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Modeling of Fractal Growth by Simulation

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Abstract: ***In the present work deals with the simulation of fractal growth patterns in electrodeposition (Diffusion limited aggregation) using concept of off lattice random walk.The simulation of electrodeposition under different electric field conditions is implemented to simulate the growth of dendritic patterns in circular cell geometry. The DLA growth in circular cell geometry is under the influence of two main driving forces, namely, the random Brownian motion of the ions and the radial ionic motion due to the applied electric field. In the simulation, the effect of radial movement of ions is superimposed over the zigzag random motion of the ions in the electrolyte. The relative influence of the random motion and radial motion is controlled by introducing a biasing parameter. It is observed that the growth patterns with lower values of bias (corresponding to lower electric field) are less crowded with limited branching and more closely resemble true DLA. As the electric field is increased (higher value of B), the growth tends to be dense and with more crowding of branches. The box counting technique was implemented to calculate the fractal dimensions of the patterns developed. The results are compared with the experimental observations.***

Keywords: Fractal, Fractal Dimension, Simulation, electrodeposition.

I. INTRODUCTION

The concept of fractal[1] has attracted the interest of scientist's form various discipline during the last decade. The complex structures/shapes studied include a broad variety of systems that span through the interdisciplinary spectrum of modern research including Life sciences /biology, chemical sciences/chemistry as well as materials sciences, computer science, image compression and geology etc. In the field of physical chemistry / heterogeneous chemistry, fractals have been observed in growth processes called as electrodeposition (Diffusion Limited Aggregation)[2]. Aggregation is one of the most familiar phenomena in physical and chemical processes. The first 'aggregation' model is based on joining the randomly walking particles to a growing cluster or nucleus. In practice aggregation process is more complex and the resulting deposits exhibit a variety of complex structures which usually exhibit statistically simple, self-similar, i.e. fractal structures [3]. Growth of many clusters in nature generate fractal patterns by a process called aggregation, crystals formed during such a growth have fractal appearance [4]. Here one particle after another, during a random walk, comes in contact and sticks to a cluster which remains fixed at a place. If these particles diffuse towards the growing cluster during random walks, the resulting process is known as Witten and Sander's diffusion-limited aggregation[5].

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Many growth processes in nature are described by the diffusion equation, which under some approximations becomes equivalent to the Laplace equation. The parameters involved are the sticking probability, pressure, temperature or electric potential and depending on the physical processes governing such processes. Solidification [6, 7] (snowflakes) and dielectric breakdown (lightening) [8] are such examples.

We present here the simulation of DLA (Diffusion Limited Aggregation) [9, 10, 11], in circular electrodeposition cell geometry, under different conditions. In this simulation, first a seed particle is placed at an origin, at the center of a circular anode. Then, one at a time, random walkers are released from the circular anode at some randomly selected location. This particle (metal ion) is allowed to undergo random walk according to the conditions imposed by the applied electric field and physical conditions in the deposition cell. When one of these particles makes contact with the aggregate (or nucleus for the first particle), the particle sticks there and a next particle is released. Cyclic boundary conditions are used i.e. when a particle reaches the outer circular anode, it is released again from the diametrically opposite point on the circular anode. The process continues till the specified number of particles are exhausted and a pattern is formed.

II. SIMULATION OF DLA USING OFF LATTICE WALK

We used the concept of off lattice walk [12] to simulate the electrodeposition [13] in which a cathode is at the center of a circular anode. The concept of 'off lattice walk' is essential as the particle is made to move partly in the random direction and partly in a specified field direction. A consequence of this fact is that the particle is not always on the grid or lattice during the course of movement. For most of the work presented, a square grid (lattice) is taken and the origin is considered to be the center of this grid. Initially a seed is placed at the origin (the cathode). Particles are released from circumference of a circle (anode) around this origin. The growth process is under the influence of a radial electric field (superimposed on random motion due to thermal agitation) [14, 15, 16] driving the particles towards the center of the circle (cathode).

