Interfaces and their models

Interfaces and surfaces are common in nature. They have many interesting properties, We will consider two aspect:

- Formation (how surfaces are formed and how they grow)
- Morphology (what is their structure)

The simples process by which a surface can be formed is called *deposition*, when particles of one substance are falling on a substrate made of another (or the same) substance.
Often this process has some *randomness* in it, and the resulting surface is *rough*.
The process of deposition known as *molecular beam epitaxy* (MBE) is of a great technological importance, as it is used to fabricate semiconducting devices and microchips. Typically, chips are manufactured by deposition of silicon and other atoms on a silicon surface.

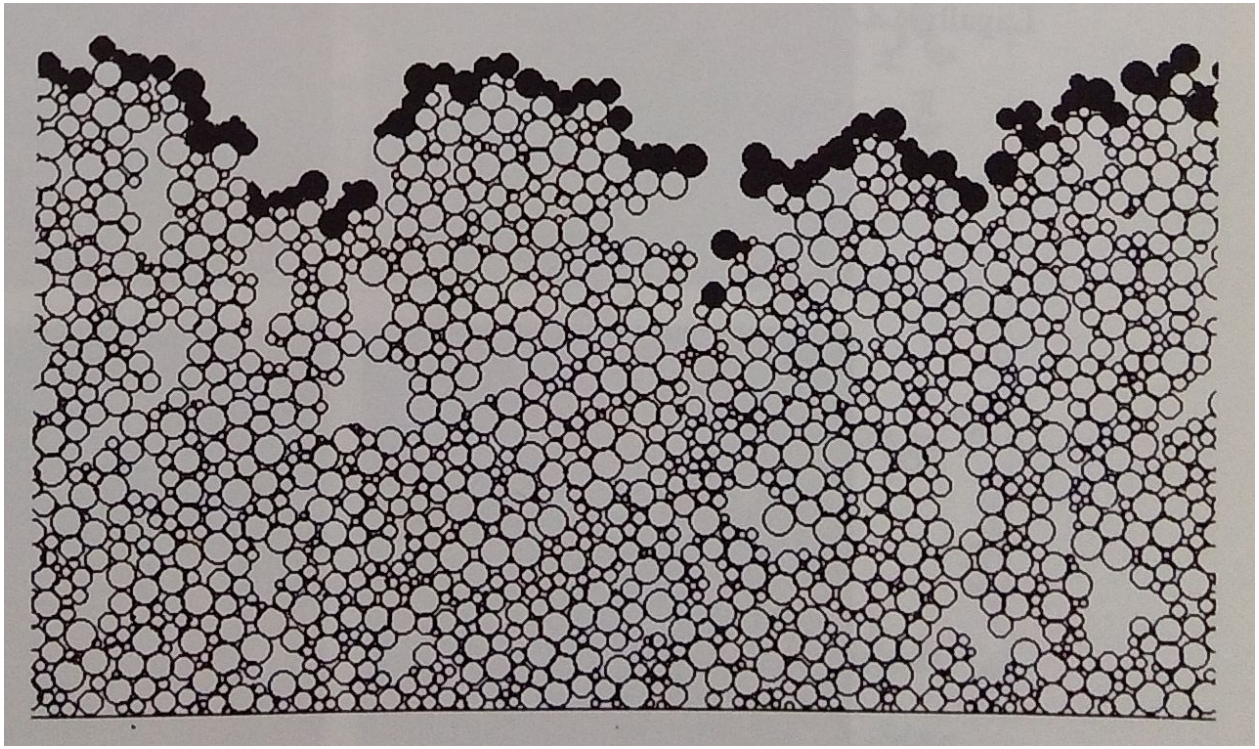
Snow deposition

The picture below shows an example of a deposition process. Snow particles are falling on a slanted glass window and form and interesting (and rough) interface.

source: A-L. Barábasi and H. E. Stanley, "Fractal Concepts in Surface Growth, Cambridge UP 1995 (FCSG).

