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2D Monte-Carlo simulation of diamond

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► **To cite this version:**

Audrey Valentin, Ovidiu Brinza, Samir Farhat, Fabien Bénédic. 2D Monte-Carlo simulation of diamond. Surface and Bulk Defects in Diamond (SBDD) XXV, Mar 2020, Hasselt, Belgium. hal-03578178

HAL Id: hal-03578178

<https://hal-cnrs.archives-ouvertes.fr/hal-03578178>

Submitted on 17 Feb 2022

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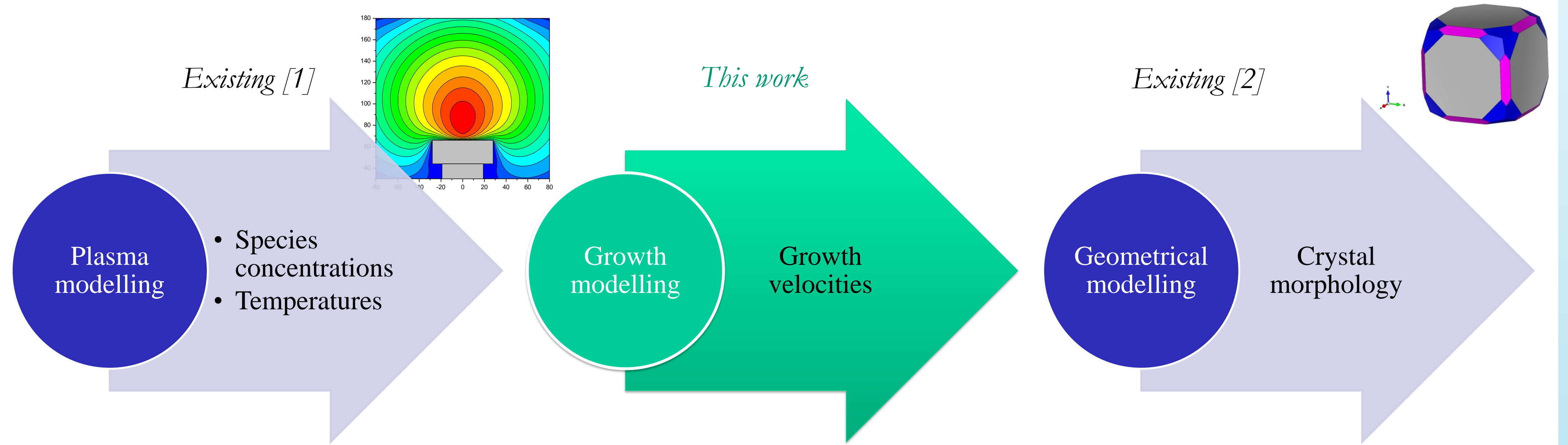
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Context

