Crystal Growth Under Strong Voltages

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Abstract

We investigate the qualitative growth of a crystal under a range of voltages, as well as how the box dimension connects to the voltage strength. The dimension is found to depend on the voltage to a certain degree.

1 Theory

The length of a measured object depends on the length of the measuring instrument. With a shorter measuring instrument it is possible to measure small segments which larger instruments cannot and therefore you will measure a longer distance with the shorter instrument.

1.1 Fractal Dimension

The dimension of an object relates to how it scales with length, and since length depends on the measuring instrument, it also relates to how it scales with different measuring instruments.

Consider a line with length L. If we divide the line into three parts, the sum of the lengths must be L:

$$L^{D_1} = 3(L/3)^{D_1},\ D_1 = 1$$

Now consider a square with side length L. If we want to measure the object using instruments with length $L/3$ we will count nine uses of such instruments to cover the object. The area covered by the square and the nine instruments must be the same:

$$L^{D_2} = 9(L/3)^{D_2},\ D_2 = 2$$

We can see here that a one dimensional object, the line, scales in one way with the measuring length while the two dimensional object, the square, scales with the measuring length in another way. What if an object scaled with the measuring length with a factor that was not an integer? Then we would have what is denoted a *fractal dimension*.

1.2 The Box Dimension

A fractal dimension can be defined in several ways. One of the easiest to work with, and the one we will use in this project, is the box dimension. The box dimension of a set F is defined as:

$$D_B(F) = \lim_{\delta \to 0} \frac{\log N_\delta(F)}{-\log \delta} \tag{1.1}$$

where δ is the side length of the measuring instruments and $N_\delta(F)$ is the number of such instruments needed to cover F. For small enough δ we have

$$N_\delta = \delta^{-D_B}$$

and if we measure an object with two differenly sizes instuments, we can calculate the box dimension D_B from:

$$\frac{N_{\delta_2}}{N_{\delta_1}} = \left(\frac{\delta_1}{\delta_2}\right)^{D_B} \tag{1.2}$$

2 Method

The biased random walk was interpreted to consist of two separate components:

1. A *normal* random walk, and

2. a bias for walking towards the voltage source

Imagining the complete process as a Gillespie procedure with uniformly distributed events in time, eight separate probabilities (reactions) was used. Four corresponding to the usual random walk events, as well as four probabilities corresponding to walking because of the voltage. The equations relating to this choice can be expressed as follows:

$$p_{rw_{l,d,r,u}} \propto C \tag{2.1}$$

$$p_{volt_{l,r}} \propto \frac{V}{r^2}|\cos\theta| \tag{2.2}$$

$$p_{volt_{u,d}} \propto \frac{V}{r^2}|\sin\theta| \tag{2.3}$$

where the indices l, d, r, u denote the different directions, C a constant chosen to be 0.25 in all cases. V marks the arbitrary voltage constant, and r^2 the squared distance from the center. θ signifies the angle between the horizontal axis and the position vector. The two angular dependent equations were set to zero whenever the particle were on the "wrong" side of the source point, i.e. the grid origin. All probabilties were normalized so that the final reaction was determined by a generated random floating point value in the interval $[0, 1)$.

For the simulations, the grid was set to increase be a specified value every time a particle collided with the crystal in few enough steps. 100000 particles were used for every separate simulations.

3 Results and Discussion

The box dimension is found to depend on the voltage constant to a certain degree. At lower voltages the dimension is slightly negatively affected, as can be seen in the leftmost part of fig. 1, although this effect is likely to be a statistical fluctuation. In contrast to this, the dimension is found to increase logarithmically with increasing voltage, with the final value ultimately convering at a box dimension of roughly 1.8.

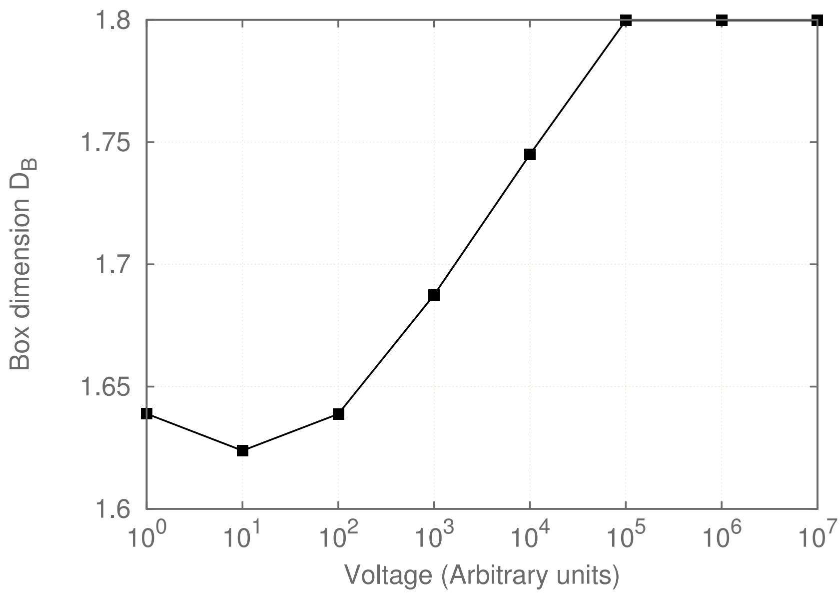

Figure 1: Fractal (box) dimension with respect to the voltage constant, which is given in arbitrary units. At high enough voltage, the dimension saturates.

