2D Monte-Carlo simulation of diamond

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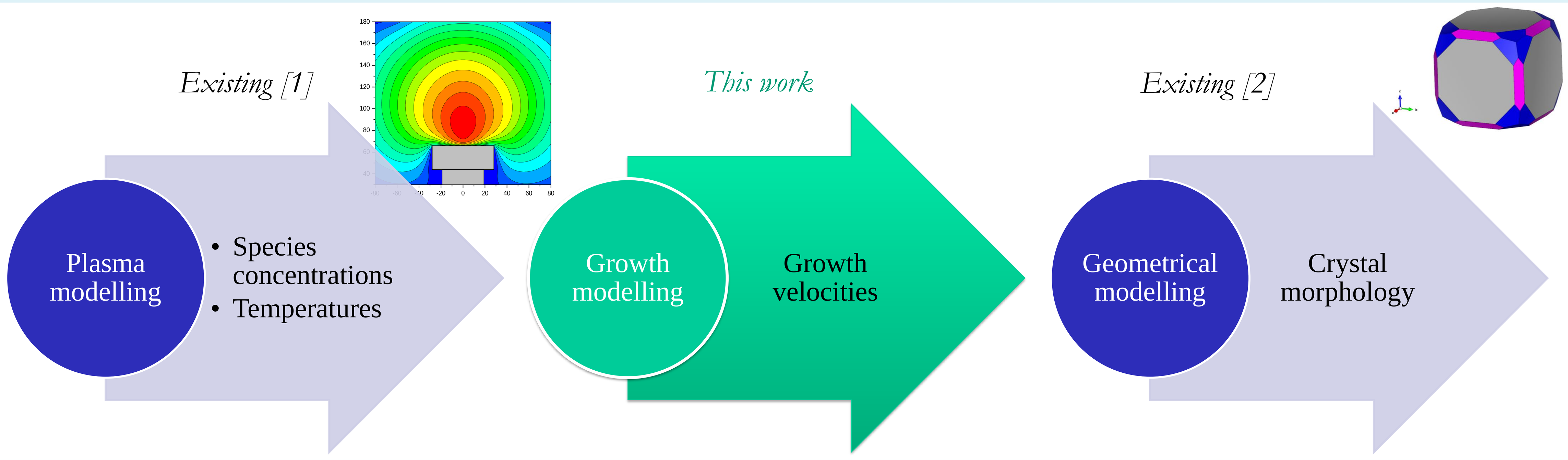
Context

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

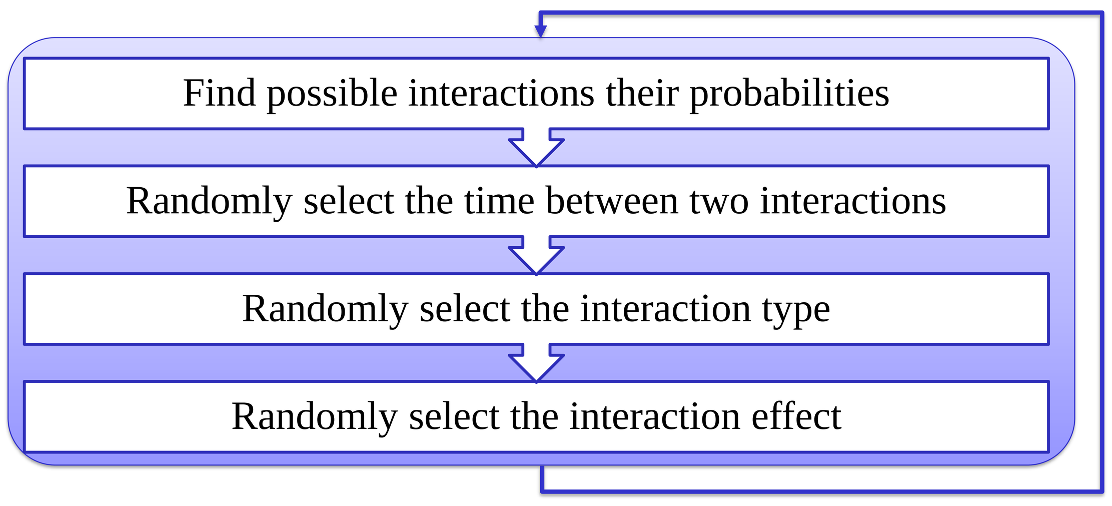
The model allies the relevant **geometric** description of [3] to the **simplicity** of [4].