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

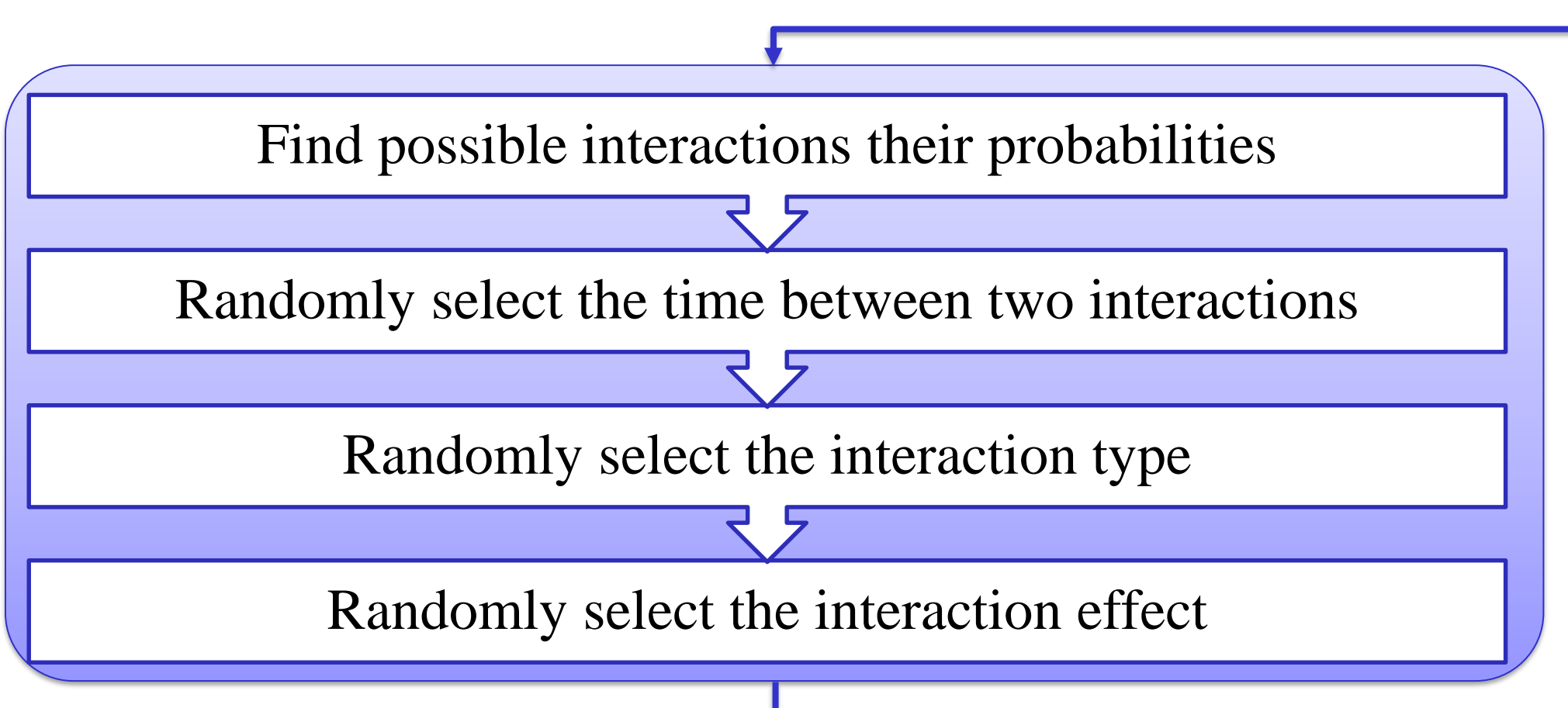
The model allies the relevant **geometric** description of [3] to the **simplicity** of [4].



