



## 2D Monte-Carlo simulation of diamond

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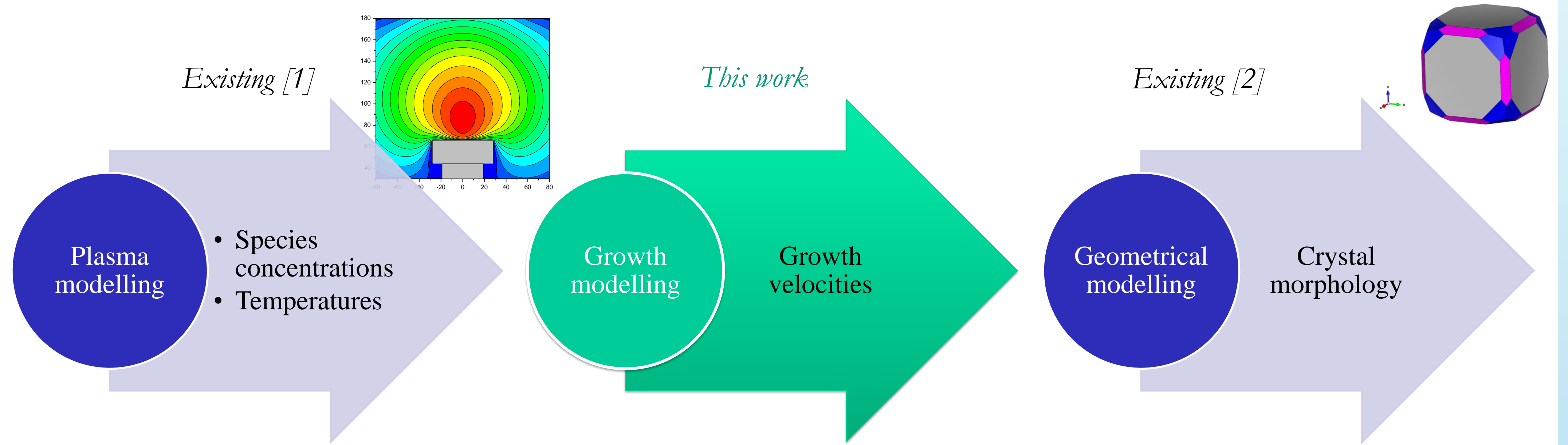


## Context

This work has 2 main objectives:

- complete the existing simulation framework to achieve **multi-scale modelling**
- obtain the growth velocities for several faces, taking **defects** into account