Figure 2 shows the resulting crystals under the different voltage values, except for the two highest ones, which were found to be effectively identical to the third to last. Clearly, the structure covers a larger part of the two-dimensional surface with increasing voltage, as is expected. That the dimensional value ultimately caps at a value of 1.8 is a consequence of the established dynamics of the system. It can be assumed that the converging value under a continous system would be sligtly higher, as our system here is bound to alternate between steps in discrete directions, and therefore are bound to have ladder-like trajectories. In a continous system, the trajectory under a strong voltage would simply be a straight line, and sligthly fewer interactions in the outer parts of the crystal could then be expected.

That the crystal assumes hyperbolic edges is also due to the discrete directions. As a particle which is instantiated in the very corners is bound to alternate between orthogonal steps, the crystal is more likely to have a larger spread in these regions; near the centers of the boundaries, the particles can walk in straighter lines, which is why the radii are smaller in these directions.

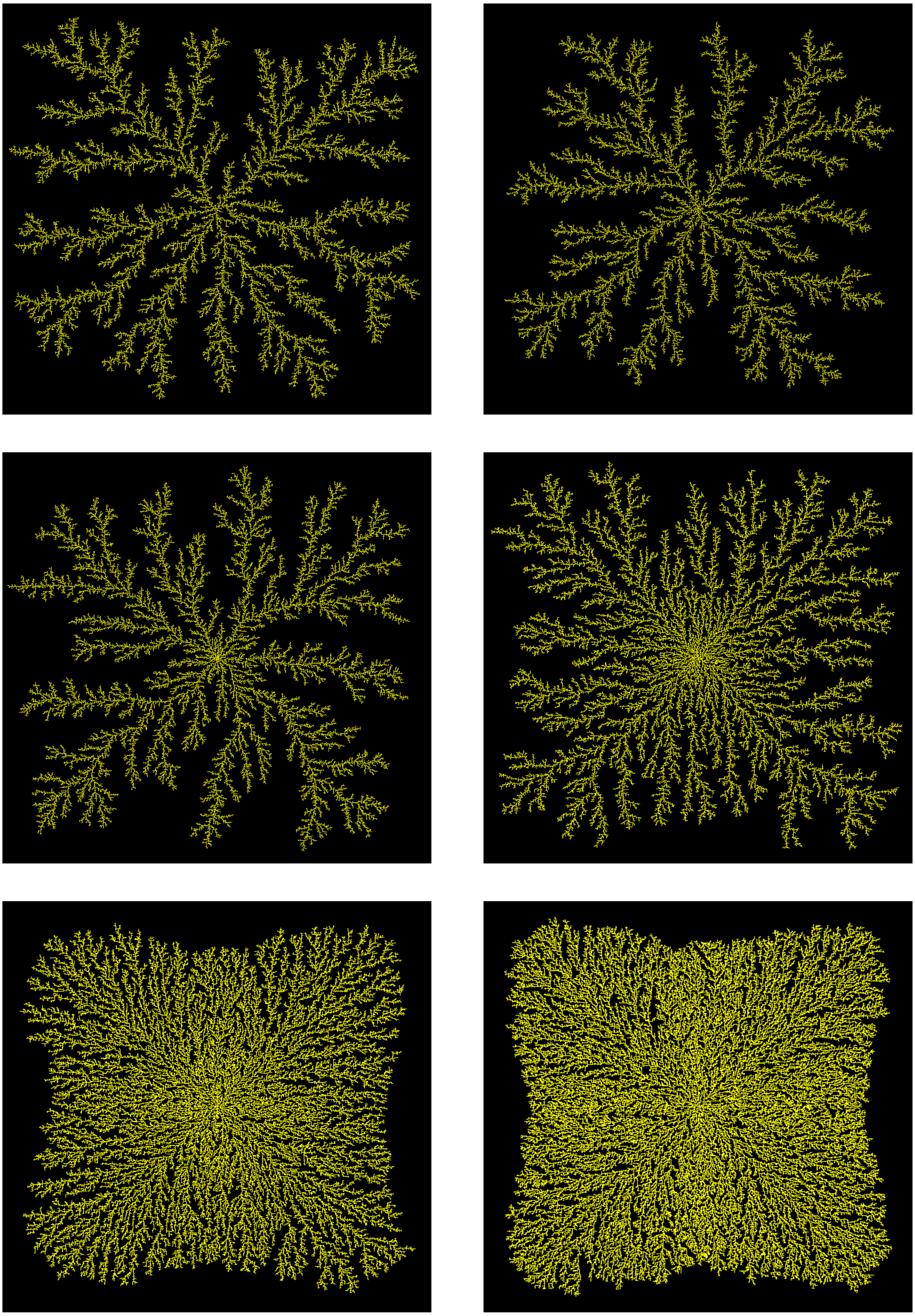

Figure 2: Crystals under increasing voltages, ranging from 0 to 100000 in powers of 10. Figures range from left to right, downwards. Note that the crystals under higher voltages are less spread out; the grid has grown less during the simulation. All simulations feature 100000 particles