The model

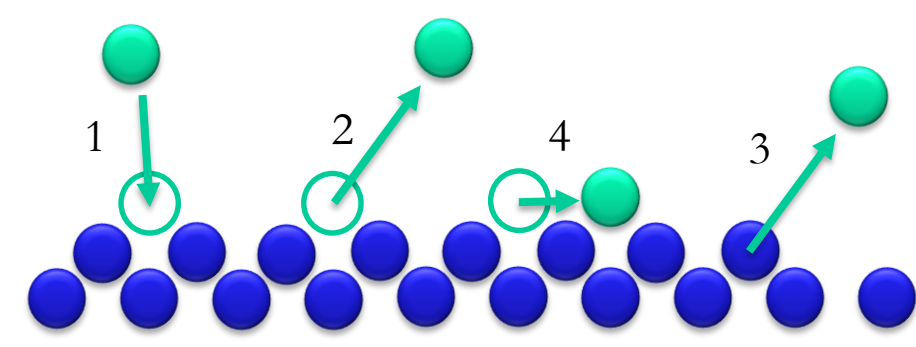
Kinetic Monte-Carlo modelling

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

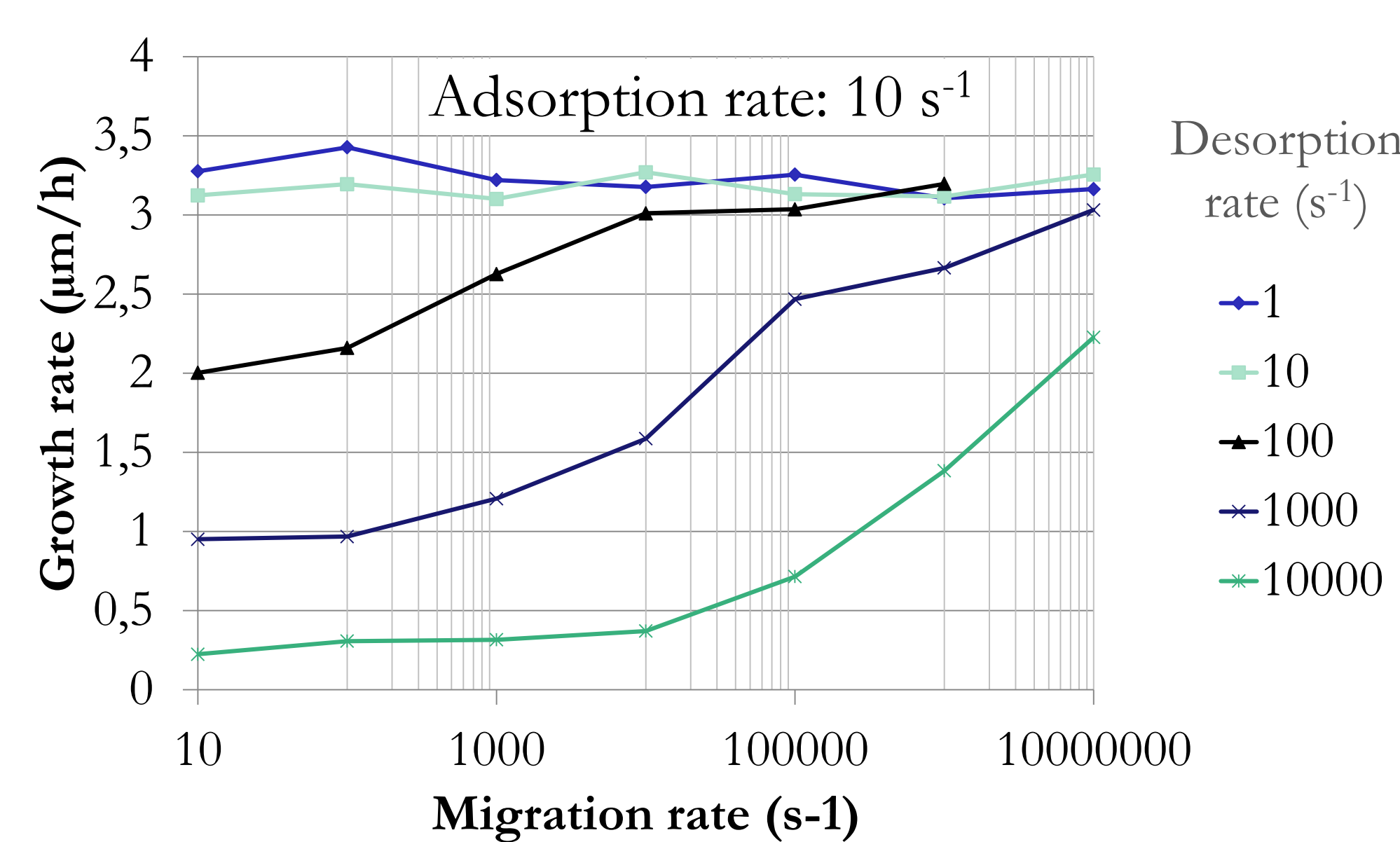
Parameters

- Adsorption rate Γ_A
- Desorption rate Γ_D
- Etching rate Γ_E
- Surface migration rate Γ_M