The model

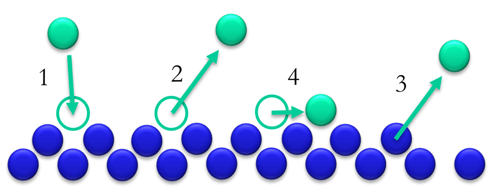
Kinetic Monte-Carlo modelling

While the layer thickness is under the max thickness:



Processes taken into account

1. Adsorption
2. Desorption
3. Etching
4. 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

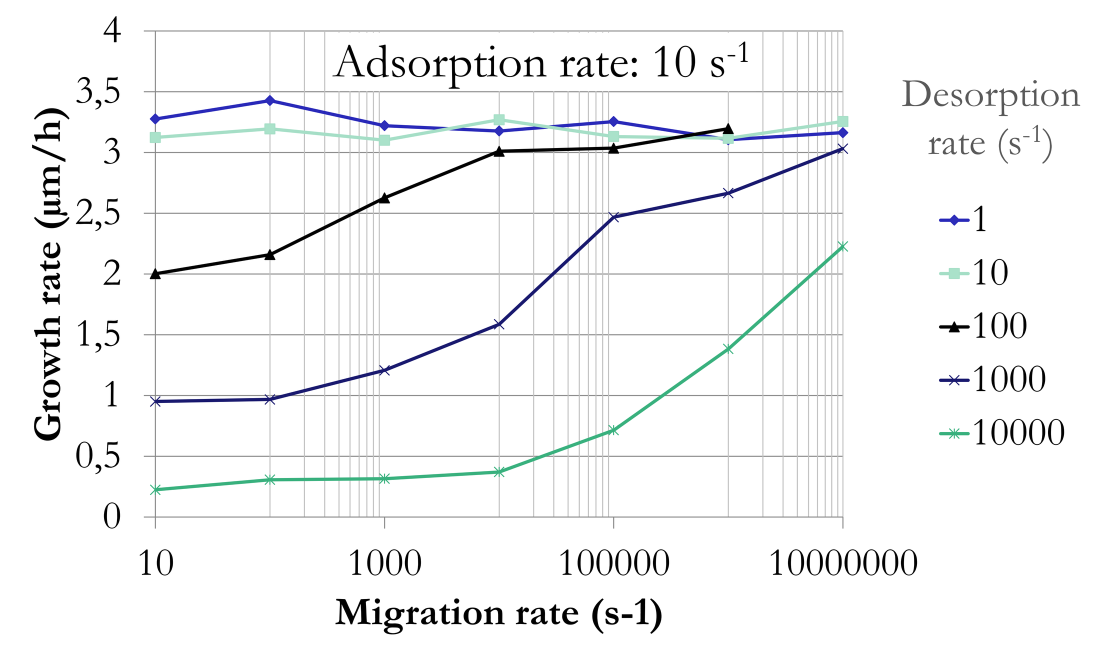
Fitted

Calculated

Influence of the parameters

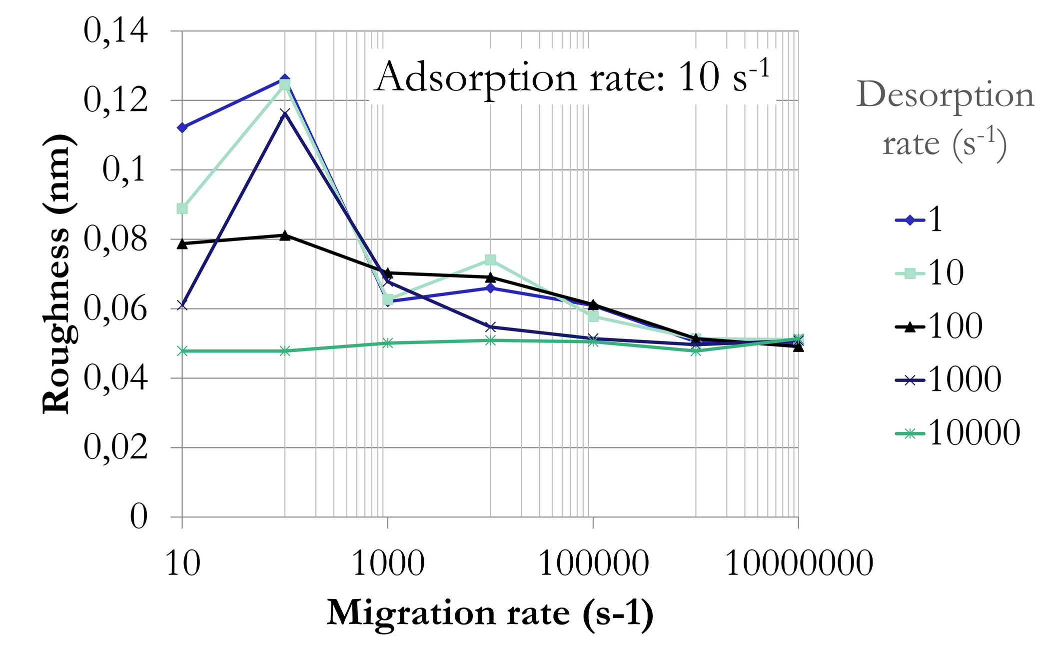
Growth rates

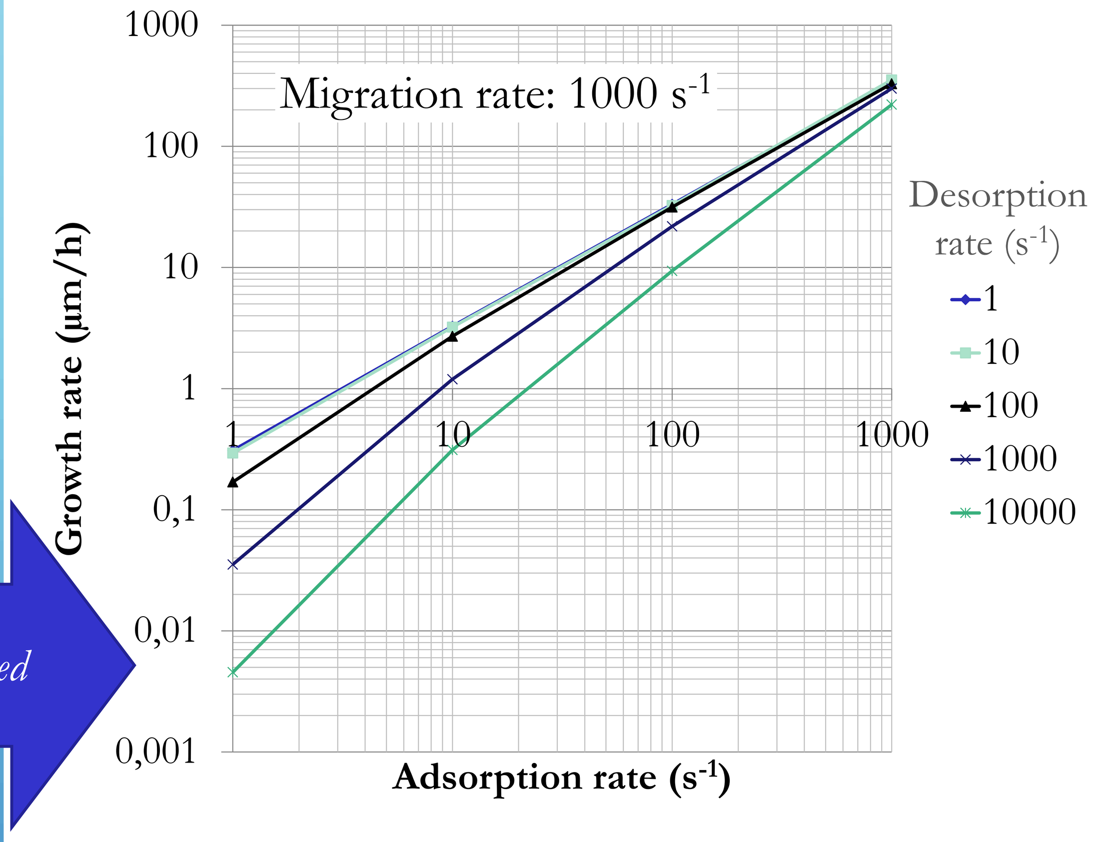
Etching turned off



