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

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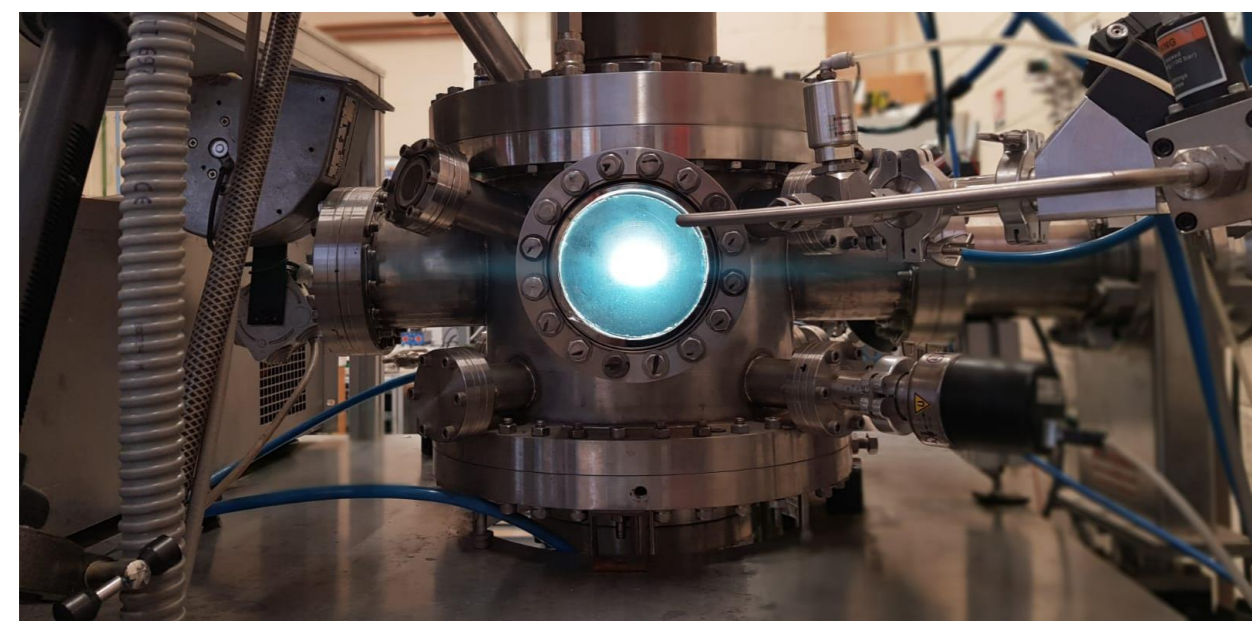
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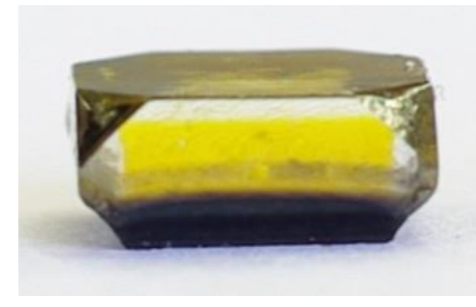