Influence of the parameters

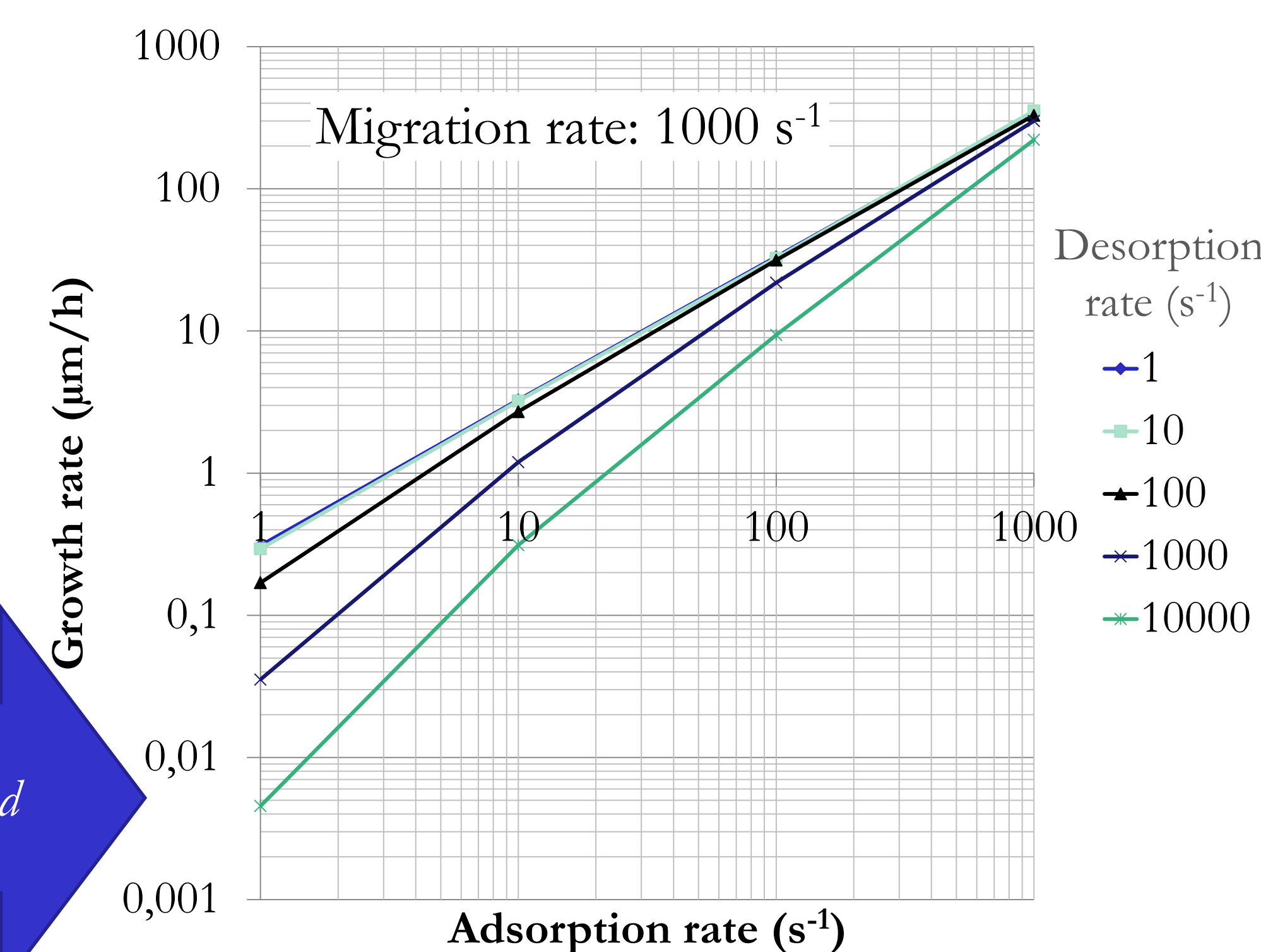
