step t is water, the state of this cell at time step $t+1$ will be ice if and only if exactly one of its neighbourhood is ice.

2.5 Discussion

The Eden Model is easy to implement in simulation and is now quite well understood from a theoretical point of view, but it can not generate dendritic crystal growth patterns. The DLA Model is very time consuming and far from satisfactorily understood, but it is used as a basis of understanding many growing patterns because it can produce much more complex behaviors to simulate real systems. However, both models can not be identified directly from experiment data, as random walks are a core component of the

model which means no deterministic models can represent them.

The Phase Field Model can generate dendritical crystal patterns and important physical mechanisms, such as curvature, anisotropy and kinetic effects are implicitly incorporated, but equations of this model are very difficult to solve, and it is almost impossible to identify such a PDE model directly from experimental data.

Wolfram's Boolean Model provides examples of abstract plates and sectors, which offers the possibility that cellular automata can generate behavior surprisingly similar to a kind of snowflake growth, and such a simple model can also be used in identification, but it does not provide global dendrite or stellar growth as each cell can only take on two values 0 or 1.

3 A New Model

In this section a new method is proposed to simulate dendritic crystal growth processes using a cellular automata model with a *Moore* or a *von Neumann* neighbourhood. Before descriping the new model, some background information on cellular automata will be introduced.

A cellular automata is composed of three parts: a neighbourhood, a local transition rule and a discrete lattice structure. The local transition rule updates all cells synchronously by assigning to each cell, at a given step, a value that depends only on the neighbourhood. In Wolfram's CA world [S.A.Wolfram, 2002], the state of each cell can only take two values: 0 or 1, which is the reason that the CA's studied are called *binary CA*. However, in the new model the state of each cell can take any real value between 0 and 1, which indicates that this model can generate much more complex behaviors than binary CA [Adamatzky, 1994, 2001].

Similar to the method used to describe excitable media using a cellular automata model [Zhao et al., 2007a,b], the proposed model divides the state of each cell into three states: *solid*, *near-solid* and *solution*. If the cell value is equal to 1, the cell denotes a *solid*. If the cell value is less than 1 and its neighbourhood has at least one *solid* cell, the cell is denoted as a *near-solid*, otherwise the cell is denoted as a *solution*. The cell value $c(r,t)(0 \leq c(r,t) \leq 1)$ can be viewed as a local concentration of solution of the considered cell, where r denotes position and t denotes the time step.

At the beginning of the simulation, each cell in the lattice is assigned the same initial value I_0. From a chemical point of view, this means that the material is dissolved in water with a specific concentration. A seed or seeds can be selected randomly as a *solid* at the beginning of the growth. The neighbourhood chosen in the present study is a *Moore* or a *von Neumann* neighbourhood, both of which belong to the square lattice type. If the status of the considered cell $c(r,t)$ is a *solid*, the value at time $t+1$ remains as 1. If $c(r,t)$ is a *near-solid*, $c(r,t+1)$, the value at time $t+1$, would be $c(r,t)$ plus a constant β plus a diffusion term $d(r,t)$. If $c(r,t)$ is a *solution*, the value of $c(r,t+1)$ would be $c(r,t)$ plus a diffusion term $d(r,t)$ without β. The diffusion term is a local weighted average of its neighbourhood by setting all *solid* and *near-solid* cells to zero. The motivation of this model is that particles in *solid* and *near-solid* states are permanently stored in the cell, and particles in *solution* move toward an average value following the concentration difference.

Consider a cell $c(r,t)$ at position r and time step t with the *Moore* neighbourhood. The value at the next time step $c(r,t+1)$ can then be described by the following CA rule.

$$c(r,t+1) = \begin{cases} 1 & c(r,t) \text{ is a } \textit{solid} \\ c(r,t) + \beta + \frac{\alpha}{16}(-8c(r,t) + \sum_{i \in P_{c(r,t)}} c(P,t)) & c(r,t) \text{ is a } \textit{near-solid} \\ c(r,t) + \frac{\alpha}{16}(-8c(r,t) + \sum_{i \in P_{c(r,t)}} c(P,t)) & c(r,t) \text{ is a } \textit{solution} \end{cases} \quad (4)$$

where $P_{c(r,t)}$ denotes the set of the neighbourhood of $c(r,t)$ only when the status is a *solution*. The symbol α is the weight of diffusion, which is normally taken as 1. If the neighbourhood is *von Neumann* structure, the model can be revised as:

$$c(r,t+1) = \begin{cases} 1 & c(r,t) \text{ is a } \textit{solid} \\ c(r,t) + \beta + \frac{\alpha}{8}(-4c(r,t) + \sum_{i \in P_{c(r,t)}} c(P,t)) & c(r,t) \text{ is a } \textit{near-solid} \\ c(r,t) + \frac{\alpha}{8}(-4c(r,t) + \sum_{i \in P_{c(r,t)}} c(P,t)) & c(r,t) \text{ is a } \textit{solution} \end{cases} \quad (5)$$

