



Growth on Imperfect Crystal Faces

Monte-Carlo Method

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Computational Physics - AP3082

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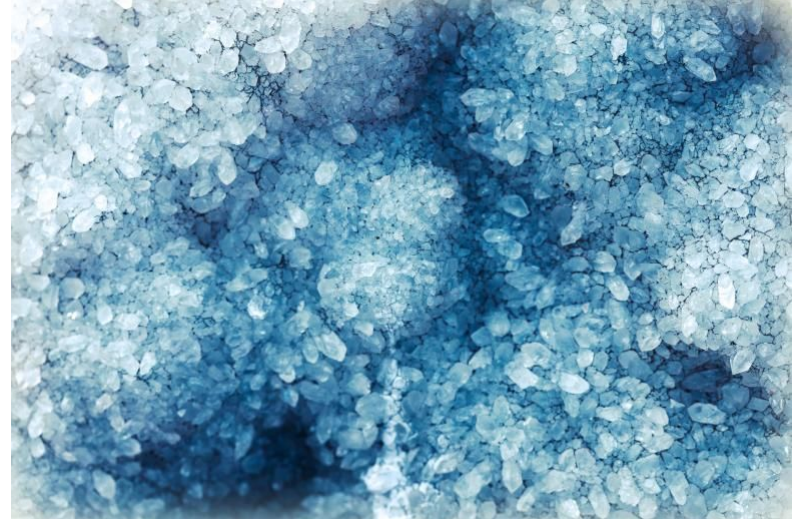
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1. Motivation

Crystal growth:

- Atomic bonding
- Atom mobility
- Surface impurities

Monte-Carlo computer simulations ideal



2. Theoretical Background

Interface interactions:

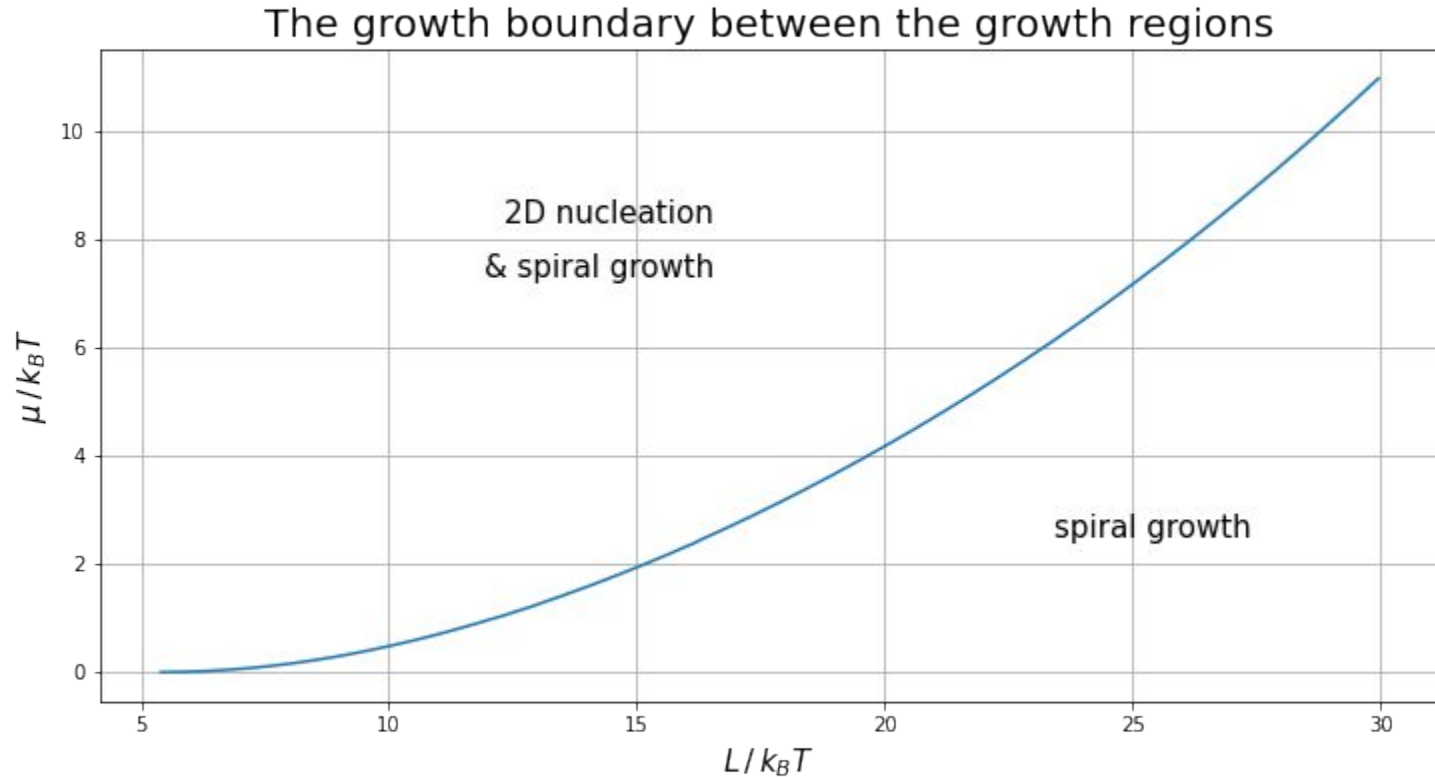
- Evaporation: $k_n^- = v \exp(-n\phi/kT)$
- Impingement: $k^+ = \exp(\Delta\mu/kT) k_3^-$
- Surface migration