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## Context

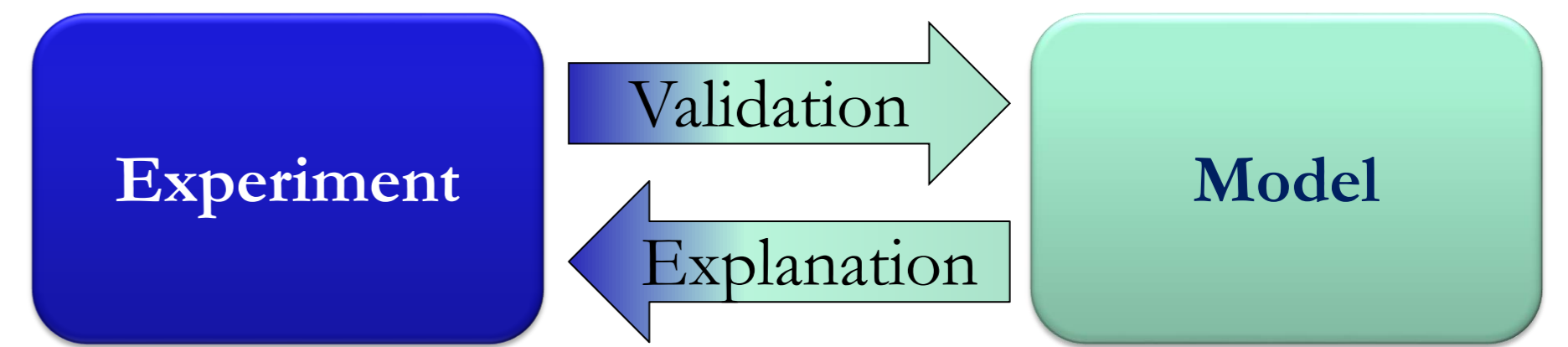


Several scales  
? Physico-chemical phenomena



### 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