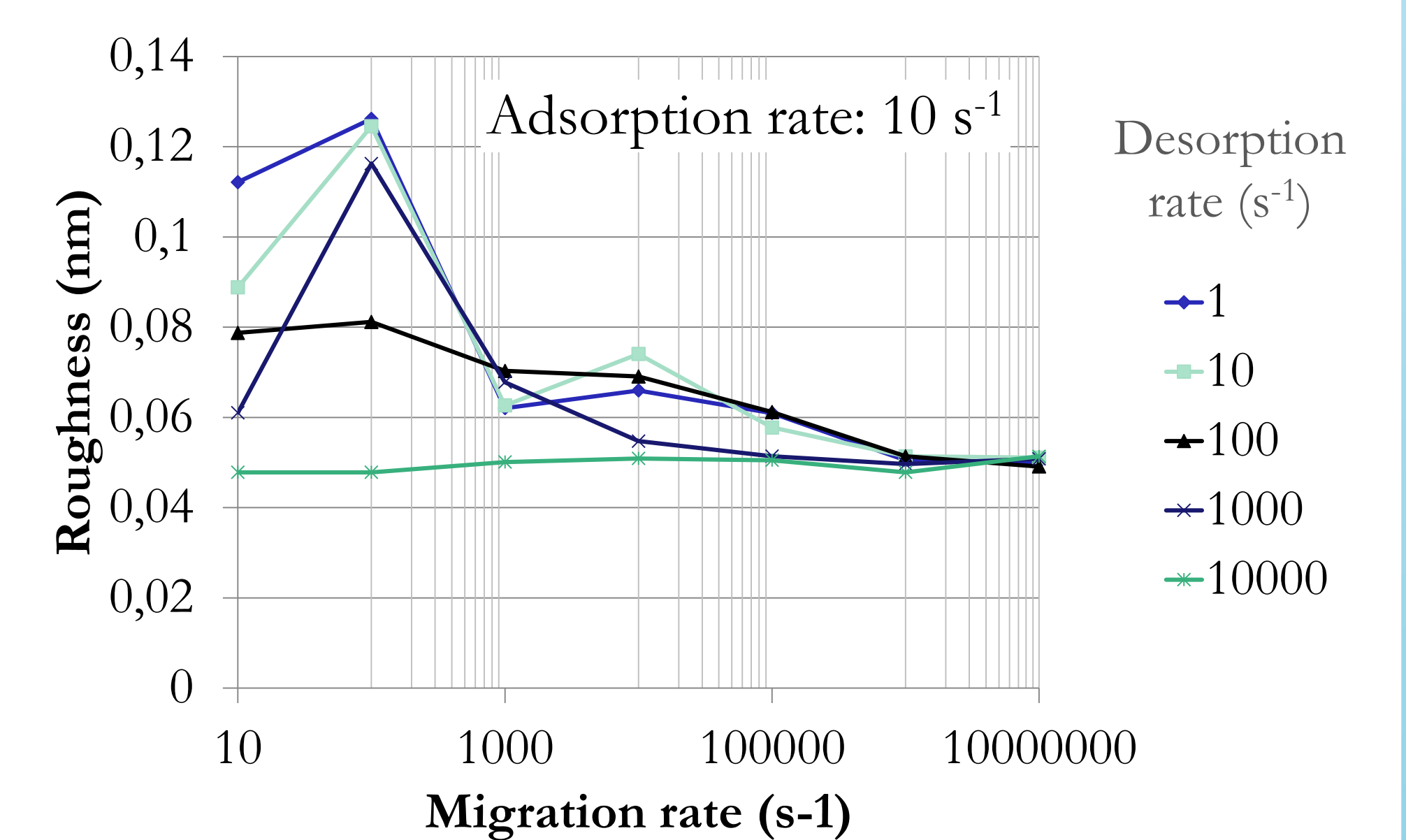
Growth rates

