I. Overall description

PixelGrowth simulator is aimed at the layered deposition of materials on surfaces. The program uses a stochastic model with a few simply defined phenomenological parameters.

The simulation produces a sequence of growth images as a function of time. The "growth image" is a 2D matrix of unit cells with assigned layer thickness at each of these cells. The "unit cell" corresponds to an arbitrary unit area in regular 2D lattice, it is set as a square shaped in the default version of the simulation. As an example, the "unit cell" can be defined as the atomic crystall lattice unit cell. The "layer thickness" is analysed in "ML" (mono-layer) indivisible units.

Simulation area limit: The analysed growth area ("frame") can be defined as a square of up to 1000x1000 unit cells of regular 2D lattice.

II. Simulation description.

The single simulation step, which is continuously repeated, consists of following actions:

1. Drawing a single unit cell from the growth area.
2. Drawing a deposition event for this unit cell. This drawing result can be "0" – means not changing or "1" – means growing a single layer (1ML) at this unit cell.
3. Update of the growth image.

Drawing of a unit cell in step 1. corresponds to the flat probability distribution, it means each unit cell has the same probability to be drawn.

Step 2. is governed by related probability parameters. This step uses a term "nearest neighbour" for a given unit cell.

The following parameters are applied in step 2.:

- \( P_N \) – "nucleation probability"
- \( P_C \) – "continuation probability"
$P_N$ is equal to the probability of drawing "1" (means deposition of 1ML) in step 2., when none of nearest neighbours is already covered by the deposited layer, which is thicker than the layer in the considered unit cell. In simple words, $P_N$ relates to the probability of "growth nucleation" event.

$P_C$ is equal to the probability of drawing "1" (means deposition of 1ML) in step 2., when at least one of nearest neighbours is already covered by the layer which is thicker than the layer in the considered unit cell. This probability can be set as a function of the number of such overgrown nearest neighbours. In simple words, $P_C$ relates to the probability of "growth continuation" event.

In a real experiment the microscopic conditions often abruptly change, if compare deposition of the first 1ML grown on the substrate with deposition of next MLs (grown on earlier deposited material). To include such a change, $P_N$ and $P_C$ parameters are additionally specified in simulations, as follows:

- $P_{N, \text{on substrate}}$ and $P_{C, \text{on substrate}}$ – are defined the same way as respectively $P_N$ and $P_C$, but only when the considered growth event means growth of the first ML in the specified unit cell.

- $P_{N, \text{on layer}}$ and $P_{C, \text{on layer}}$ – are defined the same way as respectively $P_N$ and $P_C$, but only when at least one ML was already grown in the specified unit cell.

Analogously, next pair of $P_{N, \text{on 2ML}}$ and $P_{C, \text{on 2ML}}$ can be addressed for the growth of third ML on 2MLs of deposited material.

Initial $P_N$ and $P_C$ symbols are reserved in the simulation setup as $P_N = P_{N, \text{on substrate}}$, and $P_C = P_{C, \text{on substrate}}$.

The deposition process time is measured in "number of shots" unit, which is equal to the average number of samplings of one selected unit cell, so is equal to the total number of samplings divided by total number of unit cells.

**System requirements**

PC with Windows OS and HD (1080x1920) or better screen resolution.

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