The particle is allowed to move one step at a time. One step consists of two components, the random motion and the directional radial movement towards the cathode. The simulation logic has provision to select desirable proportion of the two components. As an example, if the probability of radial movement is one part in five as compared to the random motion, the same can be described as 1 : 5 or 0.2. This parameter is called the radial bias (B). If the value of the bias is chosen 0.1 it means that the movement is such that the chance of radial movement as compared to the random motion is one part in ten. Thus this variable controls the relative strength of the radial and random movement in every step.

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During simulation, in every step the particle moves a distance equal to (1 – B) step in a random direction and a distance equal to B in the radial direction towards the cathode. This means that the particle is not always present on one of the lattice sites available, but can walk in between the lattice points. As soon as the particle reaches a point where the neighbouring site is occupied by some particle, the particle is allowed to stick. If there is no neighbouring particle present, the particle is allowed to make the next move of one step. This continues till it reaches a point with a neighbouring occupied site, it is allowed to stick and the size of the growth increases by one particle. In the event of the particle moving to a lattice site at or outside the anode (outer circle), a fresh particle is released from anode to continue the walk.

[There are three possibilities of interest in such a case. i) To release the particle from a place where the particle crosses the region ii) To release a particle on the circumference of the circle from a randomly chosen place and iii) To release the particle from a point on the circle diametrically opposite to the place where the particle crosses the region. The third condition is called 'cyclic boundary condition' and is more realistic for continuous media. During the simulation of the electrodeposition we recorded the number of steps (time) required by each particle to stick to the growth, starting from the outer circle. It is observed that the time required by the particles to stick also exhibits characters of random time series [17, 18].

Figure 1 shows a typical simulation pattern using low bias (B = 0.001), the four stages are after deposition of 300, 500, 1000 and 1500 particles. The resulting patterns are open structures with fewer branches with less crowding. Figure 2 (a, b, c and d) shows the results of box counting in the form of plot of log (N) against log(r). Plots 2 (a, b, c and d) are for the four stages of growth. Points in the figure indicate the actual data points obtained from the simulation and the straight line joining the points is the least square fit straight line for the points. Slope of the straight line gives the fractal dimension of the deposit. Table.1 gives the comparison of the estimated fractal dimensions at various stages of growth described above. It is seen that the fractal dimension approaches 1.41.