Snow deposition - model

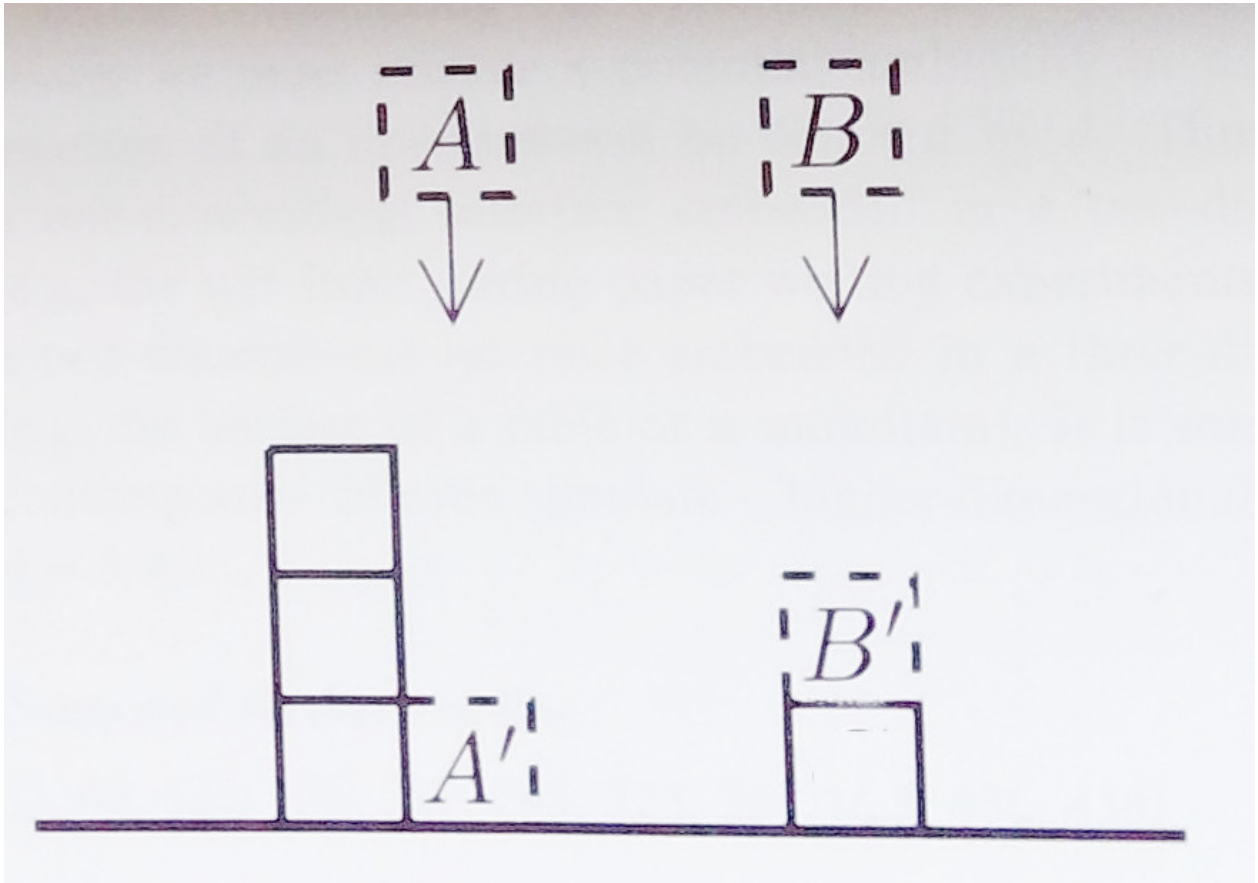
A simple model of the snow deposition can be constructed. Spherical particles with uniformly distributed random diameters fall on a surface and roll until they make contact with at least two other particles.



source: FCSG.