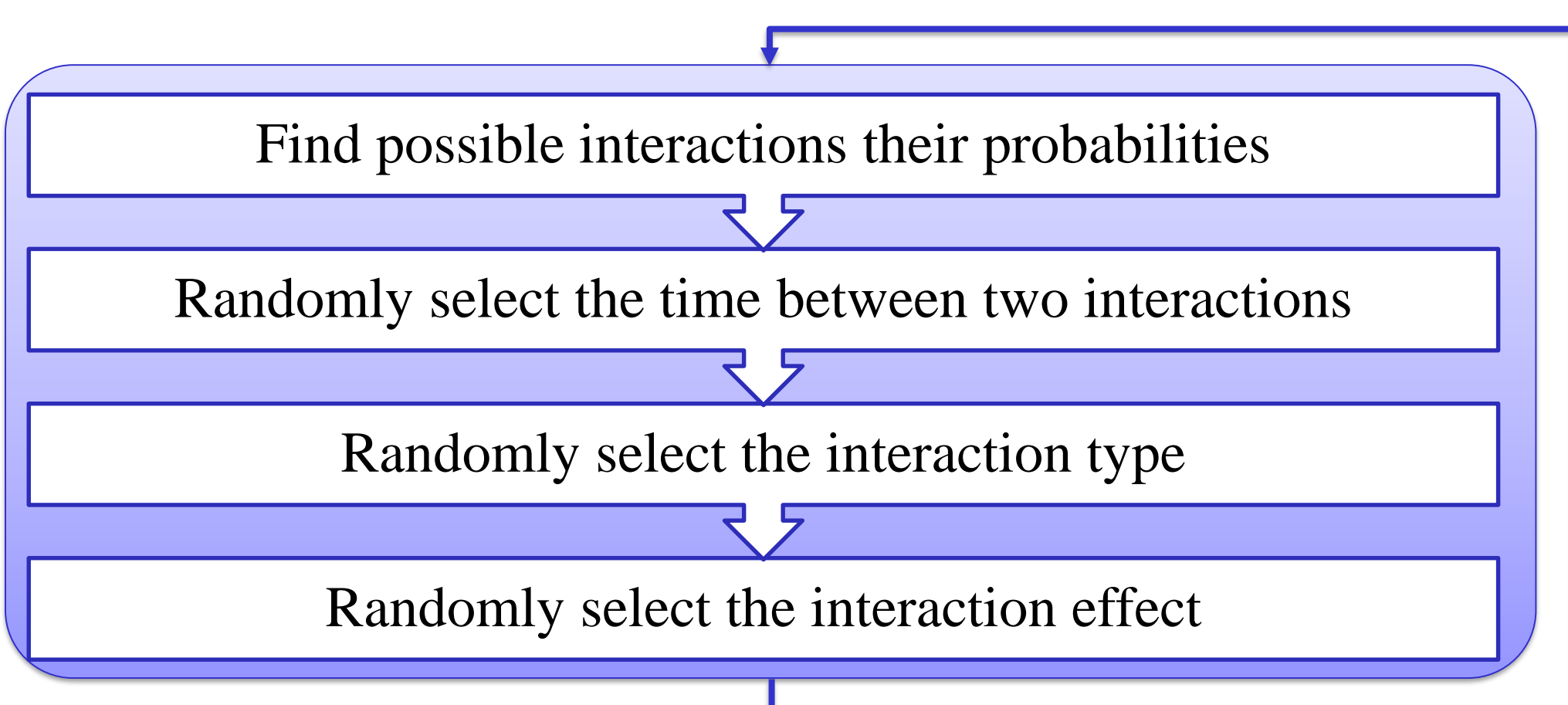
The model allies the relevant **geometric** description of [3] to the **simplicity** of [4].



## The model

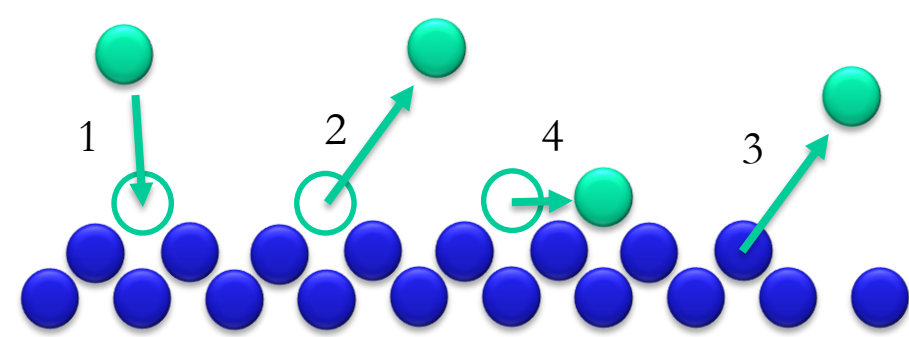
### Kinetic Monte-Carlo modelling

While the layer thickness is under the max thickness:



### Processes taken into account

- Adsorption
- Desorption
- Etching
- Surface Migration



### Crystal geometry

- (0 0 1) surface
- Projection on (1 0 0)