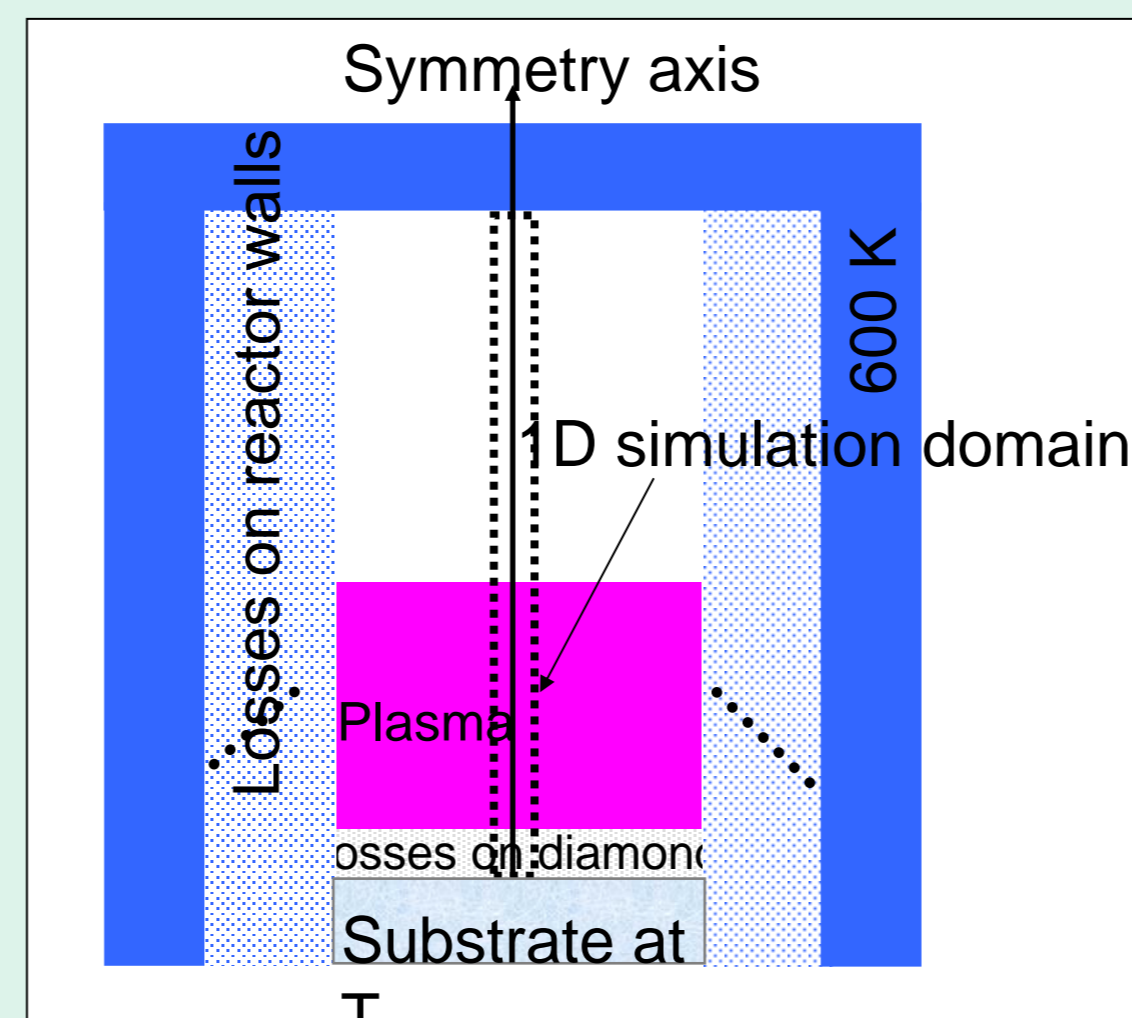


## The plasma model

### Computational details [1]

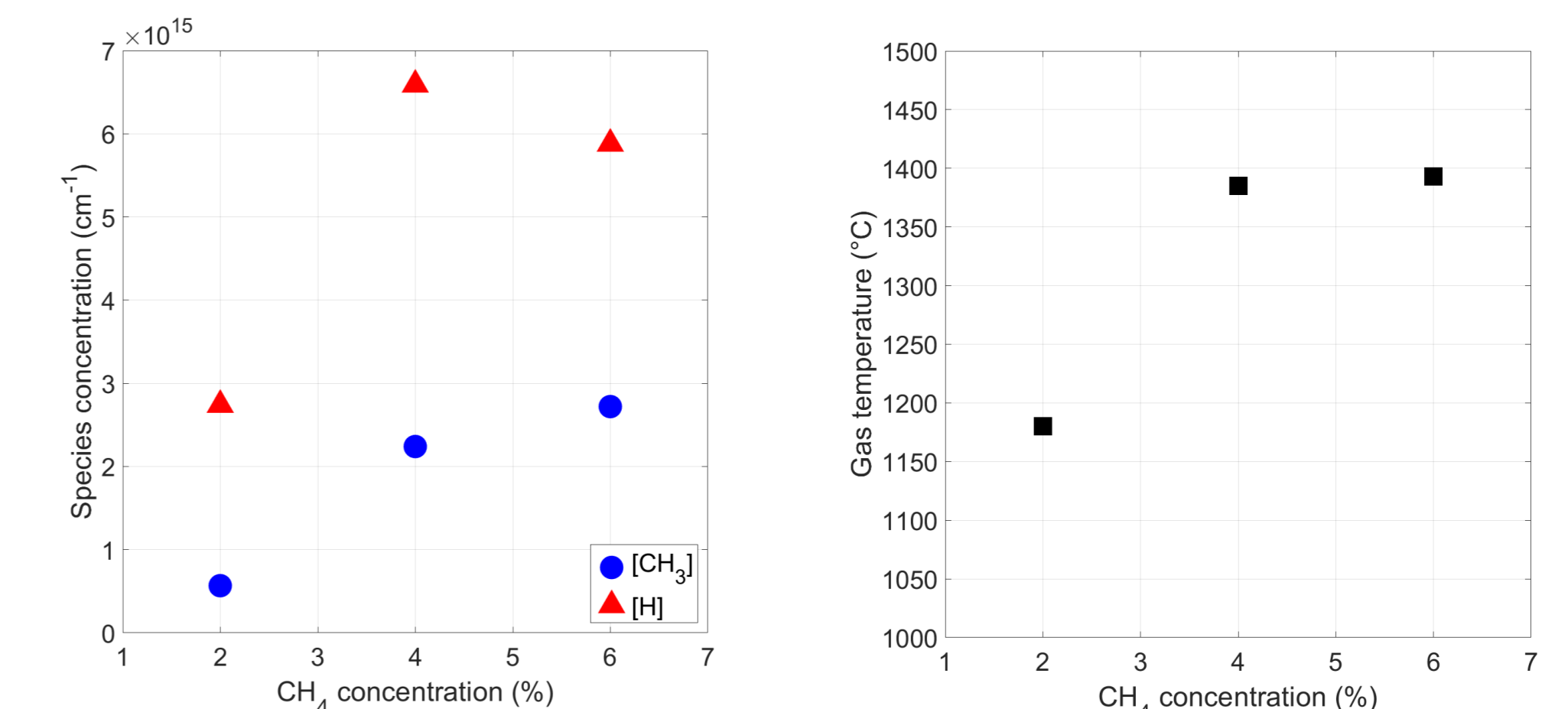
1D CH<sub>4</sub>/H<sub>2</sub> axial plasma model