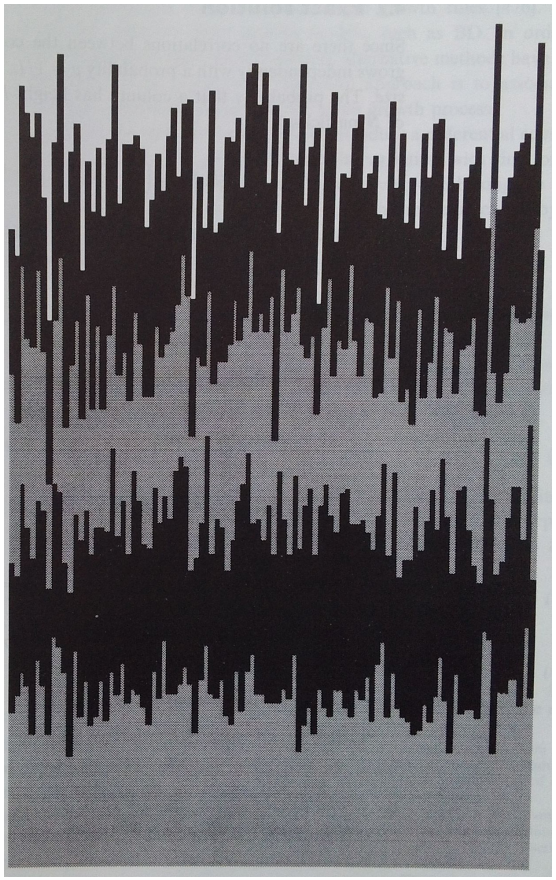
Random deposition model

The simplest mode of deposition is called *random deposition* (RD). From a randomly chosen site over the surface, a particle falls vertically until it reaches the top of the column under it, where it is deposited. Examples: the particle A will remain at A', and B at B' after deposition.



Random deposition model - simulation

Example of the simulation of RD model on a lattice of $L = 100$ columns, initially flat. The shading changes after deposition of each 4000 particles, to emphasize roughening of the surface.



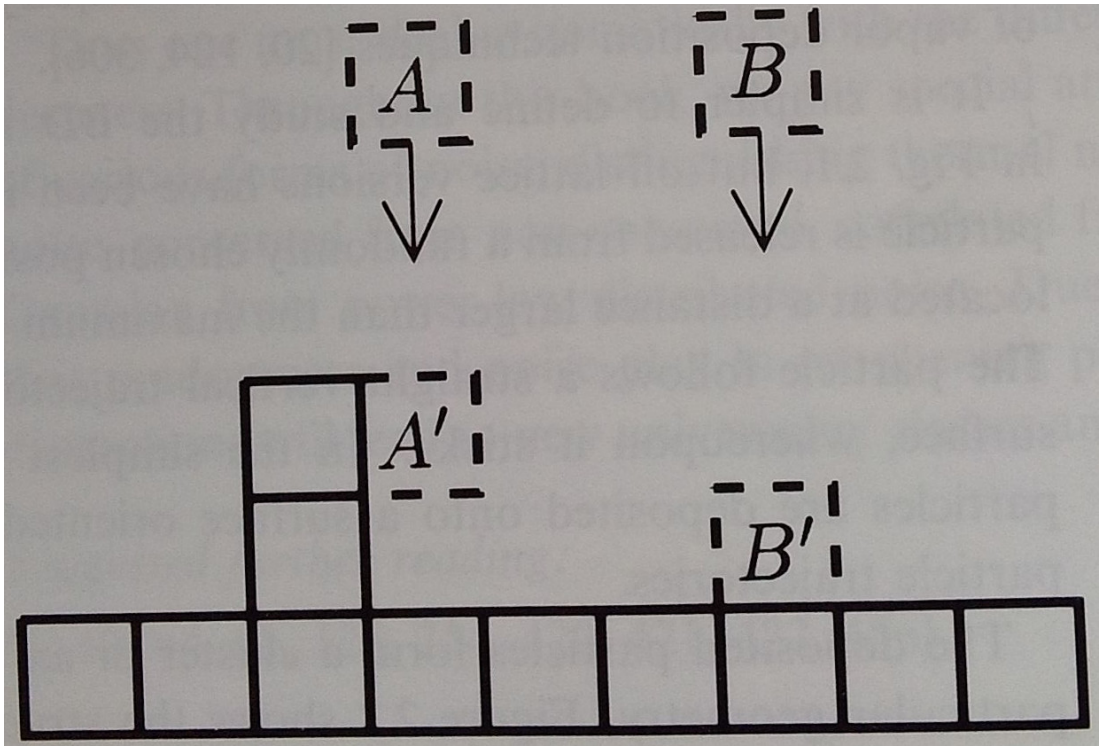
source: FCSG.