### Outputs

- Growth velocity
- Surface roughness
- Number of vacancies

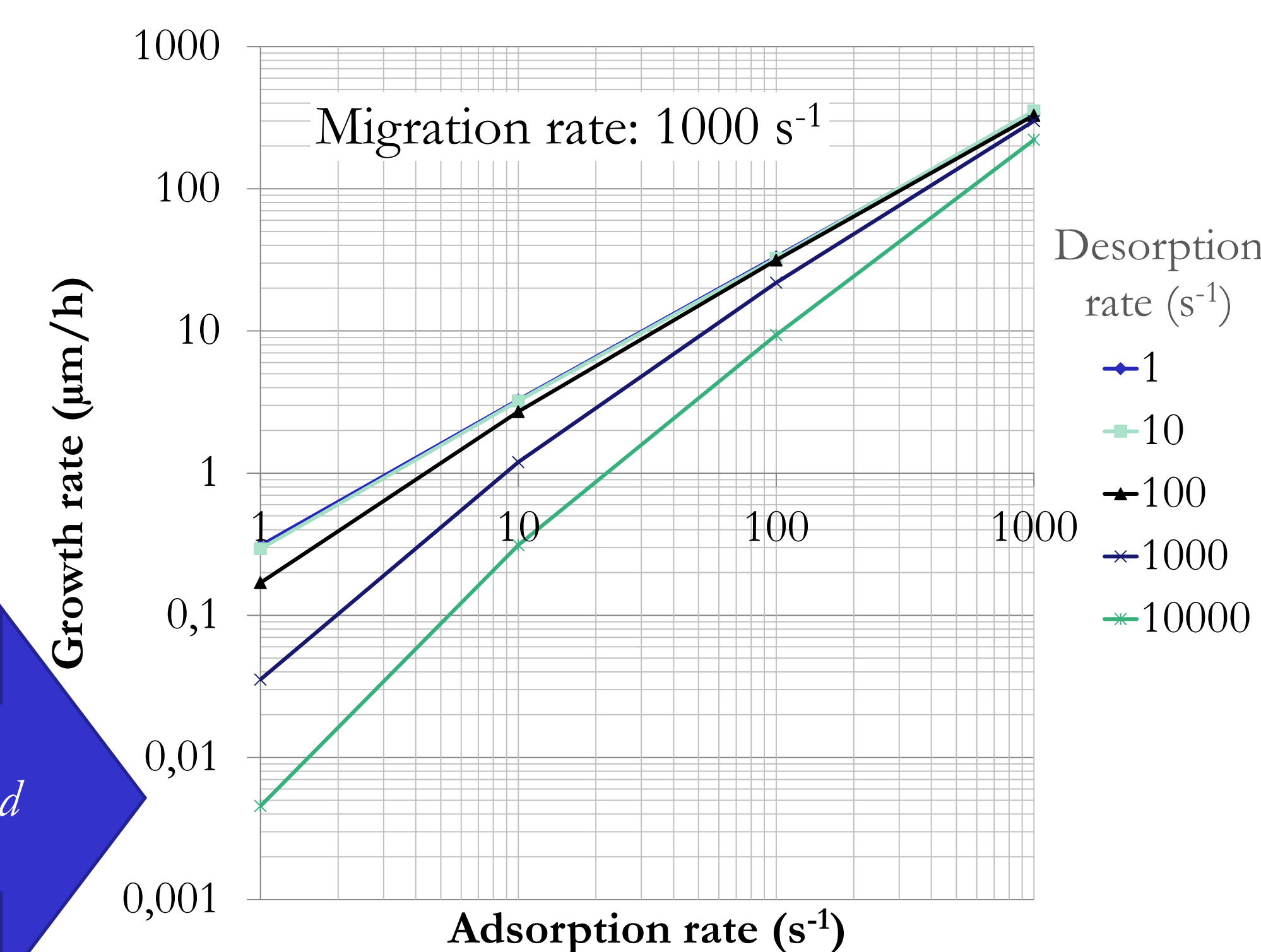
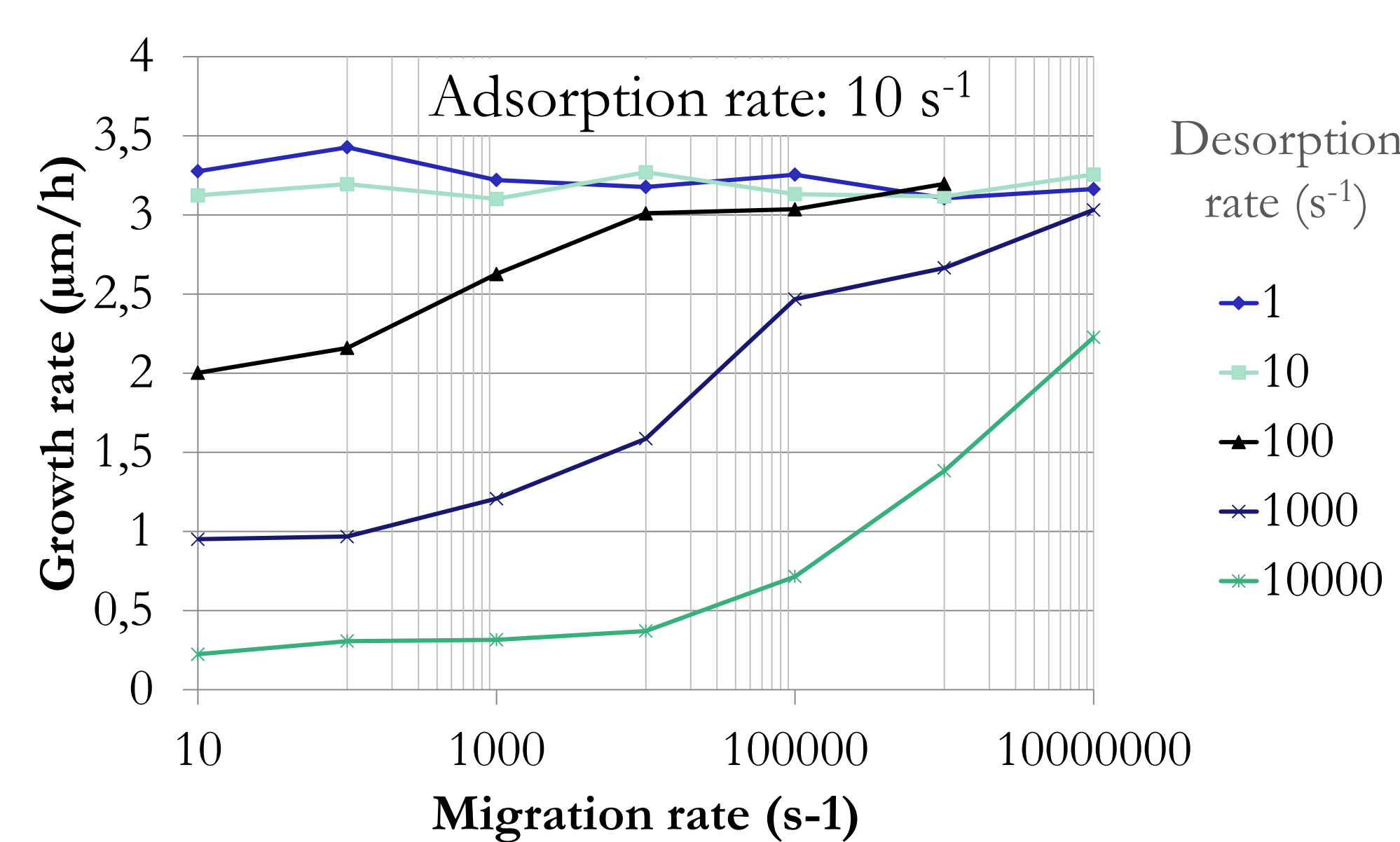
### Parameters