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

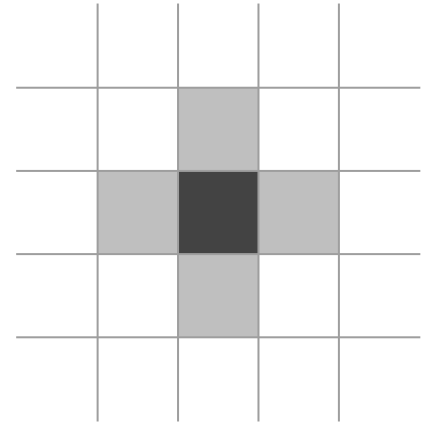
Optimize neighbour scanning by
updating the number of neighbours of
the lattice sites affected by evaporation,
impingement or migration



Interaction site



Neighbour



3. Implementation

The growth rate:

Every N_{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:

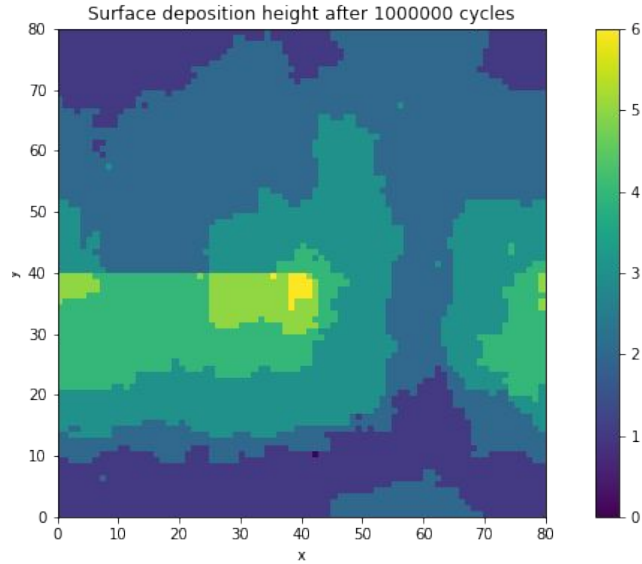
Growth rate is determined from one simulation - thus the data is correlated

The error is determined using the autocorrelation function

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

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

4. Results

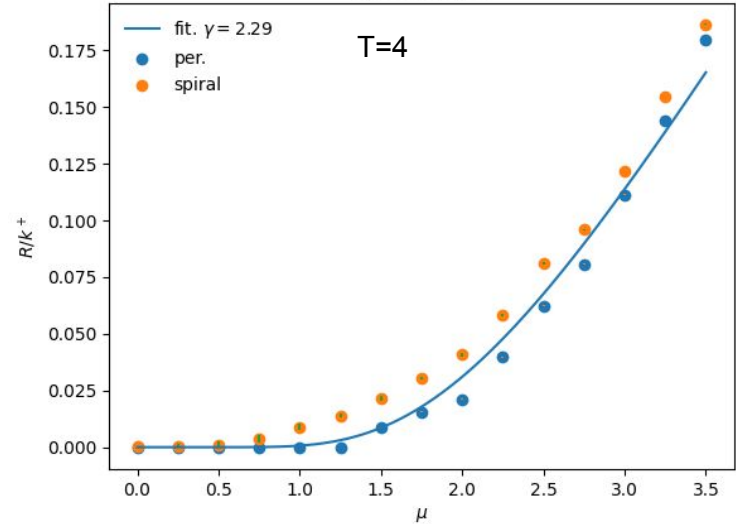
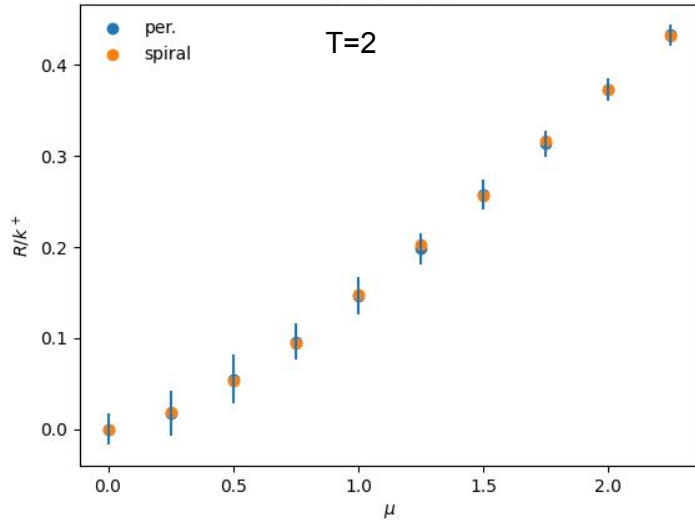


