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Multi-scale simulation of CVD diamond growth: from the experimental conditions to the crystal morphology

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Audrey Valentin, Divine Regina Kamkoum-Djouka, Ovidiu Brinza, Fabien Benedic. Multi-scale simulation of CVD diamond growth: from the experimental conditions to the crystal morphology. SBDD XXVIII, Feb 2024, Hasselt, Belgium. hal-04643855

HAL Id: hal-04643855

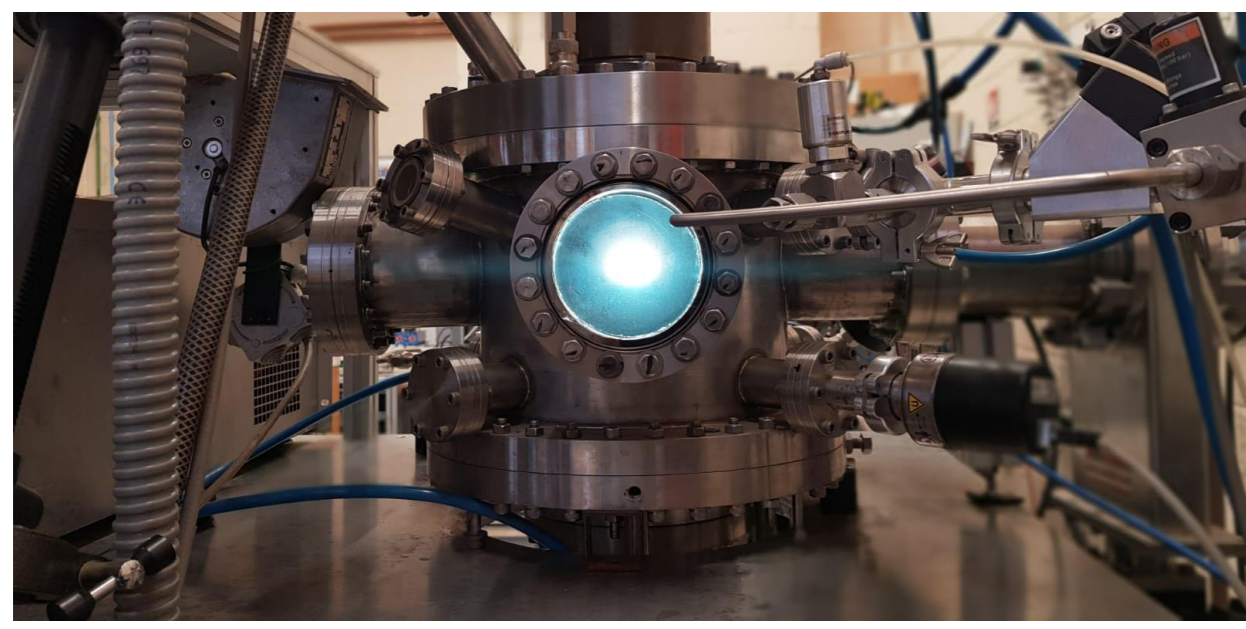
<https://hal.science/hal-04643855v1>

Submitted on 10 Jul 2024

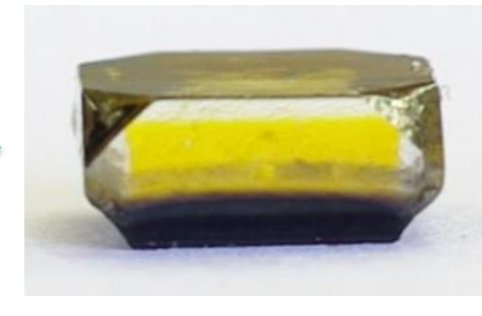
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Context