Ballistic deposition model

RD model is very simple, and it does not reproduce all essential features of real-world deposition processes.
We will now consider a little bit different model known as *ballistic deposition* (BD).

- The process takes place in a rectangular region of 2D space, with the initial surface usually flat and located at the bottom.
- The space is discrete, divided into squares (also called sites or cells).
- We choose a random position above the surface, and allow a particle to fall vertically down. The particle sticks to the first site along its path that has an occupied nearest neighbour.

Examples: the particle A will remain at A', and B at B' after deposition.



source: FCSG.

Computer simulation of DB model

Example of a simulation of BD process on a lattice of horizontal length $L = 200$. Total of 35000 particles deposited. The shading changes after each 2500 particles to bring up the changing shape of the surface (roughening).

source: FCSG.

Let $h(i,t)$ be the height of the column i at time t.
Suppose that the random position where the particle is to be deposited is i. Where will this particle land?

- If $h(i-1,t) \leq h(i,t)$ and $h(i+1,t) \leq h(i,t)$, its bottom will stick to top of column i, so that the new height of column i will be $h(i,t)+1$.
- If $h(i-1,t) > h(i,t)$, its left side will stick to the top of column $i-1$, at the same level, so that new height of column i will be $h(i-1,t)$.
- If $h(i+1,t) > h(i,t)$, its right side will stick to the top of column $i+1$, at the same level, so that new height of column i will be $h(i+1,t)$.

In general, the new height of the column i will be the largest number from the set

$$\{h(i,t)+1, h(i-1,t), h(i+1,t)\}$$

Ballistic deposition - formal description

Suppose that we perform the process of selection and height increase in a *sequential order*, one per time step. This leads us to the following mathematical description of the BD model:
At any moment t, we choose randomly a column i and increase its height according to formula

$$h(i, t+1) = \max\{h(i-1, t), h(i, t) + 1, h(i+1, t)\}$$

Note that $h(i, t) \in \mathbb{Z}^+ \cup \{0\}$.
Very important: note that at a given time step, we increase height of only *one* randomly selected column. This is different from the update scheme of cellular automata, where we update all lattice sites *at the same time*. We call this *random sequential update*, whereas in CA we had *parallel update*.