Spiral growth:

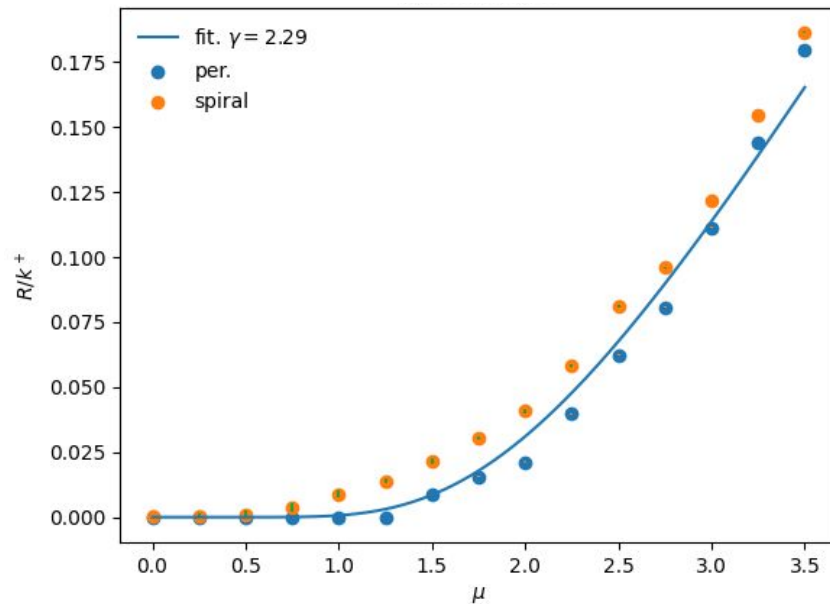
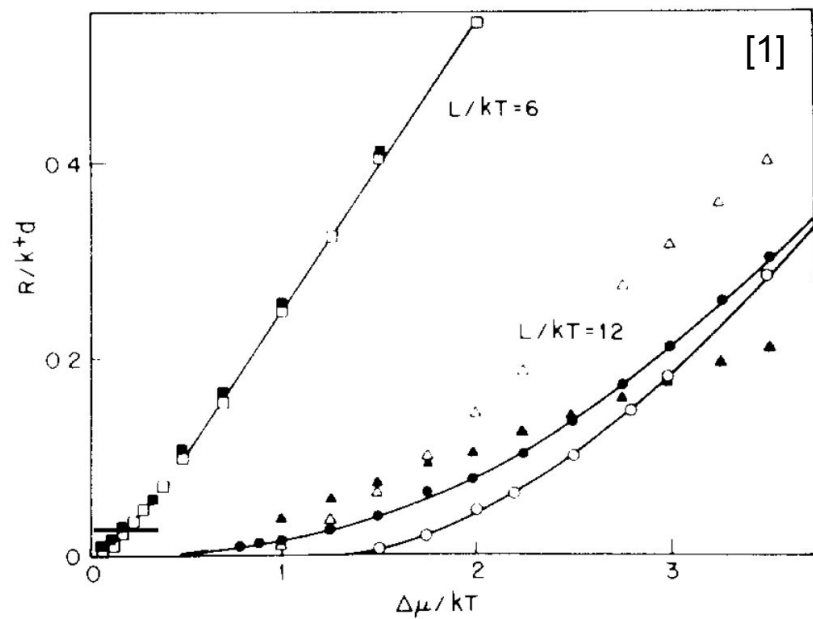
- when does a spiral grow
- what effect does it have

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

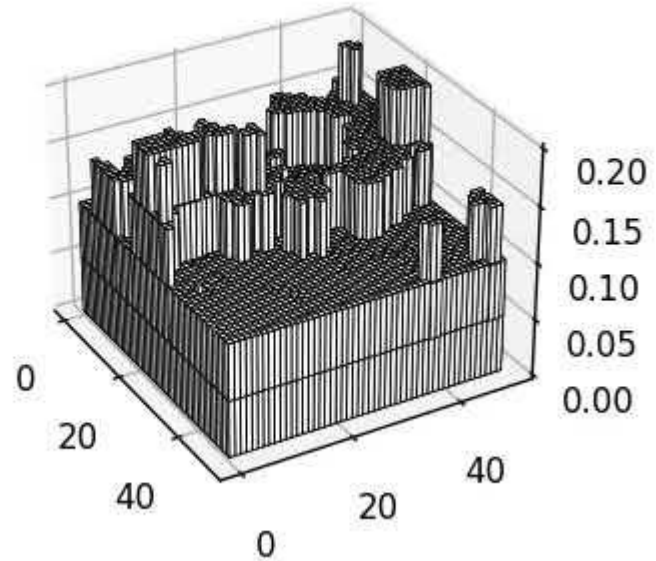
```
dims = [50,50]  
T = 6.5  
mu = 6  
N = 1e5 #attempts
```

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

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