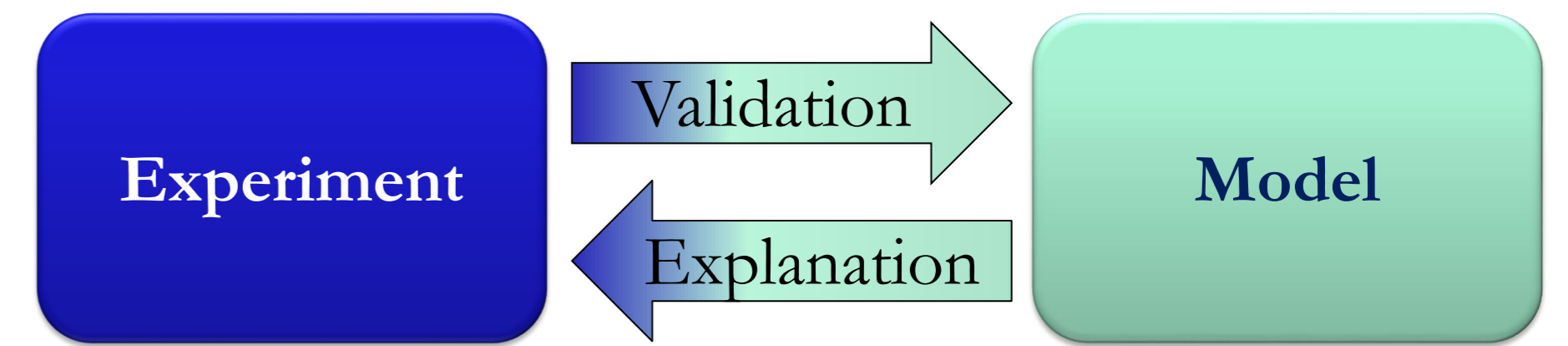


Several scales
? →
Physico-chemical phenomena



Objectives of this work

- Build a multi-scale simulation tool that reproduces the available experimental data
- Use this model to highlight the underlying mechanisms of diamond growth

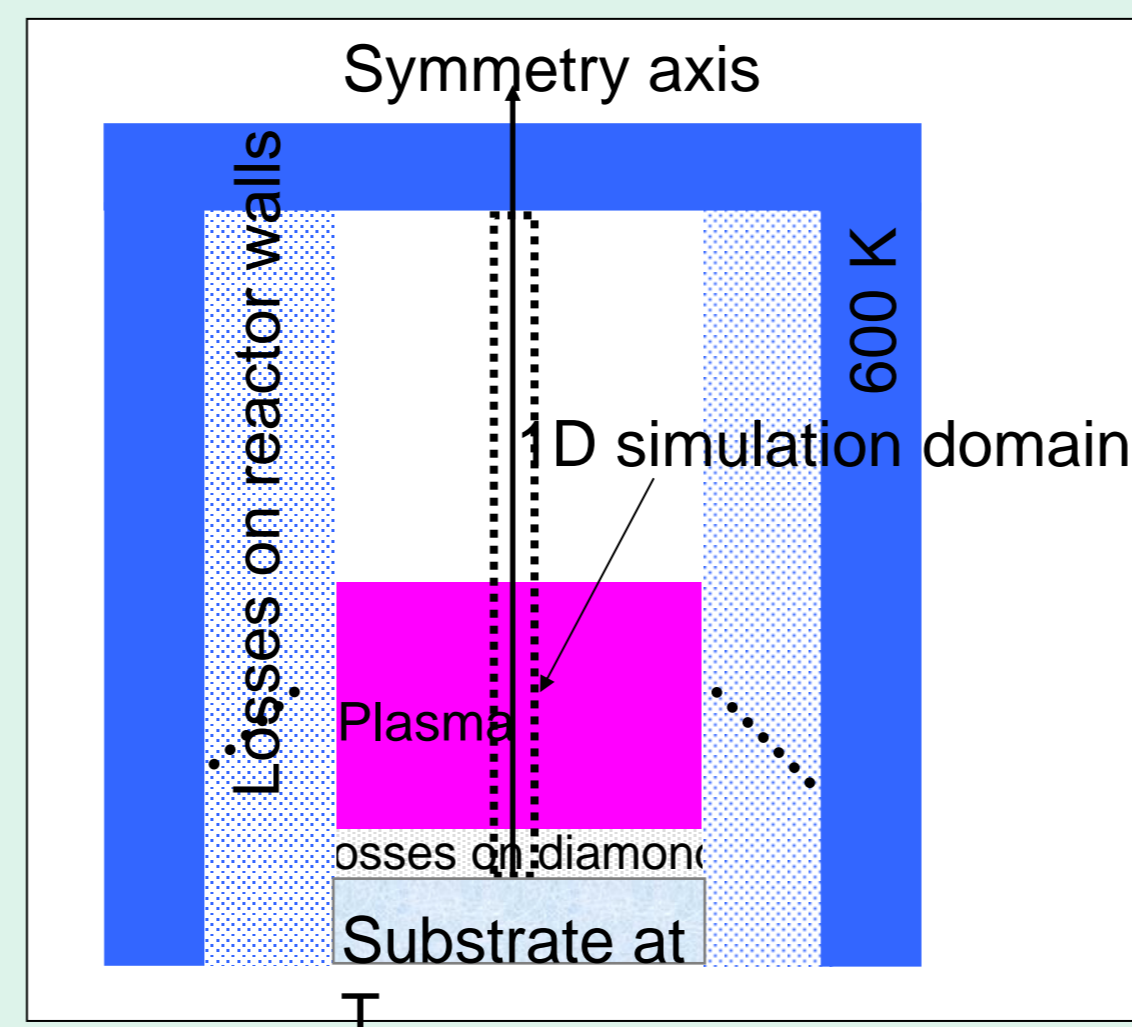


The plasma model

Computational details [1]