Five parameters are variable in this model: the lattice type, neighbourhood, initial value I_0, constant addition β and diffusion weight α. The influence of each parameter on the generated patterns will be discussed in the next section.

4 Examples and Discussion

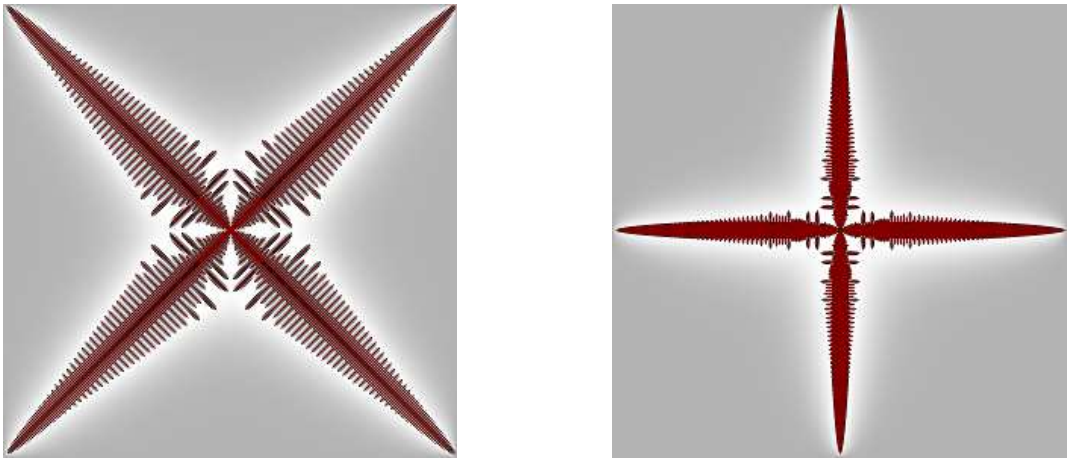
In this section, many simulation examples are employed to reveal various types of formations of dendritic patterns by varying the configuration of the model parameters. All

the patterns were generated on 300 by 300 square lattices. Simulation starts from a *seed* chosen at the center of the pattern, and grows following the rules in Equ.4 or Equ.5 until a *solid* cell approaches the boundary or the iteration time reaches 5000. In the patterns, dark pixels denote the cells close to 1 and light pixels close to 0. The *solid* cells are highlighted by the red colour.

Normally, the selection of the lattice type depends on the characteristics of the objective form. For instance, to simulate ice growth, a hexagonal lattice would be used[S.A.Wolfram, 2002, C.A.Reiter, 2005], or a more complicated type of *Quasicrystalline* structure [Chidyagwai and Reiter, 2005]. A square lattice is the most commonly used type because of its easy implementation and because it is well understood. This paper will only consider the square lattice.