Some definitions

The *mean height* of the surface is defined as

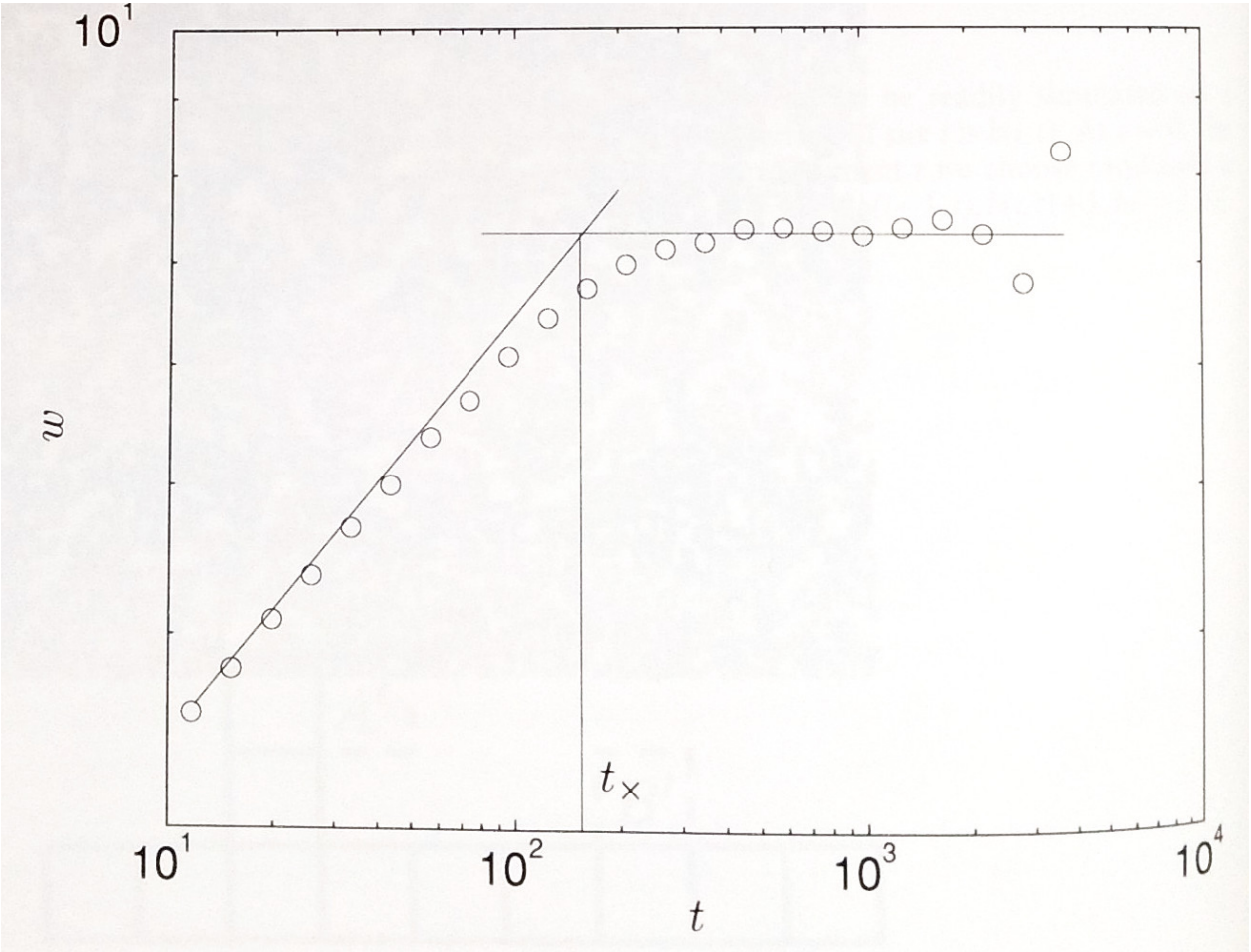
$$\bar{h}(t) = \frac{1}{L} \sum_{i=0}^{L-1} h(i,t)$$

If the deposition rate is constant, the height increases linearly with time, $\bar{h}(t) \sim t$

The *interface width* is defined as

$$w(L,t) = \sqrt{\frac{1}{L} \sum_{i=0}^{L-1} [h(i,t) - \bar{h}(t)]^2}$$

A typical plot of the width of the surface in BD model as a function of time is shown below.



source: FCSG.

- Initially, the width of the surface increases as a power of time,

$$w(L,t) \sim t^{\beta} \quad \text{if } t << t_x$$

  The exponent β is called the *growth exponent*.
- The power law behaviour does not continue indefinitely, but is followed by a saturation regime, where $w(L,t)$ approaches a *saturation value*, to be called $w_{sat}(L)$.
- The time t_x where the behavior changes from the power law regime to the saturation regime is called *crossover time*.
- Numerical experiments show that

$$w_{sat}(L) \sim L^{\alpha} \quad \text{if } t >> t_x$$

  The exponent α is called the *roughness exponent*.
- Moreover,

$$t_x \sim L^z$$

  The exponent z is called the *dynamic exponent*.