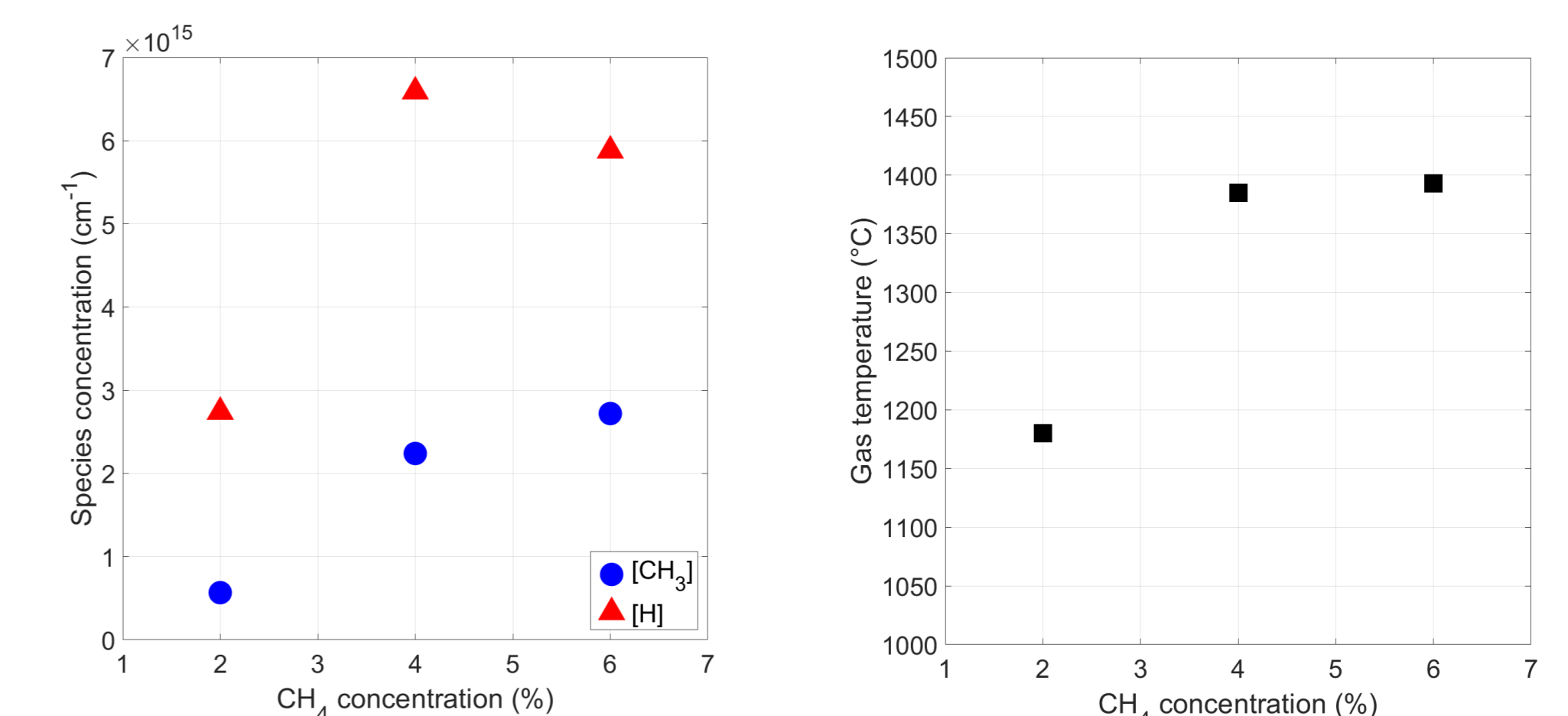
1D CH₄/H₂ axial plasma model

- Thermo-chemical model of non-equilibrium plasma:
 - 2 energy modes: T_g and eedf
 - 28 species / 131 reactions H₂, H(n=1-3), H₁₋₃⁺, CH₀₋₄, C₂H₀₋₆, CH₃₋₅⁺, C₂H₂₋₆⁺, e⁻
- Transport = diffusion
- 3 types of equations:
 - Continuity => $[X] \frac{dY_i}{dt} = \frac{W_i}{\rho} \frac{1}{r} \left(\frac{d(rF_r)}{dr} \right)$