Etching turned off



Roughness

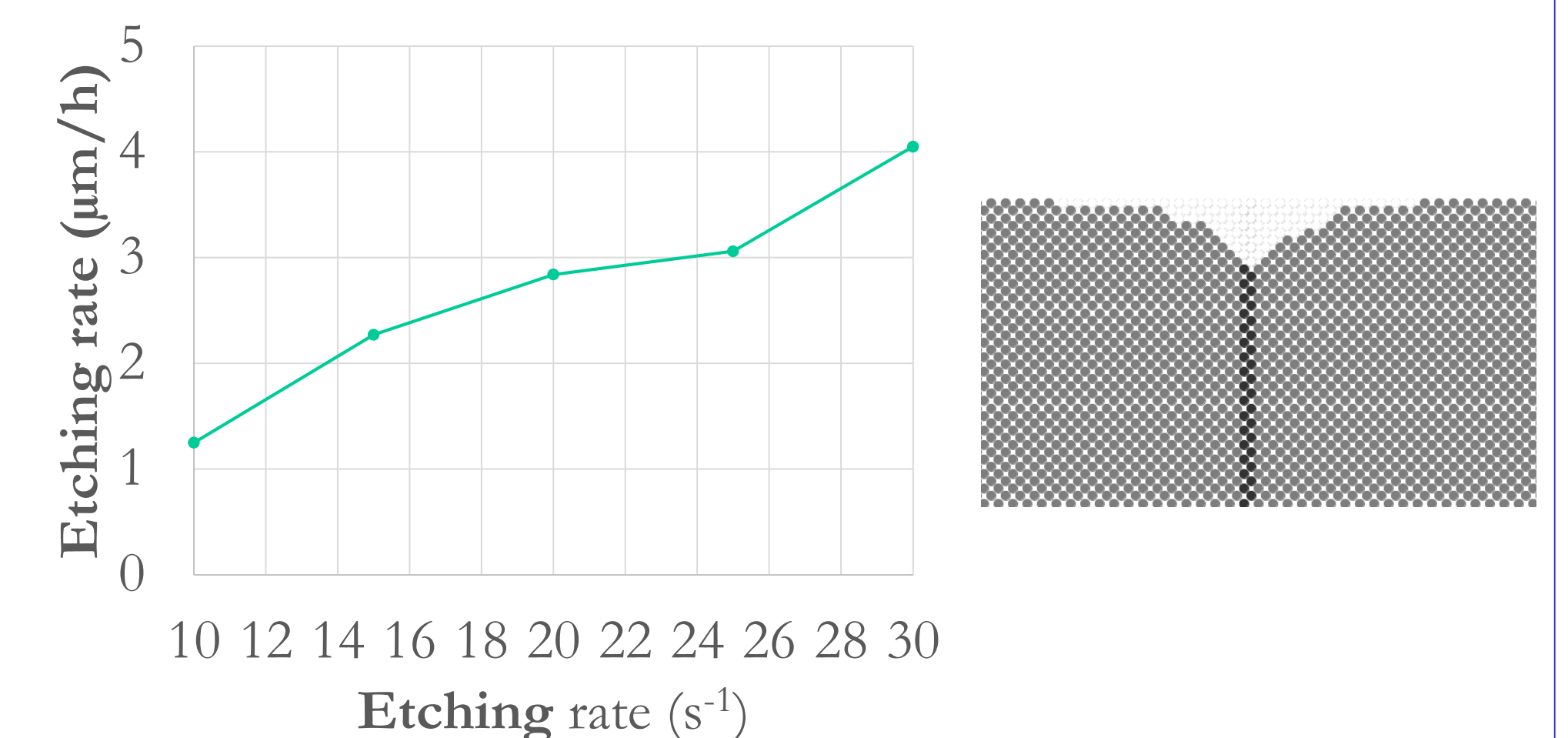
Etching turned off



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 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]