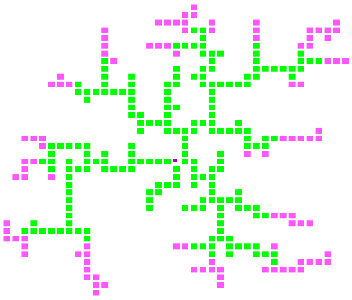

Figure 1(a- d) Showing four stages of simulation pattern for low bias

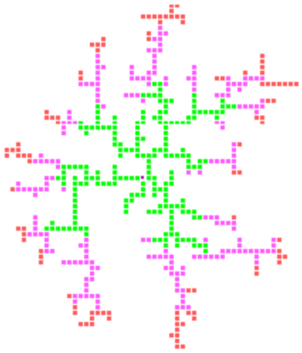

Fig a) Stage 1 Number of Particles deposited 300 B=0.001

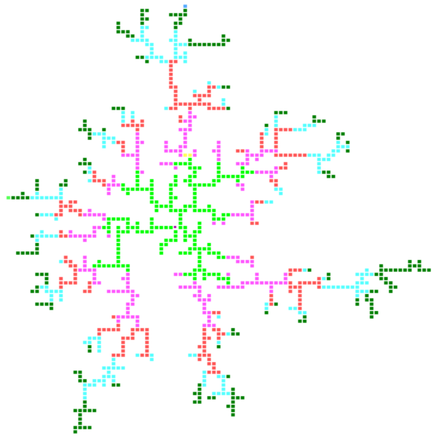

Fig b) Stage 2 Number of Particles deposited 500 B=0.001

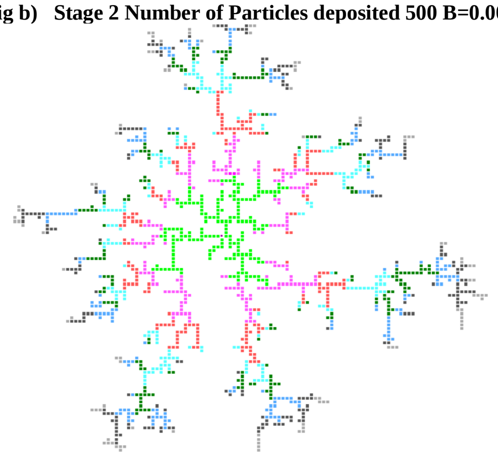

Fig c) Stage 3 Number of particles deposited 1000 B=0.001

Fig d) Stage 4 Number of Particles deposited 1500 B=0.001 Plot for four stage of simulation Pattern for B = 0.001

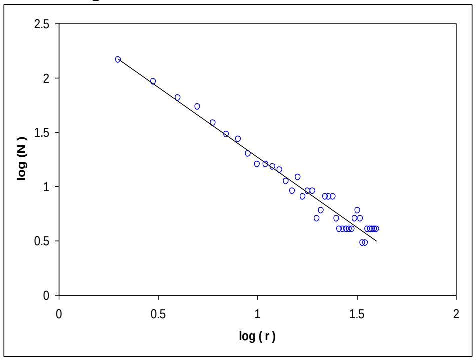

Fig 2 a Plot of box counting of first stage of simulation for B=0.001

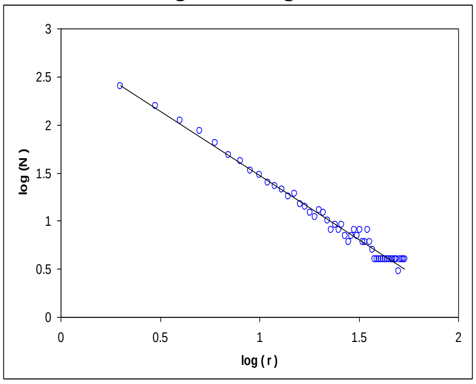

Fig 2 b Plot of box counting of second stage of simulation for B=0.001

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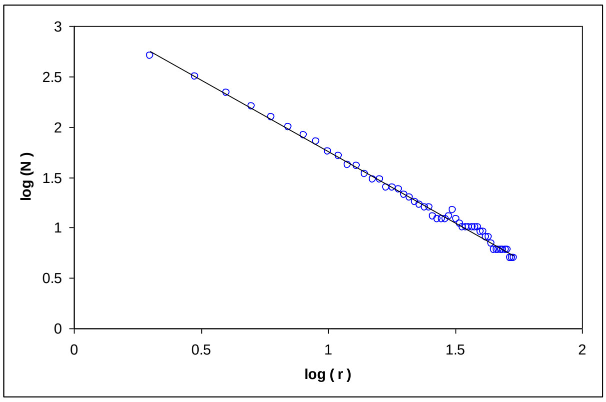

Fig 2 c Plot of box counting of third stage of simulation for B=0.001

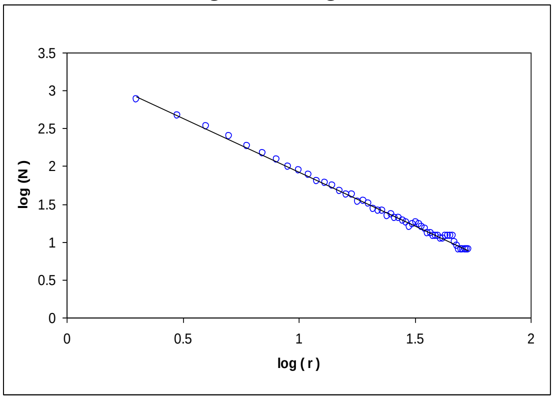

Fig 2 d Plot of box counting of fourth stage of simulation for B=0.001

Table 1 Gives the comparison of the estimated fractal dimensions at various stages of growth described in fig .7 [a –d]