What is the value of exponents α, β and z? It turns out that while these exponents can be estimated rather easily from numerical simulations, they exact values, in general, are very difficult to compute, and form most models (except the simplest ones) their exact value is unknown, or, at best, is only conjectured. Nevertheless, we will show that for RD model, they can be calculated easily. Let us recall basic definitions first:

$$\bar{h}(t) = \frac{1}{L}\sum_{i=0}^{L-1} h(i,t) \quad \text{(mean height)}$$

$$w(L,t) = \sqrt{\frac{1}{L}\sum_{i=0}^{L-1}[h(i,t) - \bar{h}(t)]^2} \quad \text{(interface width)}$$

$$w(L,t) \sim t^{\beta} \quad \text{if } t << t_x \quad \text{(growth exponent)}$$

$$w_{sat}(L) \sim L^{\alpha} \quad \text{(roughness exponent)}$$

$$t_x \sim L^{z} \quad \text{(dynamic exponent)}$$

Calculation of exponents in RD model

In RD, there are no correlations between columns, and every column grows independently with probability $p = 1/L$. The probability that a column has height h after N steps (N depositions) is

$$P(h, N) = \binom{N}{h} p^h (1-p)^{N-h}$$

.

Define the time to be the mean number of deposited layers, $t = N/L$. Then the mean height is

$$\langle h \rangle = \sum_{h=1}^{N} h P(h, N) = Np = \frac{N}{L} = t$$

Moreover, one can show that (exercise)

$$\langle h^2 \rangle = \sum_{h=1}^{N} h^2 P(h, N) = Np(1-p) + N^2 p^2$$

Calculation of exponents in RD model - continued

$$w^2(t) = \langle (h - \langle h \rangle)^2 \rangle = \langle h^2 \rangle - \langle h \rangle^2 = Np(1-p) + N^2p^2 - N^2p^2$$

$$w^2(t) = Np(1-p) = \frac{N}{L}\left(1 - \frac{1}{L}\right)$$

For large L, $1 - 1/L \approx 1$, thus

$$w^2(t) \sim \frac{N}{L} = t$$

$$w(t) \sim t^{1/2}$$

$$\beta = \frac{1}{2}$$

In RD model, the surface width increases indefinitely without saturation, $w_{sat}(L) = \infty$. It is common to say that also $\alpha = \infty$, although it really means that α is undefined. Similarly, dynamic exponent z is undefined.

Exponents α and β in BD model

For BD model, the exponents have the following values, obtained numerically

$$\alpha = 0.45 \pm 0.02$$

$$\beta = 0.33 \pm 0.006$$

It is now commonly believed that the exact values of these exponents for BD model are