 - Electron energy => $T_e \frac{\partial \bar{E}_e}{\partial t} = [PMW - Q_{e-e} - Q_{e-x}] \frac{1}{\rho} \left[\frac{1}{r} \frac{d}{dr} (rF_r^{(NR)}) \right] \frac{1}{\rho}$
 - Total energy => $T_g \frac{\partial \bar{E}}{\partial t} = [PMW - Q_{rad} - S_p] \frac{1}{\rho} \left[\frac{1}{r} \frac{d}{dr} (rF_r^{(NR)}) \right] \frac{1}{\rho}$



Results

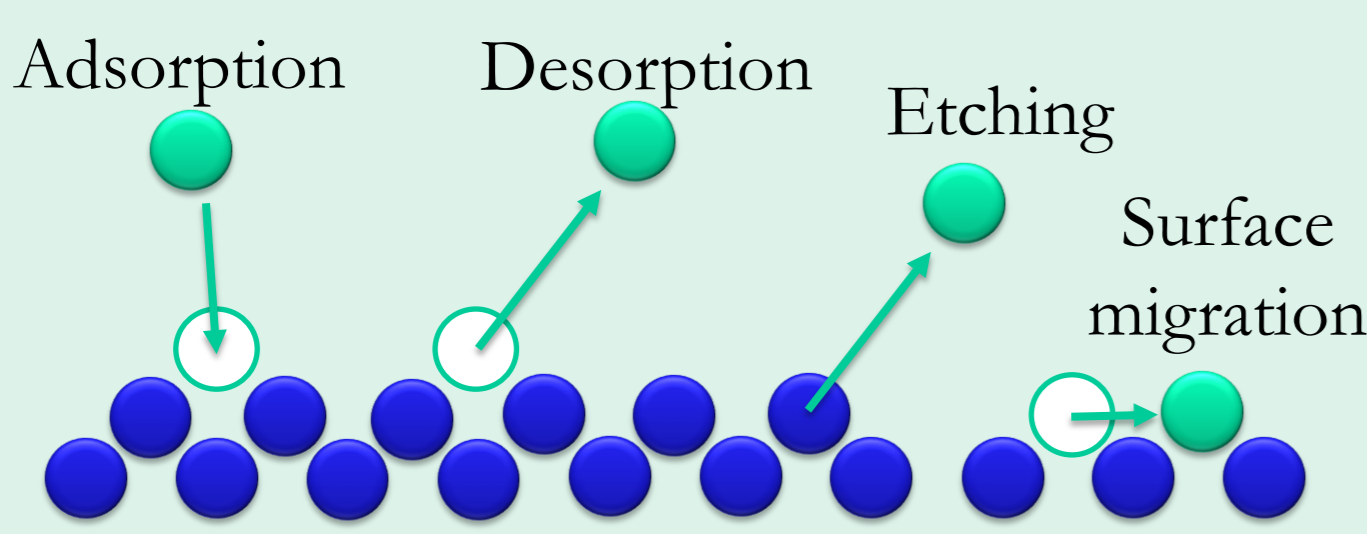
Concentrations and temperatures taken 1 mm from the diamond surface