- Adsorption rate  $\Gamma_A$
- Desorption rate  $\Gamma_D$
- Etching rate  $\Gamma_E$
- Surface migration rate  $\Gamma_M$

## Influence of the parameters

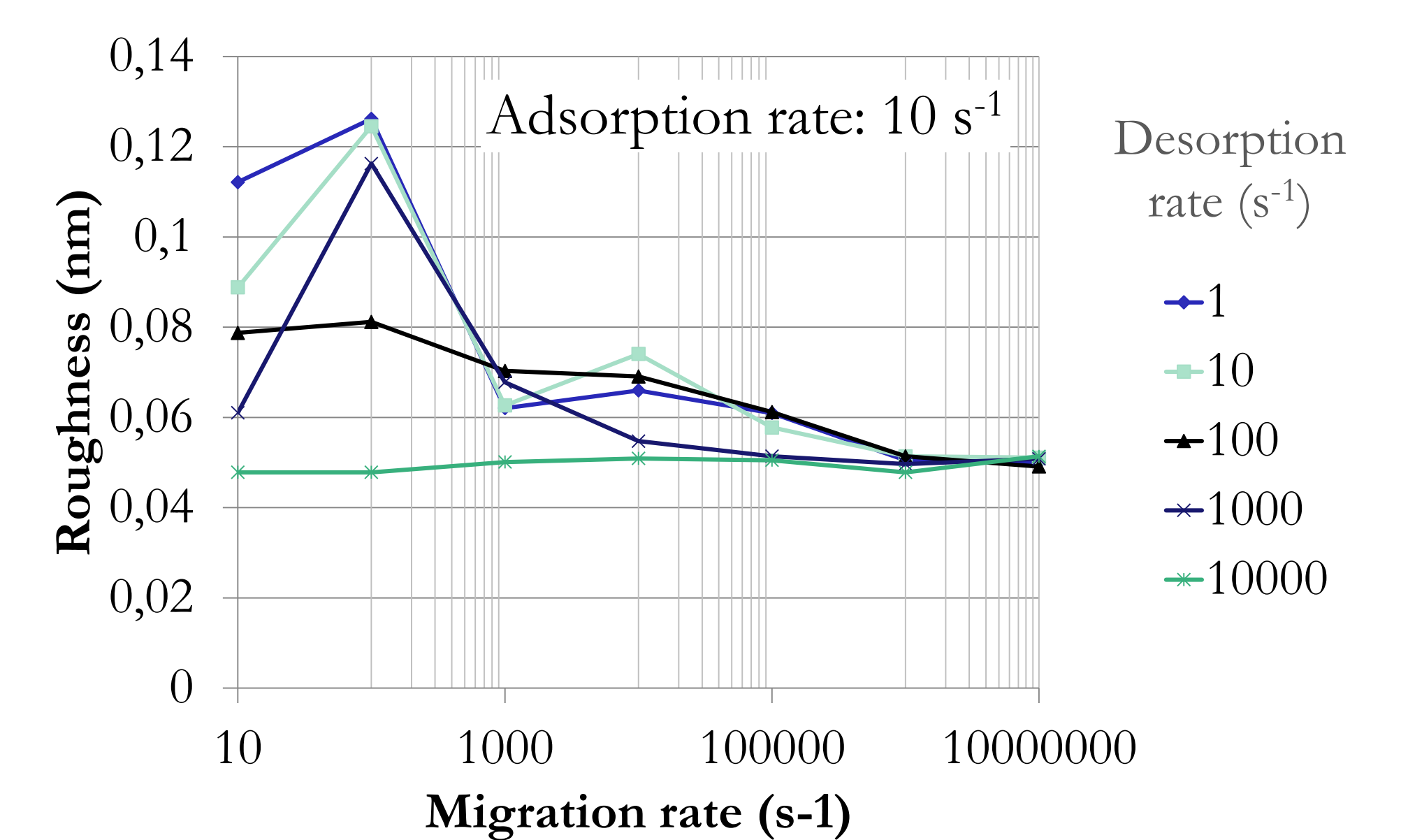
### Growth rates

Etching turned off



### Roughness

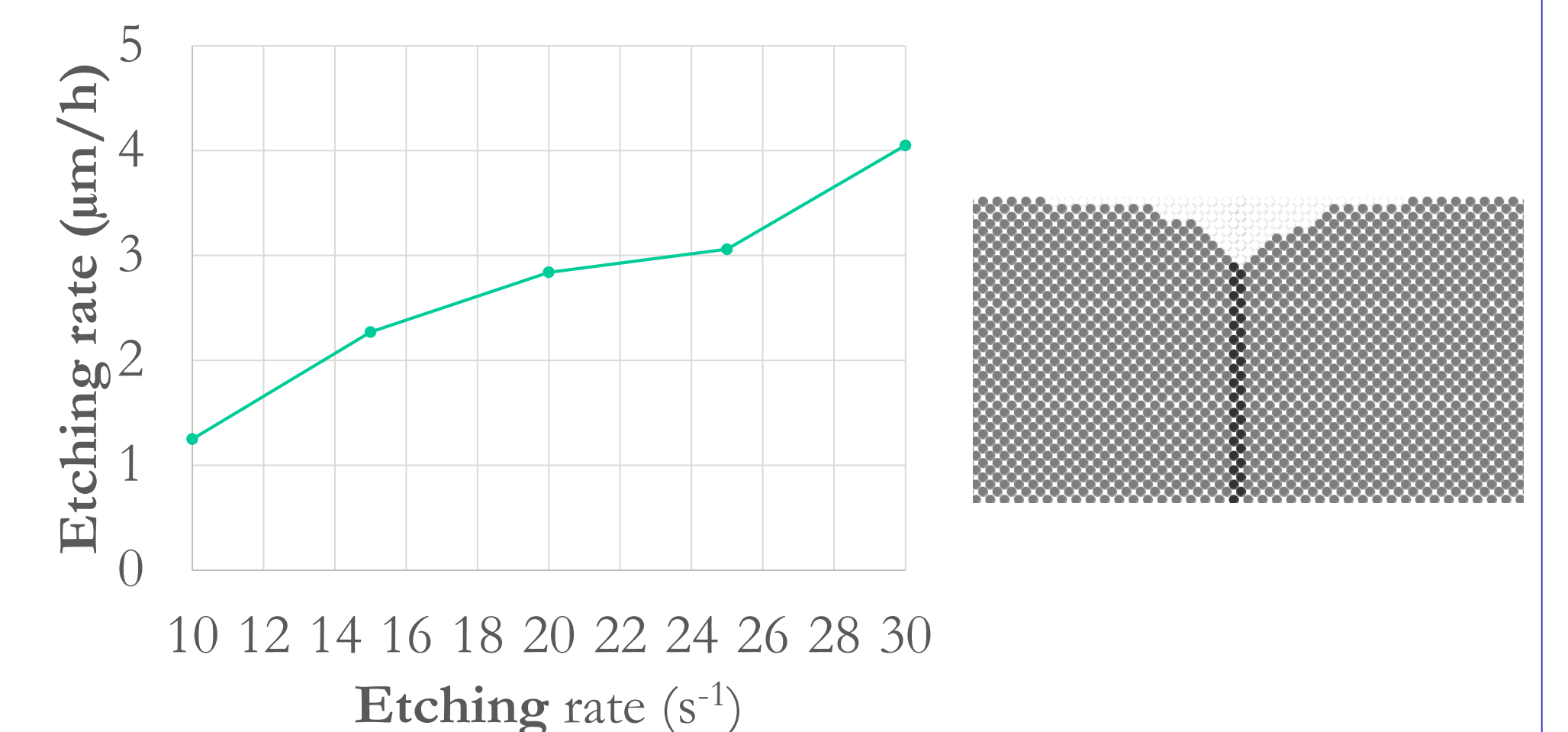
Etching turned off



### Etching velocities

Adsorption turned off

Etching of a layer with a line of defects



## Comparison to experiment

### Conditions

- Adsorption and migration rates are taken from [4-6]
- Desorption rate is fixed to  $10^5 \text{ s}^{-1}$

### Results

- The order of magnitude and the tendencies are correct
- The growth rates are overestimated but closer to experiment than results obtained with desorption rates calculated with [4-5]