$$\alpha = \frac{1}{2}$$

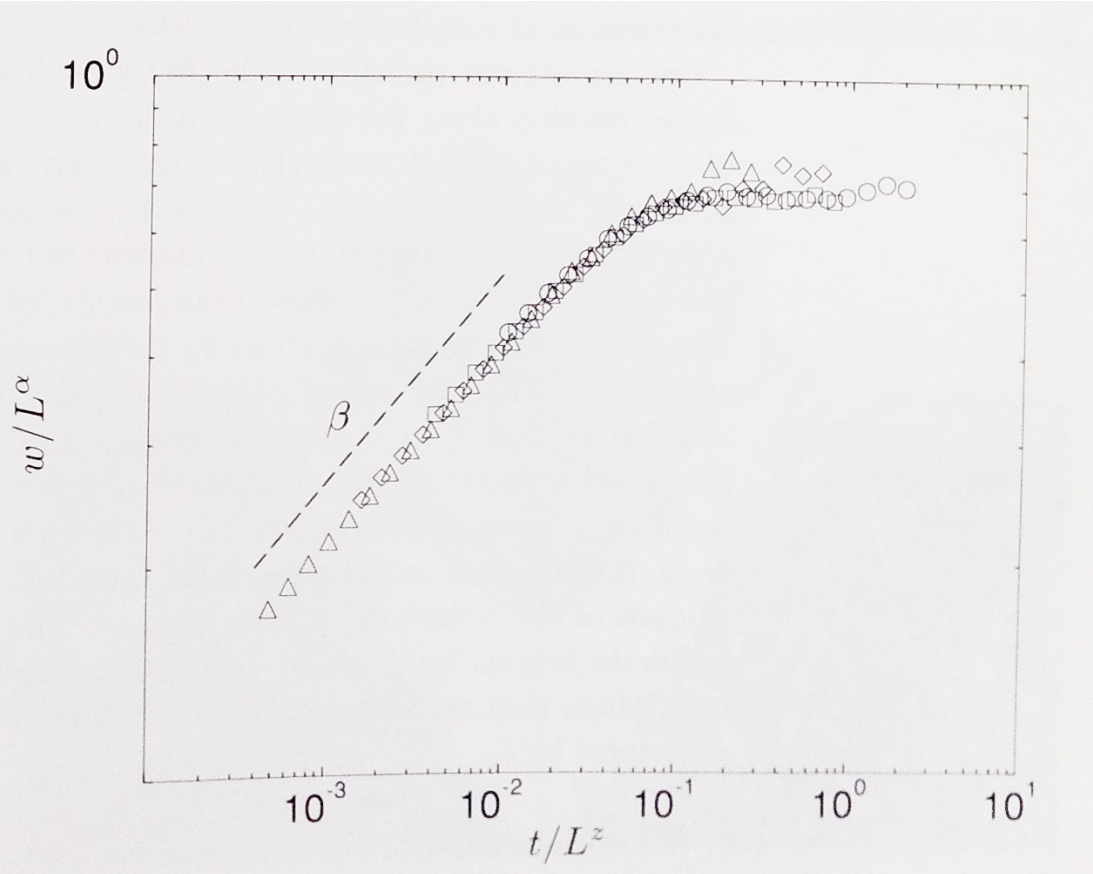
$$\beta = \frac{1}{3}$$

These values can be obtained from the so-called renormalization group theory applied to Kardar-Parisi-Zhang equation which describes nonlinear growth of surfaces assuming continuous time and space. One should emphasize that these are non-rigorous (approximate) calculations, and the formal proof that $\alpha = \frac{1}{2}$ and

Historical remark

The founder of renormalization group theory is Kenneth G. Wilson (1936 – 2013), winner of the Nobel Prize in Physics in 1982.

Renormalization group calculations are well beyond the scope of this course (see FCSG if you are interested).
We will show, however, how can the third exponent z be calculated if α and β are known. The following observation is crucial: *Plotting $w(L,t)/w_{sat}(L)$ as a function of t/t_x will result in curves which appear to be universal regardless of L.* Plot below shows these curves for lattice sizes $L = 100, 200, 400, 800$.



Dynamic scaling

This means that

$$\frac{w(L,t)}{w_{sat}(L)} \sim f\left(\frac{t}{t_x}\right)$$

where f is called a *scaling function*. Using $w(L,t) \sim t^{\beta}$, $w_{sat}(L) \sim L^{\alpha}$, $t_x \sim L^z$ we obtain

$$w(L,t) \sim L^{\alpha} f\left(\frac{t}{L^z}\right)$$

(the above is called Family-Vicsek scaling relation). Also,

$$w(L,t) \sim t^{\beta}$$

When $t = t_x$, the first of these equations gives

$$w(L,t_x) \sim L^{\alpha} \cdot const$$

while the second one yields

$$w(L,t_x) \sim t_x^{\beta}$$

This means $t_x^{\beta} \sim L^{\alpha}$, or $t_x \sim L^{\alpha/\beta}$, thus $z = \frac{\alpha}{\beta}$

Scaling law

The equation

$$z = \frac{\alpha}{\beta}$$

is called a *scaling law*. Although we obtained it in a non-formal way, it seems to be valid for all known surface deposition models. Renormalization group theory confirm this law too. It is still waiting for a rigorous mathematical proof.
For BD model it yields $z = \frac{3}{2}$, and numerical experiments confirm this value.
For RD model, since $\alpha = \infty$, we can say that $z = \infty$ as well.