TU Delft

Growth on Imperfect Crystal Faces

Monte-Carlo Method

A. Francke, M.W. Glorie, J. Sangers

Computational Physics - AP3082
June 8 2022

Table of content

1. Motivation
2. Theoretical Background
3. Implementation
4. Results
5. Discussion
6. Conclusion & Outlook

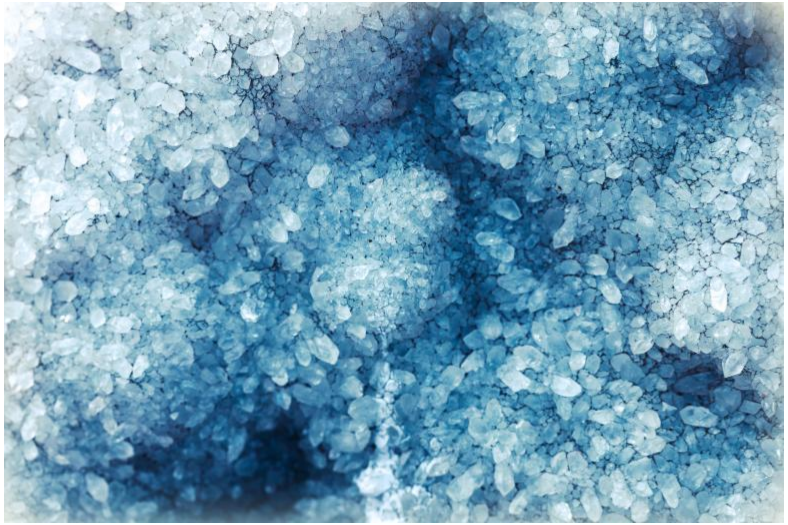
1. Motivation

Crystal growth: -Atomic bonding

-Atom mobility

-Surface impurities

Monte-Carlo computer simulations ideal



2. Theoretical Background

Interface interactions:

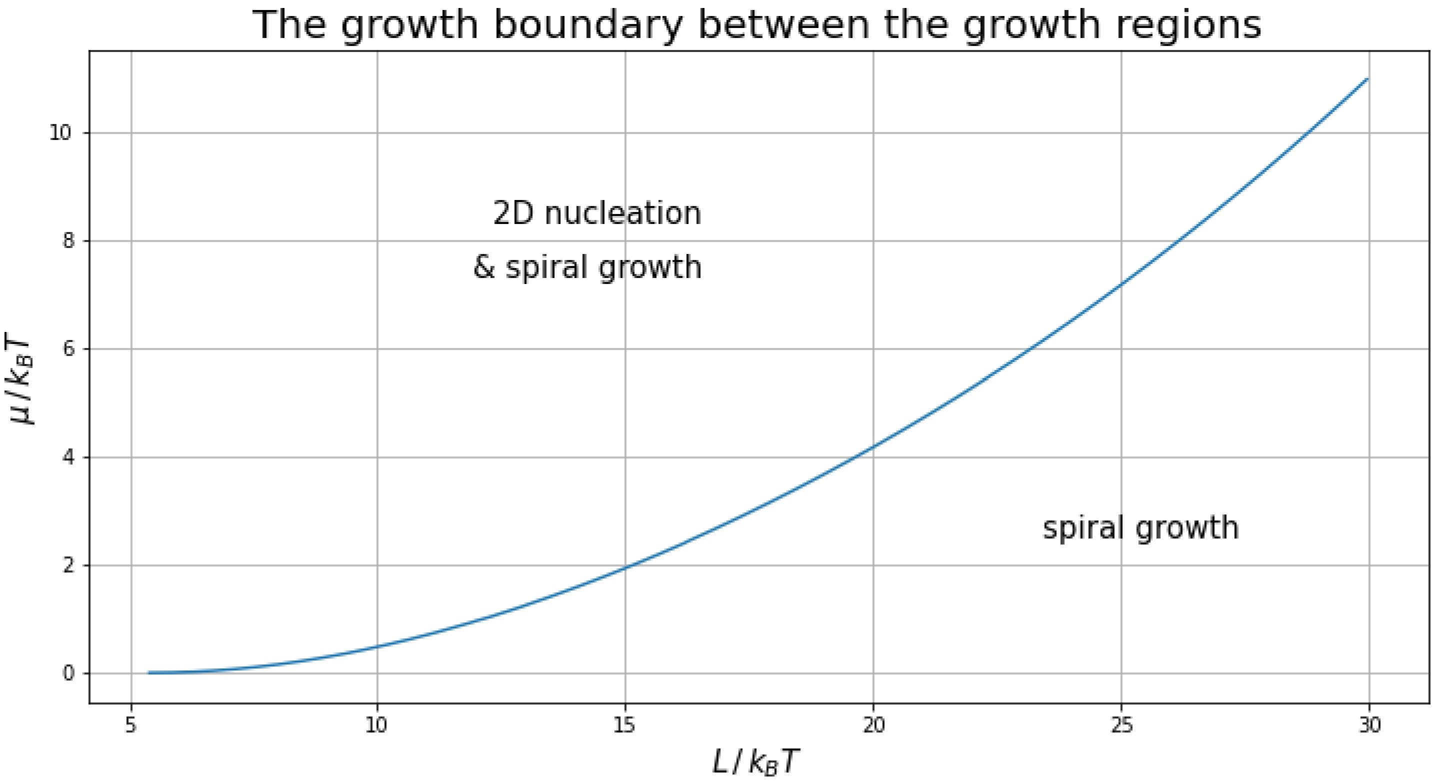
- Evaporation: $$k_n^- = v \exp(-n\phi/kT)$$
- Impingement: $$k^+ = \exp(\Delta\mu/kT)\, k_3^-$$
- Surface migration