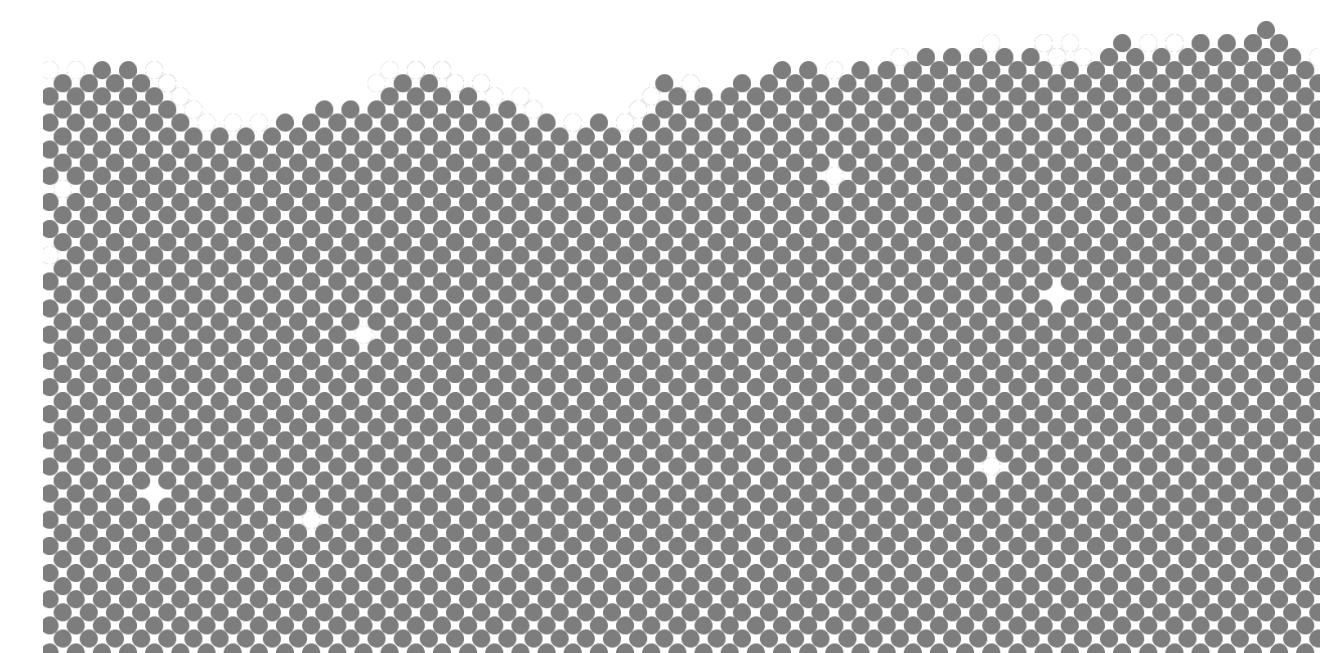
(200 mbar / 3 kW)

Conditions		Growth rates (μm/h)	
[CH <sub>4</sub> ]	T (°C)	Experimental [7]	Simulated
2 %	850	1.5	5.6
4 %		5.5	6.5
6 %		11	10
8 %		15	25.5
4 %	750	3.5	2.7
	850	5.5	6.5
	950	11	17.15