The Kinetic Monte-Carlo model

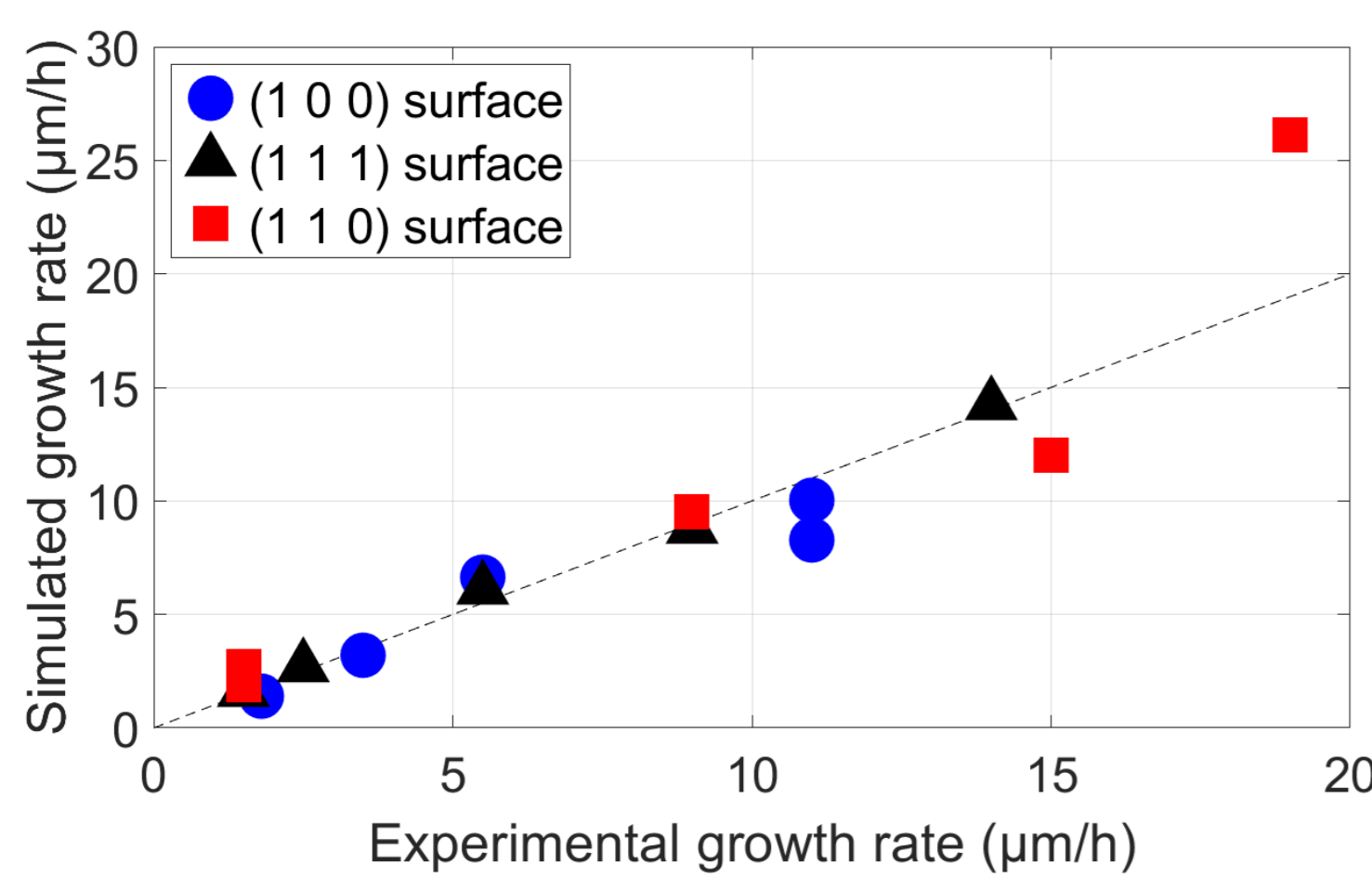
Computational details [2]

- 4 processes taken into account with frequencies calculated from the plasma model
- Realistic geometry with dimer bond formation at the surface