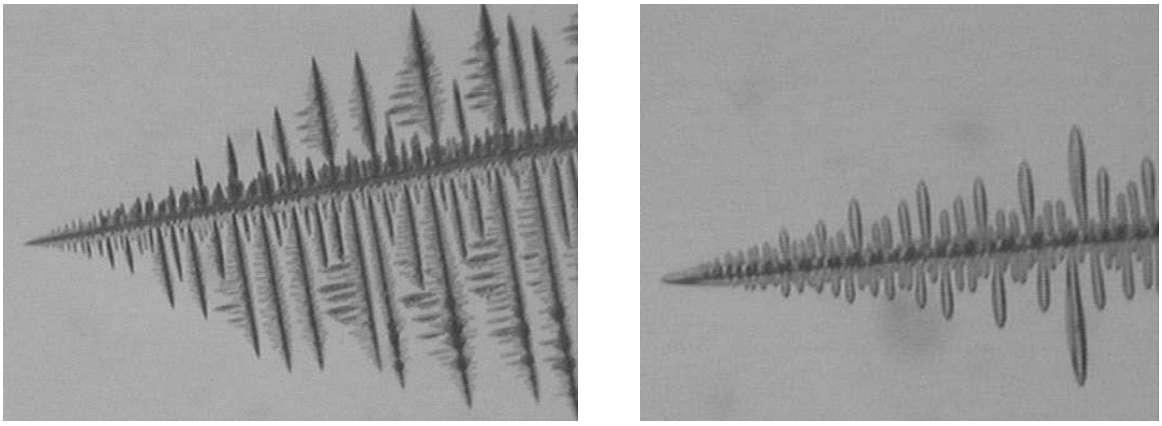
Neighbourhood selection is one of the most important steps in CA modelling and identification [Zhao and Billingse, 2006]. Figure 1 shows two patterns generated under the *Moore* and *von Neumann* neighbourhoods respectively by setting $I_0 = 0.3$, $\beta = 0.0001$ and $\alpha = 1$. Both patterns demonstrate typical dendritic crystals. The stem in the pattern with a *von Neumann* neighbourhood has a Greek-cross structure, but the stem with a *Moore* neighbourhood has a St.Andrew's cross structure, which illustrates that the skeleton of the simulated crystal depends on the structure of the selected neighbourhood. Figure 2 shows two snapshots of a crystal obtained from a NH_4Br solidification experiment. There is a high degree of visual similarity between the simulation and the real pattern suggesting that the proposed model has encouraging potential to represent this interesting phenomena.

Figure 3 shows a group of patterns generated by varying the initial value I_0 and constant addition β and fixing the *Moore* neighbourhood and $\alpha = 1$. The patterns clearly show that when $\beta \geq 0.005$, the crystals are on a plate form regardless of the value of I_0, and $\beta < 0.005$ and $I_0 \leq 0.03$ give rise to dendritic crystals. In Figure 1.(a), secondary dendrites and even tertiary dendrites are visible. It is predictable that if the growth space and time are large enough, higher order dendrites will appear. Moreover, space between adjacent secondary dendrites tends to decrease for increasing β. When $\beta = 0.005$, secondary dendrites almost disappear. Figure 3.(a),(f),(k),(p) also show that the length of the secondary dendrites increases following the increment of I_0 with the same β. When $I_0 > 0.03$ sector forms appear again because secondary dendrites are so long that they



(a) (b)

Figure 1: Growth forms on different neighbourhoods by setting $I_0 = 0.3$, $\beta = 0.0001$ and $\alpha = 1$. (a) Moore; (b) von Numann



(a) (b)

Figure 2: Snapshots from a crystal growth experiment using NH_4Br.