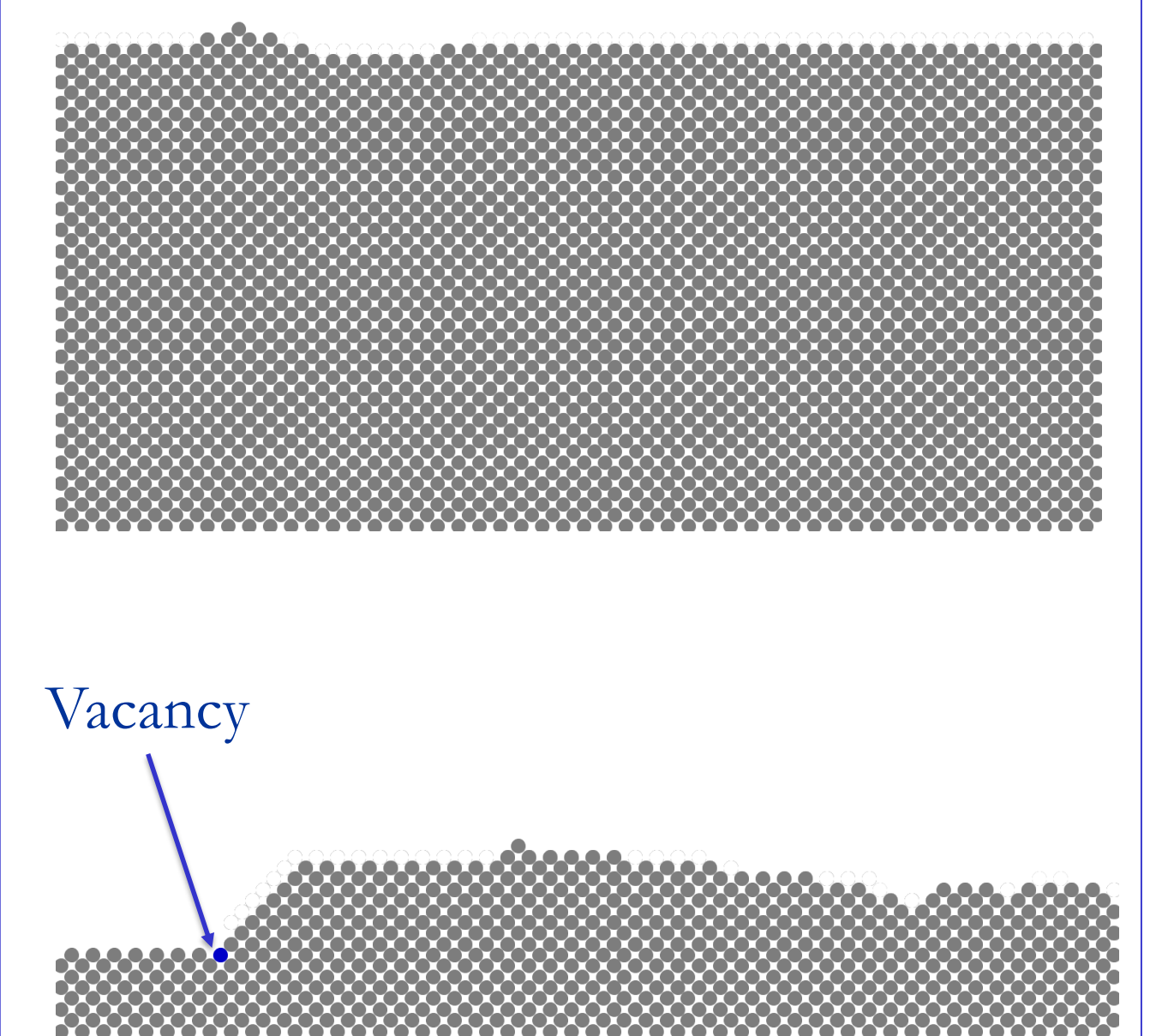
## Surface morphologies

- Increase of migration and/or desorption leads to a smoother surface
- Vacancies appear at low migration and desorption rates
- Vacancies are responsible for the appearance of macro-steps

$$\begin{aligned} \Gamma_A &= 10 \\ \Gamma_D &= 10 \\ \Gamma_E &= 0 \\ \Gamma_M &= 100 \end{aligned}$$



$$\begin{aligned} \Gamma_A &= 10 ; \Gamma_D = 10000 \\ \Gamma_E &= 0 ; \Gamma_M = 10000 \end{aligned}$$



## Conclusion and perspectives

- The results are consistent with simulations by other authors [3-6]
- Taking into account the crystal geometry leads to the appearance of vacancies and faces
- The rate calculation must be improved
- Defects (impurities and dislocations) and misorientation will be taken into account

## References

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- [3] M. Grujicic, M. & S. G. Lai, Journal of Materials Science 35, 5359–5369 (2000).
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- [6] A. Netto & M. Frenklach, Diamond and Related Materials 14, 1630–1646 (2005).
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