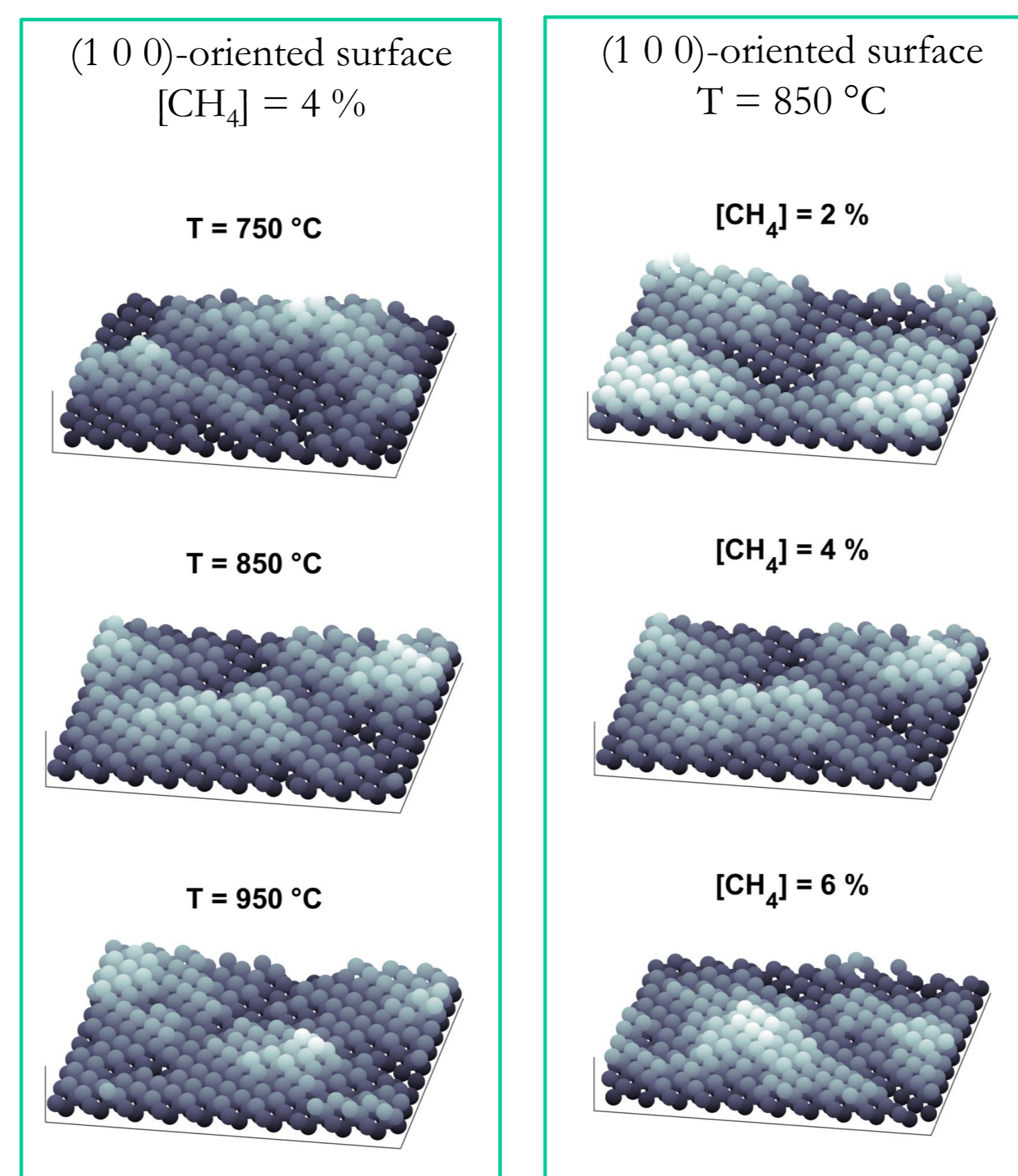
Growth rates

Comparison to experimental data from [4]