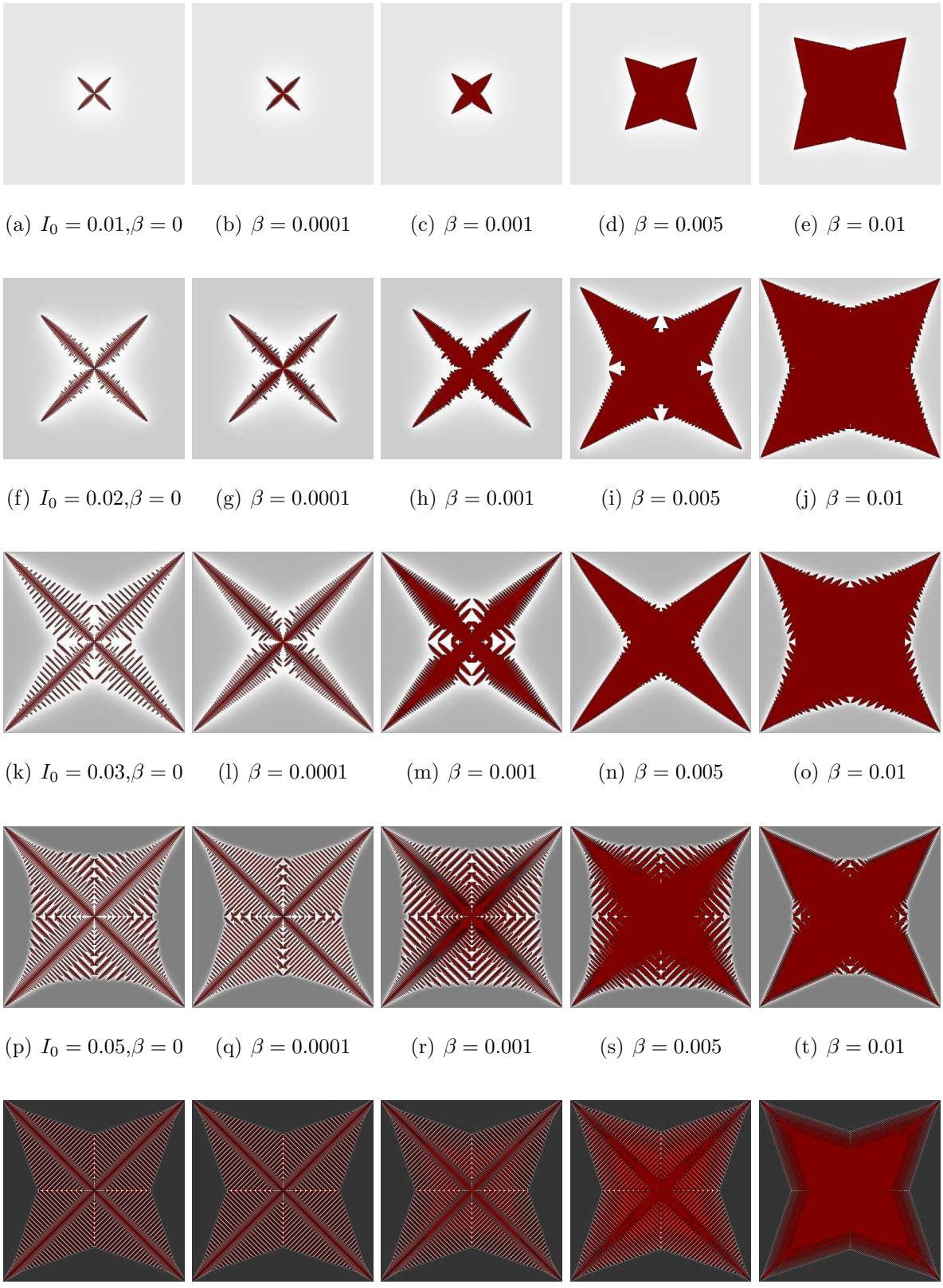
touch together.

It can also be seen from Figure 3 that the growth speed of the crystals varies from different initial values and constant additions. When β and I_0 are both small the growth is very slow, but when both of them are large, the growth is fast. To quantitatively investigate the relationship between these factors, average tip growth speed was measured and employed in this section. The average tip speed is defined as the Euclidean distance from final tip position to the center(the position of the initial seed) divided by the elapsed time step. Many examples were implemented to establish that the tip growth speed is almost stable during the evolution when all parameters are fixed. Figure 4 shows tip speed values over time for three examples. Although a slight oscillation occurs in each example, the trend-lines are almost horizonal, which indicates tip speed can be represented by *average tip speed* introduced here. Note the patterns generated are 4-fold symmetrical, hence, only the tip of one of four branches was considered. Figure 5.(a) shows the trend of averaged tip speed following increments in I_0 with fixed β, and Figure 5.(b) shows the trend by varying β and fixing I_0. Figure 5 illustrates tip growth speed is nearly linear with β and nearly parabolic to I_0.

To study the effectiveness from diffusion weight α to crystal dendrite forms, many patterns were generated by changing α from 0.6 to 2 when $I_0 = 0.3, \beta = 0.0001$, and these are shown in Figure 6. Figure 7 shows the tip speed trend following the increments of α. There is no remarkable rule connecting dendrite length and space between dendrites with respect to α, but Figure 7 clearly indicates tip growth speed is nearly linear with respect to α.