Roughness

Etching turned off

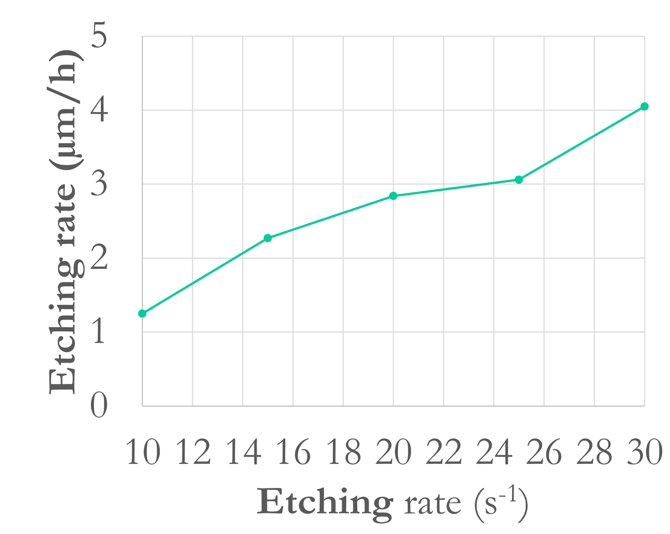


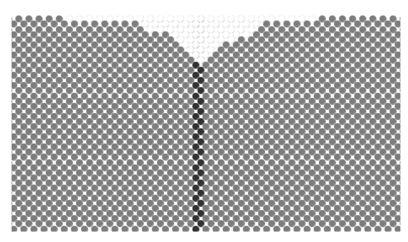


Etching velocities

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 tendancies are correct
- The growth rates are overestimated but closer to experiment than results obtained with desorption rates calculated with [4-5]

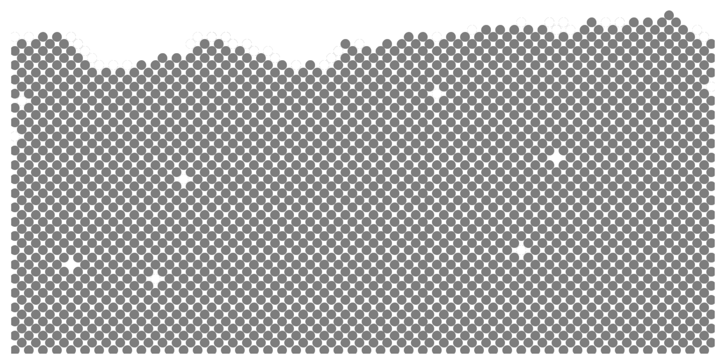
(200 mbar / 3 kW)

Conditions		Growth rates (µm/h)	
[CH_4]	T (°C)	Experimental [7]	Simulated