Table 1

Sr. No	Stage of Growth	Fractal Dimension	Number of particles Attached
1	First stage	1.28	300
2	Second stage	1.32	500
3	Third stage	1.41	1000
4	Fourth stage	1.41	1500

III. SIMULATION OF THE EFFECT OF CELL VOLTAGE

The simulation of electrodeposition can be simplified as the combined effect of two competing process i.e. random Brownian motion due to thermal agitation and a central motion of ions due to the applied electric field. The relative proportion of the two is controlled by the bias parameter B. An increase in the value of B corresponds to a higher value of applied voltage to the cell or the electric field. It is observed that the growth patterns simulated under lower electric field conditions (lower values of B) appear to be more open structures with fewer or limited branching, having lower fractal dimension. Whereas the patterns obtained at higher values of B exhibit dense and crowded branching and the fractal dimension of the simulated growth is on the higher side indicating excess complexity of shape associated with the pattern.

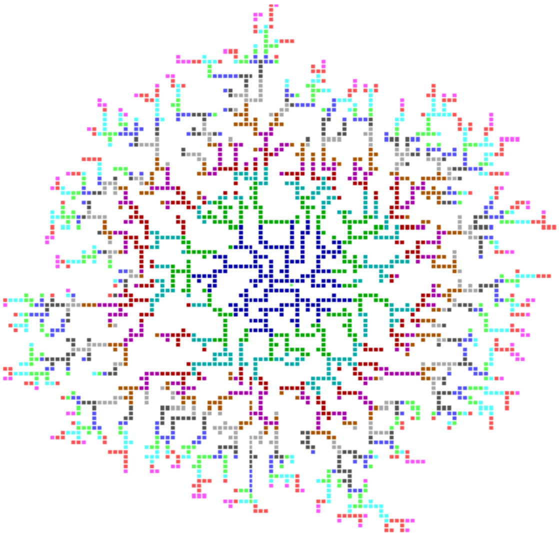
Fig 3 Simulation of electrodeposition for B = 0.05

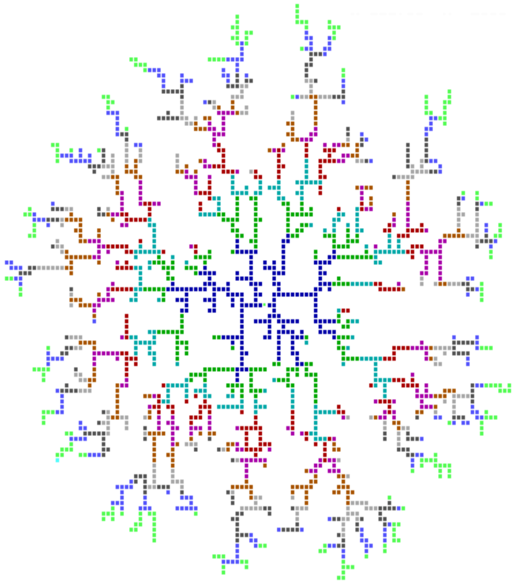
Fig 4 Simulation of electrodeposition for B = 0.1

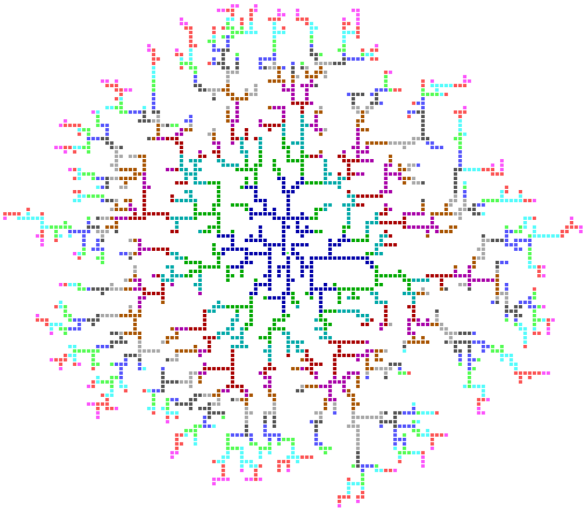
Fig 5 Simulation of electrodeposition for B = 0.25