5 Conclusions

A new simulation model of dendritic crystal growth based on the *Moore* and *von Neumann* neighbourhoods in a cellular automata type model has been introduced. In the new model, each cell in the lattice can take any real value between 0 and 1 rather than just binary values, which indicates more complex behaviors can be generated than traditional CA. By defining the state of each cell into three status, the transition rule can be described in a polynomial form, as shown in Equ.4, which has the potential to be understood from a chemical point of view. Simulation results show this model can gen-



(a) $I_0 = 0.01, \beta = 0$ (b) $\beta = 0.0001$ (c) $\beta = 0.001$ (d) $\beta = 0.005$ (e) $\beta = 0.01$

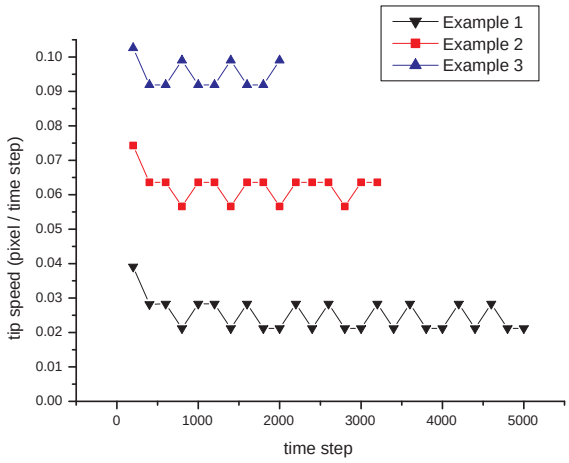
(f) $I_0 = 0.02, \beta = 0$ (g) $\beta = 0.0001$ (h) $\beta = 0.001$ (i) $\beta = 0.005$ (j) $\beta = 0.01$

(k) $I_0 = 0.03, \beta = 0$ (l) $\beta = 0.0001$ (m) $\beta = 0.001$ (n) $\beta = 0.005$ (o) $\beta = 0.01$

(p) $I_0 = 0.05, \beta = 0$ (q) $\beta = 0.0001$ (r) $\beta = 0.001$ (s) $\beta = 0.005$ (t) $\beta = 0.01$

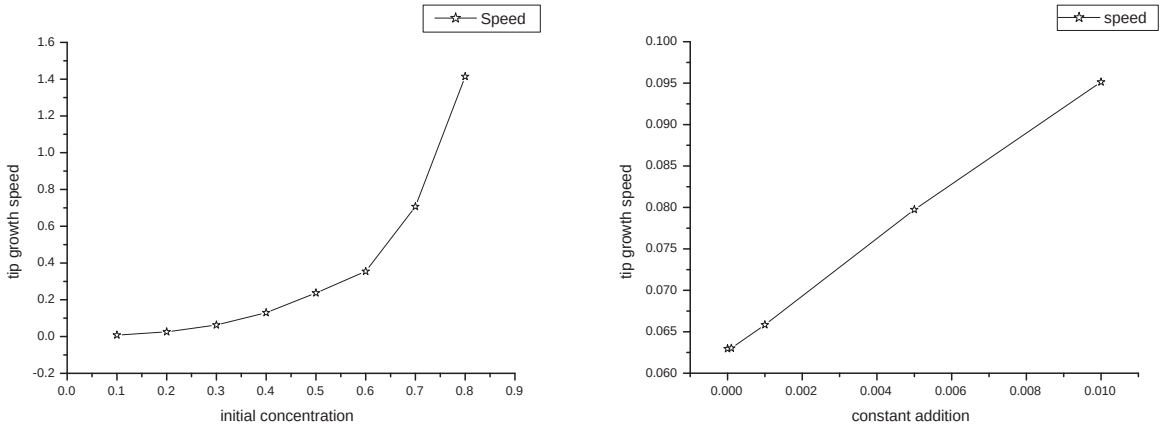
(u) $I_0 = 0.08, \beta = 0$ (v) $\beta = 0.0001$ (w) $\beta = 0.001$ (x) $\beta = 0.005$ (y) $\beta = 0.01$

Figure 3: Growth forms on different initial values I_0 and constant addition β with a *Moore* neighbourhood and $\alpha = 1$.



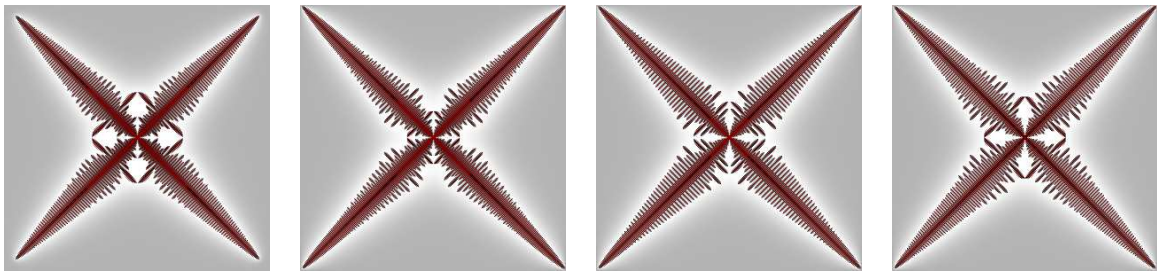
(a)