2 %	850	1.5	5.6
4 %	850	5.5	6.5
6 %	850	11	10
8 %	850	15	25.5
4 %	750	3.5	2.7
4 %	850	5.5	6.5
4 %	950	11	17.15

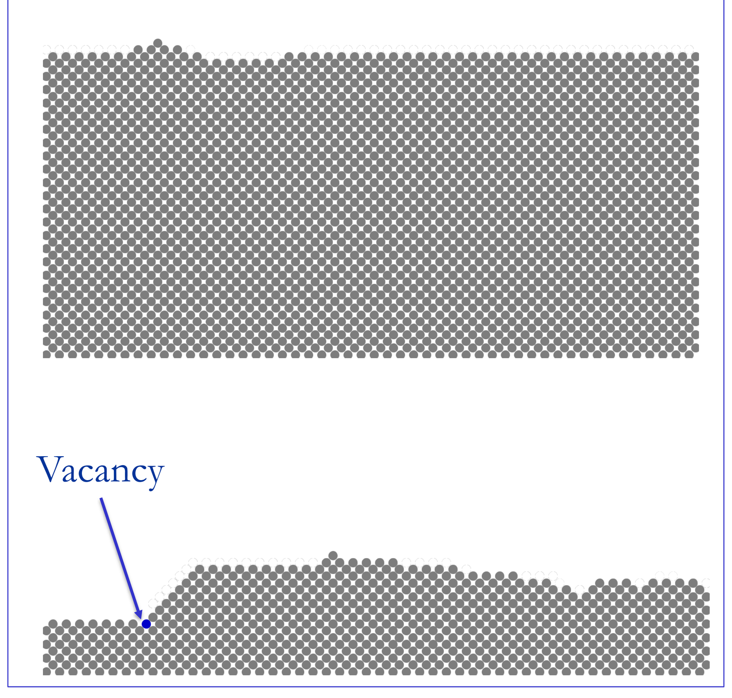
Surface morphologies

- 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

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



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



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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