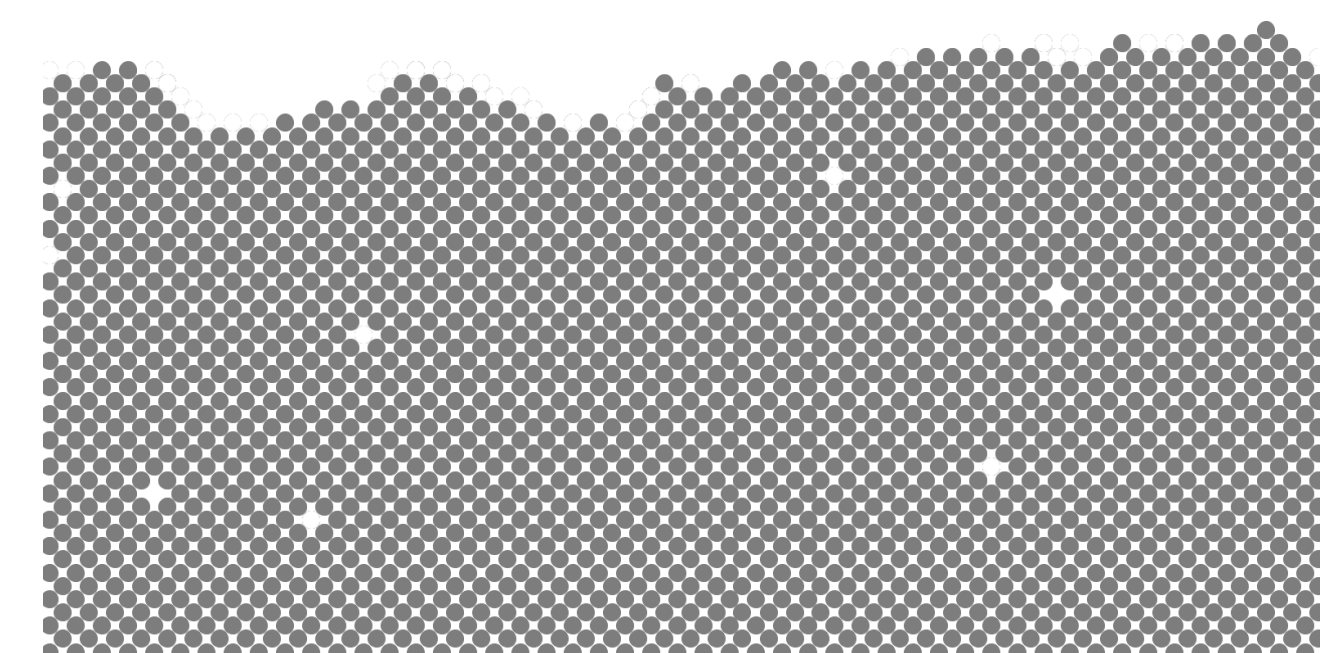
(200 mbar / 3 kW)

Conditions		Growth rates (µm/h)	
[CH ₄]	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