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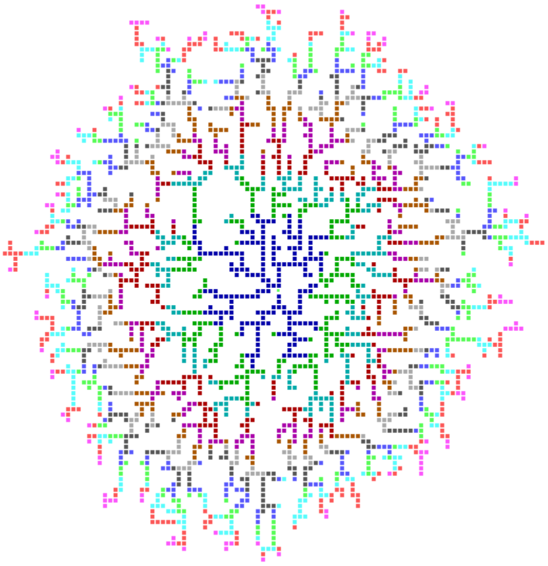

Fig 6 Simulation of electrodeposition for B = 0.3

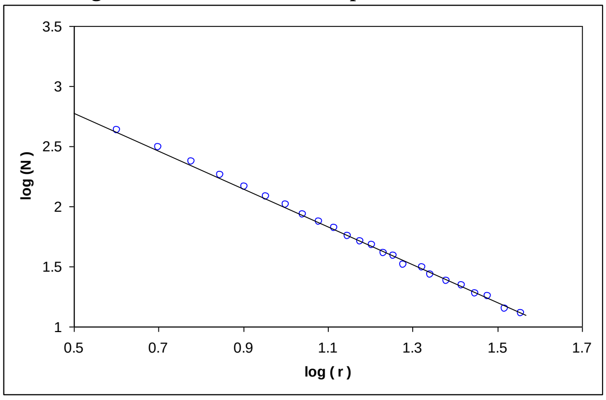

Fig 7 Plot of log (N) against log (r) for bias B=0.05

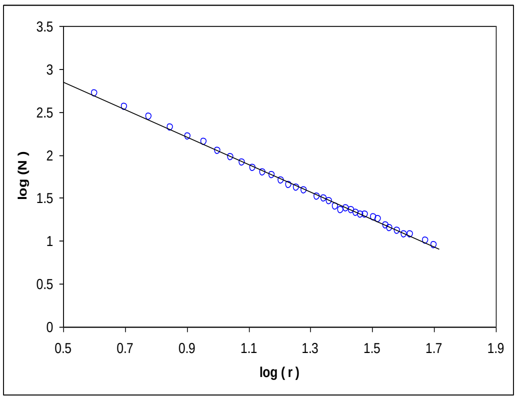

Fig 8 Plot of log (N) against log (r) for bias B=0.1

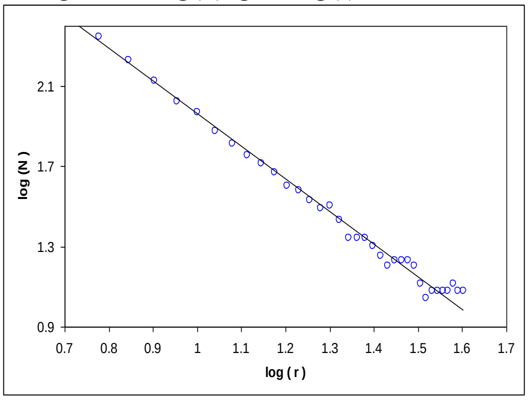

Fig 9 Plot of log (N) against log (r) for bias B=0.25

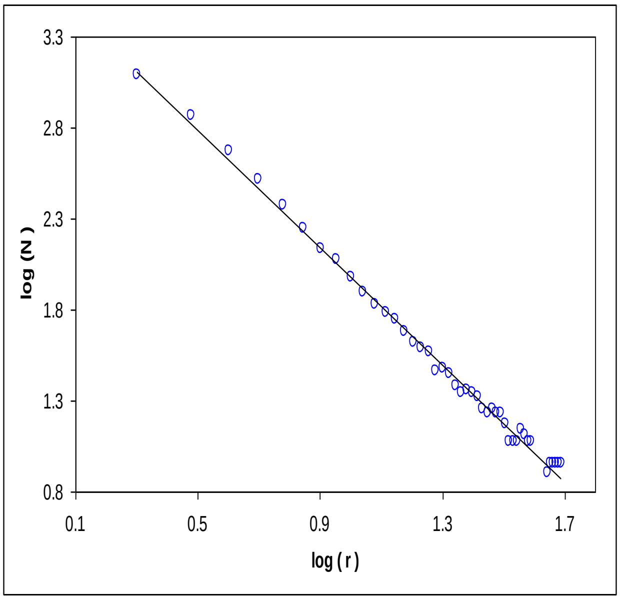

Fig 10 Plot of log (N) against log (r) for bias B=0.3

Figures 3, 4, 5 and 6 are the simulation of electro deposition under increasing electric field conditions with a value of B = 0.05, 0.1, 0.25 and 0.3 respectively. It is clearly seen from the figures that the growth patterns under lower values of B are less crowded with limited branching. As the electric field is increased (higher value of B), the growth tends to be dense and with more crowded branching. This is in agreement with the experimental observations of electrodeposition in circular cell geometry using different cell operating voltages.

Box counting was implemented to fully grown patterns of all the four cased described above and the results are presented in Figures 7, 8, 9 and 10 as a plot of log (N) versus log(r). Points in the plot are the actual data points from the box counting of simulated pattern and the straight line joining the points is the least square fit to these points. Fractal dimension of the deposit (simulated pattern) is obtained from the slope of the straight line.

It is seen from figures 3-10 that the complexity of the shape of growth patterns increases with an increase in the electric field or the value of 'B'. Also an increase in applied cell voltage or increase in value of bias 'B' results in an increase in value of the value of 'D' the fractal dimension indicating the increased complexity of the structure and texture of the simulated electrodeposit. Table 2 shows a comparison of the values of fractal dimensions estimated from the box counting of the simulated patterns of figure 3-6. The simulated growth pattern for lower value of bias (B = 0.001) i.e. Figure 1 can be compared with actual electrodeposition