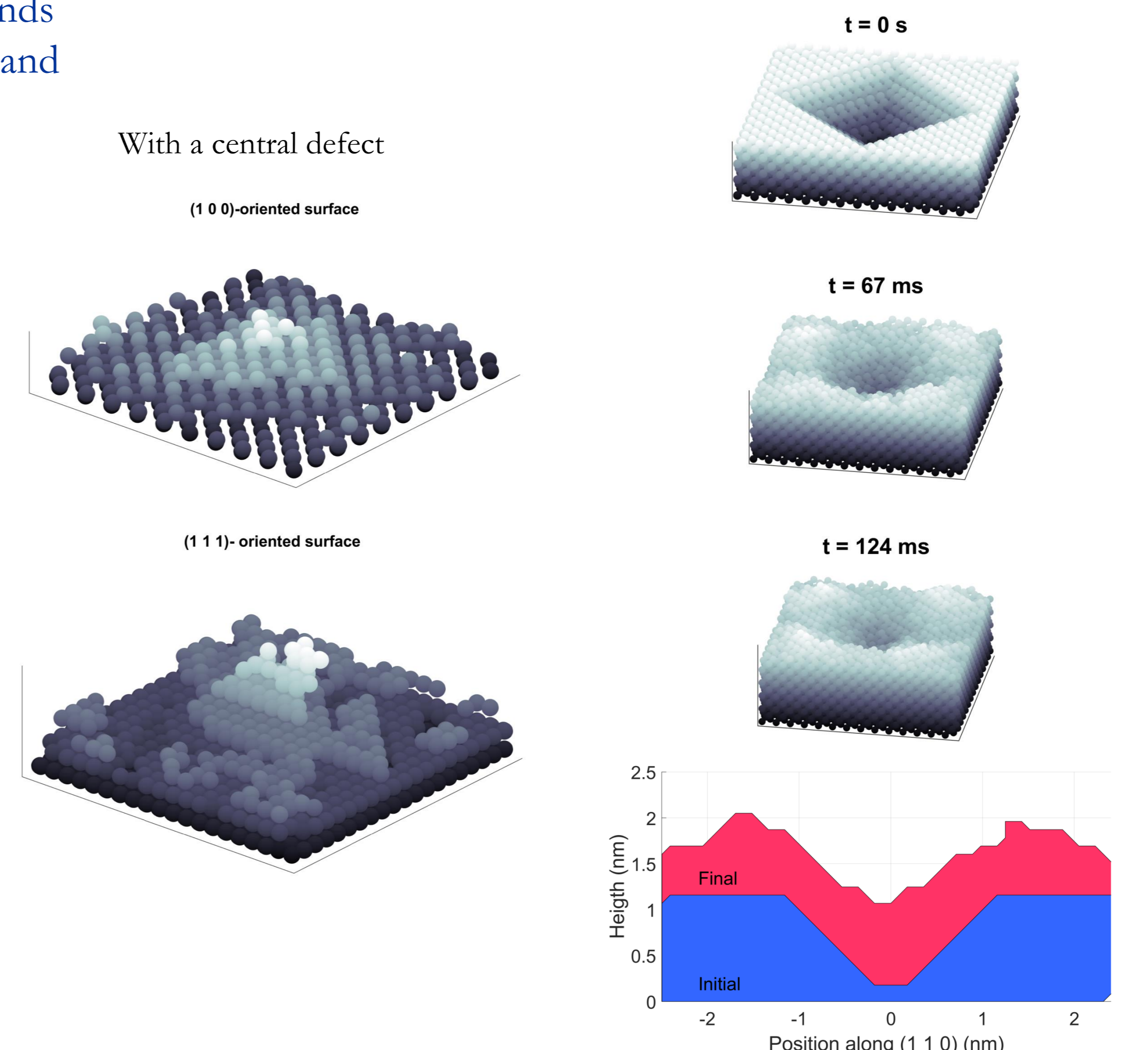
Surface morphologies

- Straighter step edges when the temperature increases or the methane concentration decreases
- (1 0 0)-oriented surfaces: pyramid-shaped islands
- (1 1 1)-oriented surfaces: triangular-shaped island



Growth in a nanometric etch pit

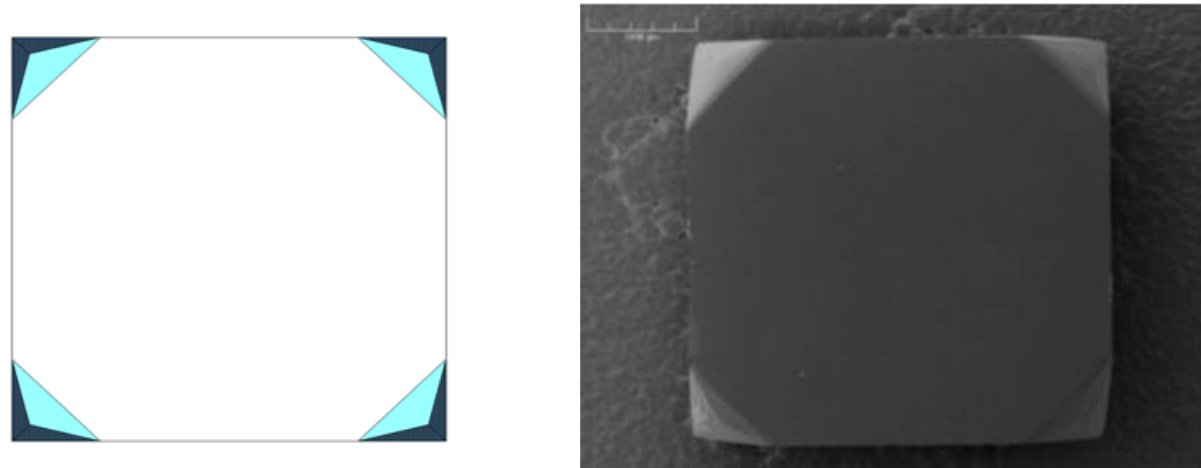
- Flat bottom
- (1 1 1) faces only



The geometric model

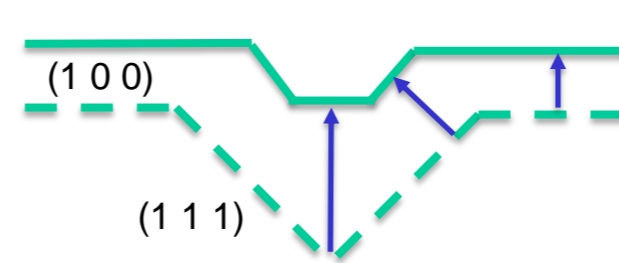
Computational details [3]