Figure 4: Trend of tip growth speed by time of three examples. Example 1: $\beta = 0.0001, \alpha = 1, I_0 = 0.35$; Example 2: $\beta = 0.0001, \alpha = 1, I_0 = 0.3$;Example 3: $\beta = 0.0001, \alpha = 1, I_0 = 0.2$;

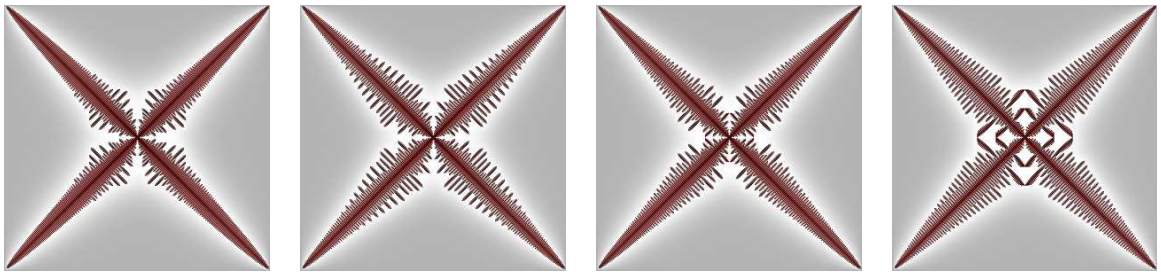


(a) (b)

Figure 5: (a)Trend of tip growth speed following increments of I_0 with $\beta = 0.0001, \alpha = 1$; (b) Trend of tip growth speed following increments of β with $I_0 = 0.3, \alpha = 1$.

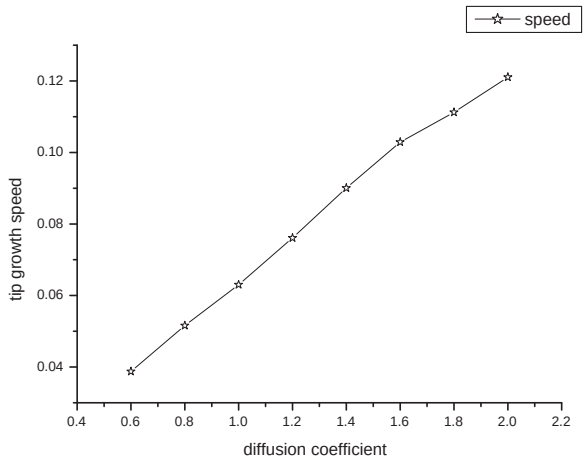


(a) $\alpha = 0.6$ (b) $\alpha = 0.8$ (c) $\alpha = 1.0$ (d) $\alpha = 1.2$



(e) $\alpha = 1.4$ (f) $\alpha = 1.6$ (g) $\alpha = 1.8$ (h) $\alpha = 2.0$

Figure 6: Growth forms for different diffusion coefficients α, and fixed I_0 and β.



(a)

Figure 7: Trend of tip growth speed following increments of α with $I_0 = 0.3, \beta = 0.0001$.

erate typical dendritic crystal patterns that are very close to real data from experiments by setting the appropriate model parameters. Normally, the neighbourhood is chosen as a *Moore* neighbourhood with $0 < I_0 \leq 0.03$ and $\beta < 0.005$, and the results also show that the diffusion weight α does not significantly affect the crystal form, but does affect growth speed.

As a very important parameter in studying crystal growth, tip growth speeds were measured and analysed under different I_0, β, α. Results show β and α are nearly linear with respect to speed, and I_0 is nearly parabolic with respect to speed. Cooling temperature and the initial concentration of the solution will also have a significant effect on the speed of crystal growth and other characteristics of the dendritic form. In future research, studies the relationship between I_0, β, α and speed will be studied to further investigate the impact of these characteristics on dendritic crystal growth from physically controlled system variables.

Acknowledgment

The authors gratefully acknowledge that part of this work was financed by Engineering and Physical Sciences Research Council(EPSRC), UK.

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