under low cell voltage conditions. Similarly comparison of Figure 3 and actual electrodeposition under higher cell voltage conditions shows that in both the cases the effect of increase in cell voltage is identical. Of course, there is difference between the two patterns; the one obtained using actual electrodeposition and the other is of simulation. And also that electrodepositions under certain operating condition are identical in terms of appearance and fractal character, however they are not replica of each other.

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In electrodeposition at a constant applied cell voltage, as the growth size increases, the distance between cathode and anode is reduced which results in an increase in electric field during later stages of electrodeposition. This results in an increase in branching during the developed stage of the electrodeposits.

Table 2

Sr. No	Figure NO.	Bias Value B	Fractal Dimension
1	3	0.05	1.56
2	4	0.1	1.59
3	5	0.25	1.60
4	6	0.3	1.63

Table 2 shows a comparison of the values of fractal dimensions estimated from the box counting of the simulated patterns of figure 3-6.

IV. CONCLUSION

A theoretical model based on the DLA theory of electrodeposition is presented to study the effect of different cell operating conditions on growth of simulated fractal pattern. It is observed that fractal growth at low bias B= 0.001 shows open structure with fewer number of branches with less crowding and low fractal dimension D= 1.41. As the bias is increased (higher value of B=0.3), the growth tends to be dense and with more crowded branching. The complexity of the shapes of growth patterns increases with an increase in the value of 'B'. This is consistent and in agreement of the actual electrodeposition using increased applied cell voltage, which results in an increase in the fractal dimension 'D' indicating the increased complexity of the structure and texture of the simulated pattern. The fractal dimensions shown in Table – 2 are in close agreement with actual fractals grown from copper sulphate solution under different cell operating voltage conditions[].

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