- Calculation of the faces positions from their growth rates
- Usually applied to macroscopic cases with experimentally obtained growth rates

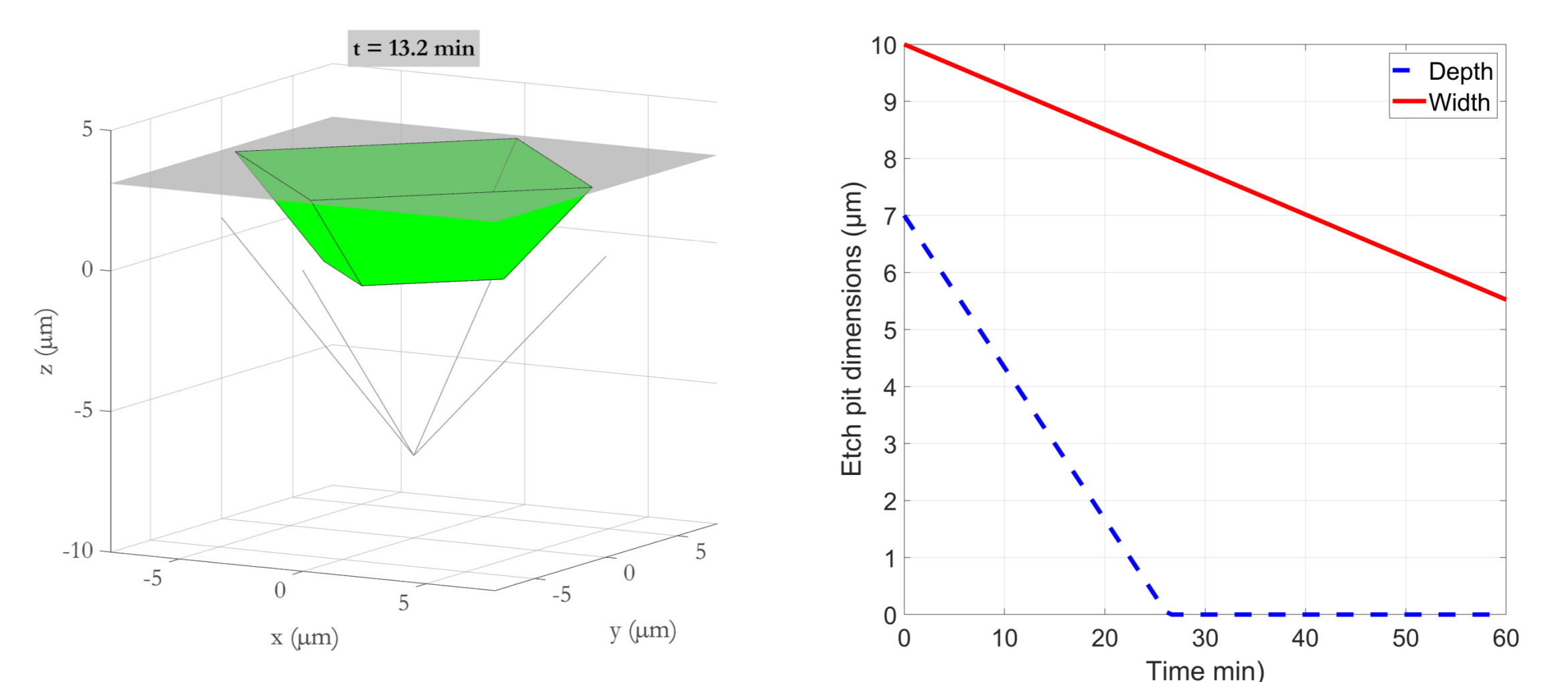


Growth in a micrometric etch pit

- Growth rates inside the etch pits obtained from the KMC model



- Application of the geometric model for etch pits of realistic dimensions



Perspectives

Short term

- Addition of the (1 1 3) surfaces in the KMC model
- Application of this framework to different conditions and reactors

Long term

- Study of point defects
- Study of extended defects
- Application to the etching process

References

- [1] G. Lombardi *et al.*, J. Appl. Phys. **98**, 053303 (2005).
- [2] A. Valentin *et al.*, Diam. Relat. Mater. **123**, 108865 (2022).
- [3] F. Silva *et al.*, Phys. Status Solidi A **203**, 3049 (2006).
- [4] O. Brinza *et al.*, Phys. Status Solidi A **205**, 2114 (2008)

Acknowledgement

The ANR project Trampoline (ANR-22-CE51-0019) is gratefully acknowledged for funding