2. Theoretical Background

Interface interactions:

- Evaporation: $$\tilde{k}_n^- = \exp(-n\tilde{T})$$
- Impingement: $$\tilde{k}^+ = \exp(\Delta\tilde{\mu})\,\tilde{k}_3^-$$
- Surface migration

2. Theoretical Background



3. Implementation

Divide the surface atoms in subsets based on the number of neighbours of each atom

Select a subset with probability p_n

Choose a lattice point from the subset

Choose from of interaction with a probability proportional to their interaction rate

$$p_n = N_n(k_n^- + k^+) / \sum_{i=1}^{5} N_i(k_i^- + k^+)$$

3. Implementation

Simulate dislocation by introducing scanning matrices

At the boundaries periodic boundary conditions were applied

Dislocation

1	1	1	1	1
1	1	1	1	1
1	1	1	1	1
1	1	1	1	1
1	1	1	1	1

Surface matrix

0	0	0	2	0
0	0	0	2	0
0	0	0	2	0
0	0	0	0	0
0	0	0	0	0

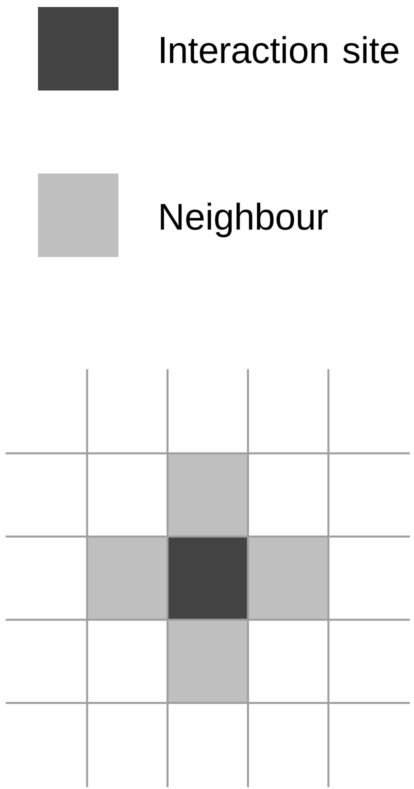
Forward scanning matrix

0	0	-2	0	0
0	0	-2	0	0
0	0	-2	0	0
0	0	0	0	0
0	0	0	0	0

Backward scanning matrix

3. Implementation

Optimize neighbour scanning by updating the number of neighbours of the lattice sites affected by evaporation, impingement or migration



3. Implementation

The growth rate:

Every $N_{\mathbf{cycles}}$ the crystal surface is stored

$$\Delta h_i = 1/N_{\text{cycles}}(\langle h\rangle_{i+1} - \langle h\rangle_i)$$

$$R/k^+d = 1/n\sum_{i=0}^{n}\Delta h_i$$

Growth rate error:

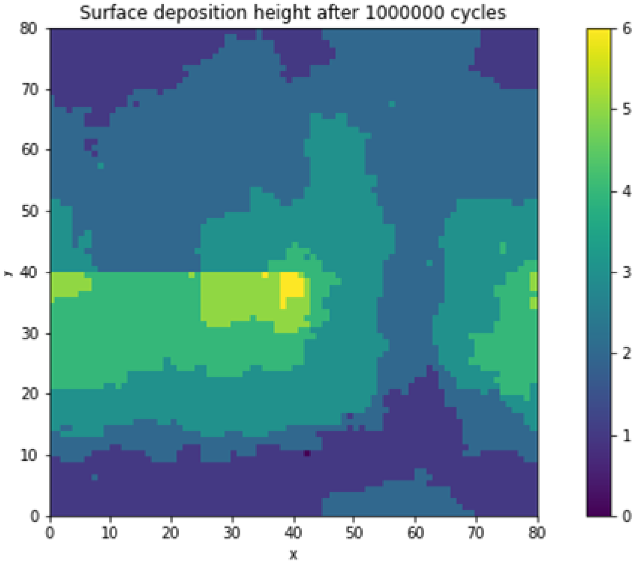
Growth rate is determined from one simulation - thus the data is correlated

The error is determined using the autocorrelation function

$$\chi_A(t) = \frac{1}{\sigma_A^2}\sum_n (A_n - \langle A\rangle)(A_{n+t} - \langle A\rangle)$$

$$\sigma_A = \sqrt{\frac{2\tau}{N}\left(\langle A^2\rangle - \langle A\rangle\right)}$$

4. Results

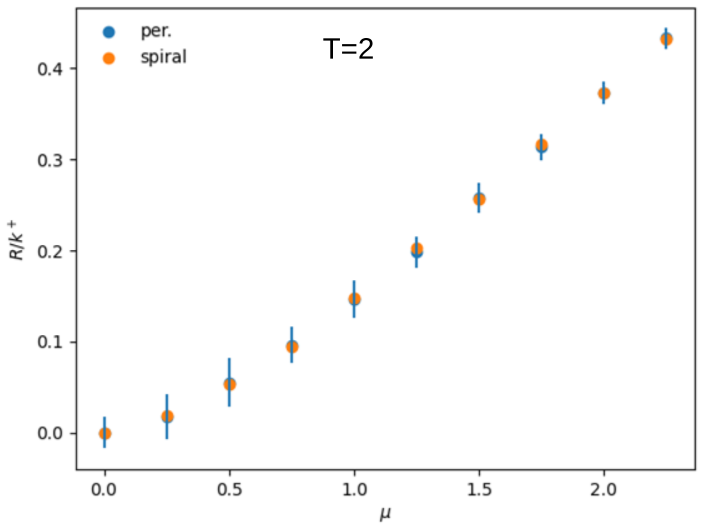


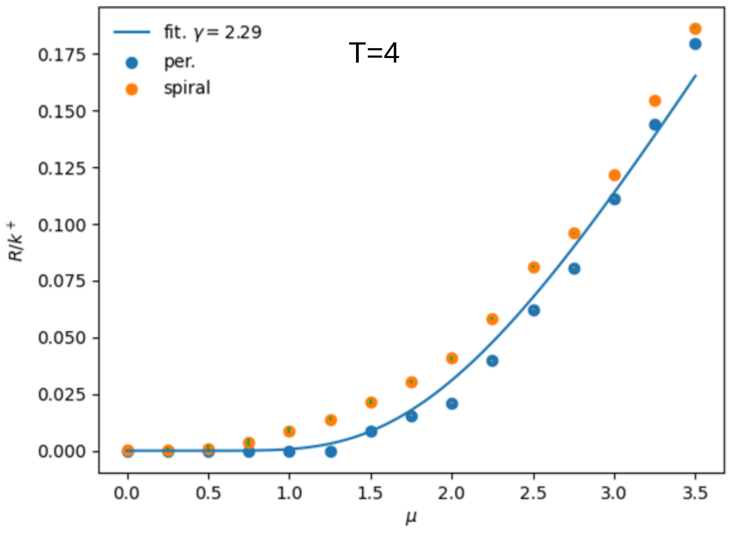
Spiral growth:

- when does a spiral grow
- what effect does it have

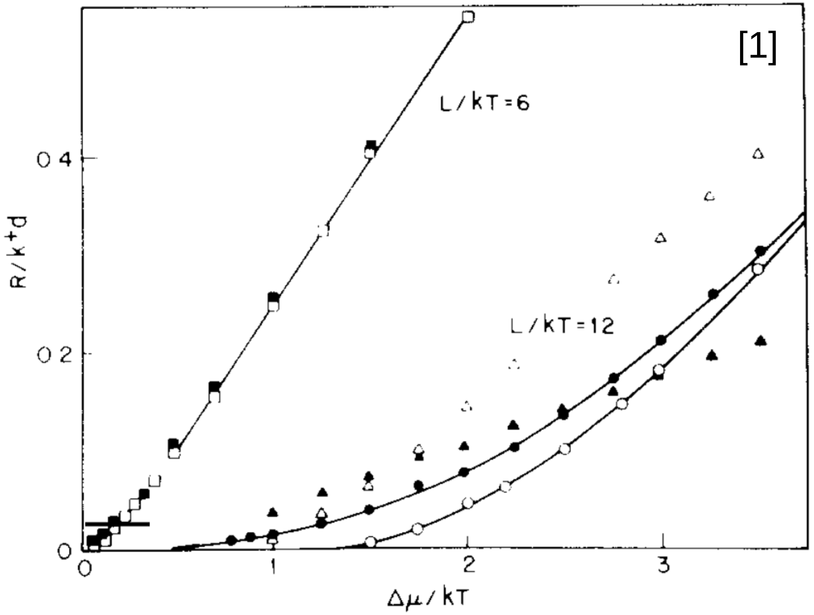
4. Results

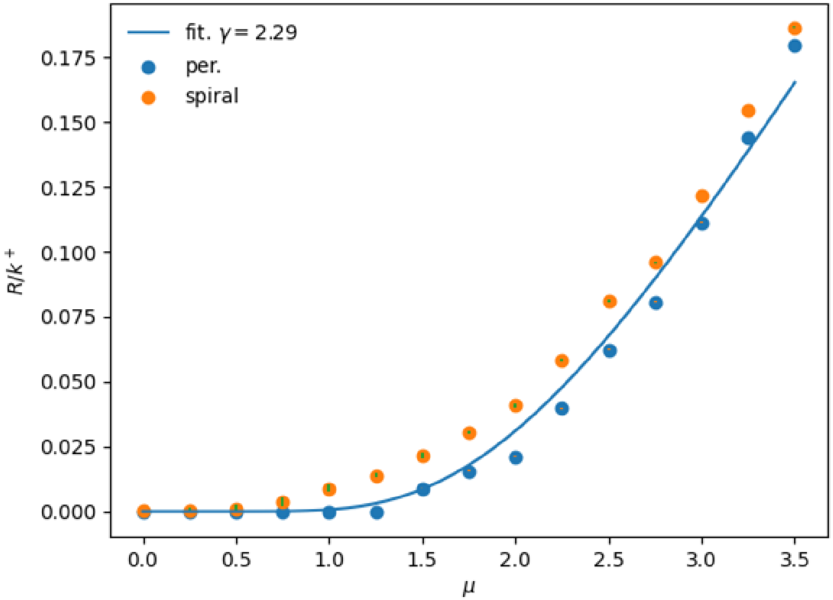
Only in a small range of T do we see the contribution of spiral growth





5. Discussion





6. Conclusion & Outlook

- The results in the paper were replicated
- Spiral growth contributes to growth rate in a small window of temperatures.

With more time…

- …we would like to have simulated with surface migrations and analysed these results

7. Short video

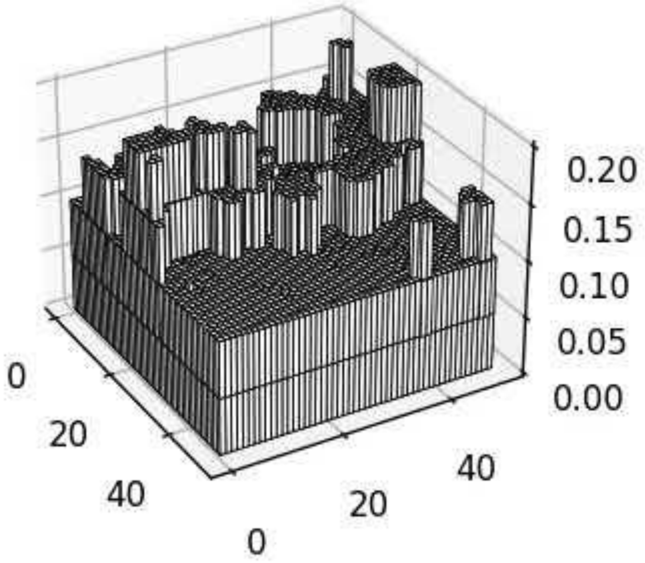
```
dims = [50,50]
T = 6.5
mu = 6
N = 1e5 #attempts

defect introduced at
[0,25]->[15,25]
```

Can see:

- Periodic BC
- Plateaus of growth
- Clumps of critical size stay

spirals can’t be seen due to small simulation space



Source:

[1] G.H. Gilmer, *Growth on imperfect crystal faces: I. Monte-Carlo growth rates*, Journal of Crystal Growth, Volume 36, Issue 1 (1976), Pages 15-28,

Thank you for your attention

A. Francke, M.W. Glorie, J. Sangers