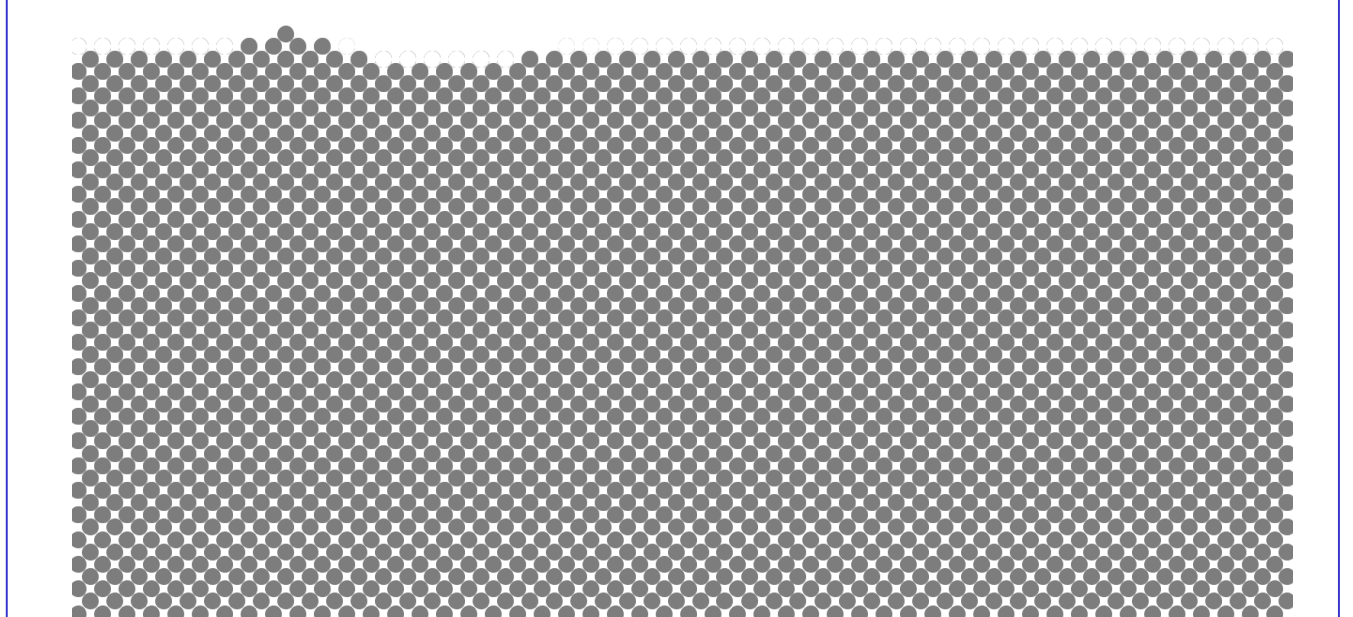
Surface morphologies

- 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

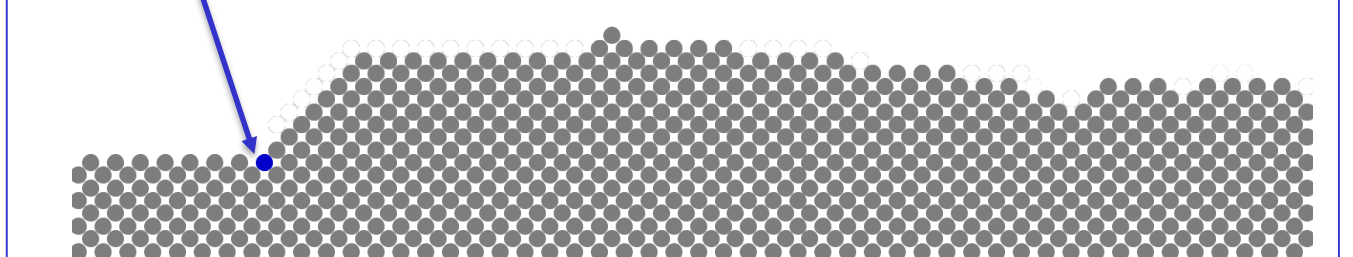
$\Gamma_A = 10$
 $\Gamma_D = 10$
 $\Gamma_E = 0$
 $\Gamma_M = 100$



$\Gamma_A = 10$; $\Gamma_D = 10000$
 $\Gamma_E = 0$; $\Gamma_M = 10000$



Vacancy



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

- [1] S. Prasanna *et al.* Plasma Sources Sci. Technol. 26, 097001 (2017).
- [2] F. Silva *et al.* Physica Status Solidi (a) 203, 3049–3055 (2006).
- [3] M. Grujicic, M. & S. G. Lai, Journal of Materials Science 35, 5359–5369 (2000).
- [4] P. W. May *et al.* J. Phys.: Condens. Matter 21, 364203 (2009).
- [5] W. Rodgers *et al.* Chem. Phys. 142, 214707 (2015).
- [6] A. Netto & M. Frenklach, Diamond and Related Materials 14, 1630–1646 (2005).
- [7] O. Brinza *et al.* Physica Status Solidi (a) 205, 2114–2120 (2008).