- Thermo-chemical model of non-equilibrium plasma:
  - 2 energy modes: T<sub>g</sub> and eedf
  - 28 species / 131 reactions H<sub>2</sub>, H(n=1-3), H<sub>1-3</sub><sup>+</sup>, CH<sub>0-4</sub>, C<sub>2</sub>H<sub>0-6</sub>, CH<sub>3-5</sub><sup>+</sup>, C<sub>2</sub>H<sub>2-6</sub><sup>+</sup>, e<sup>-</sup>
- 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 =>  $T_g \frac{\partial \bar{E}_g}{\partial t} = [PMW - Q_{rad} - S_p] \frac{1}{\rho} \left[ \frac{1}{r} \frac{d}{dr} (rF_r^{(NR)}) \right] \frac{1}{\rho}$



### Results

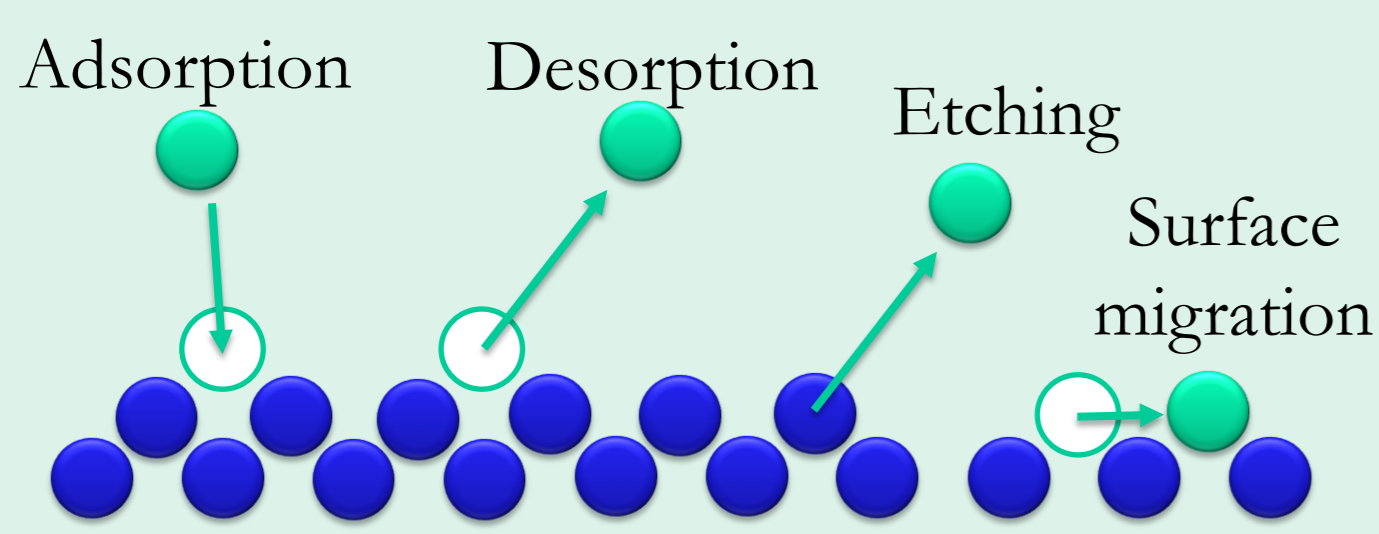
Concentrations and temperatures taken 1 mm from the diamond surface



## The Kinetic Monte-Carlo model

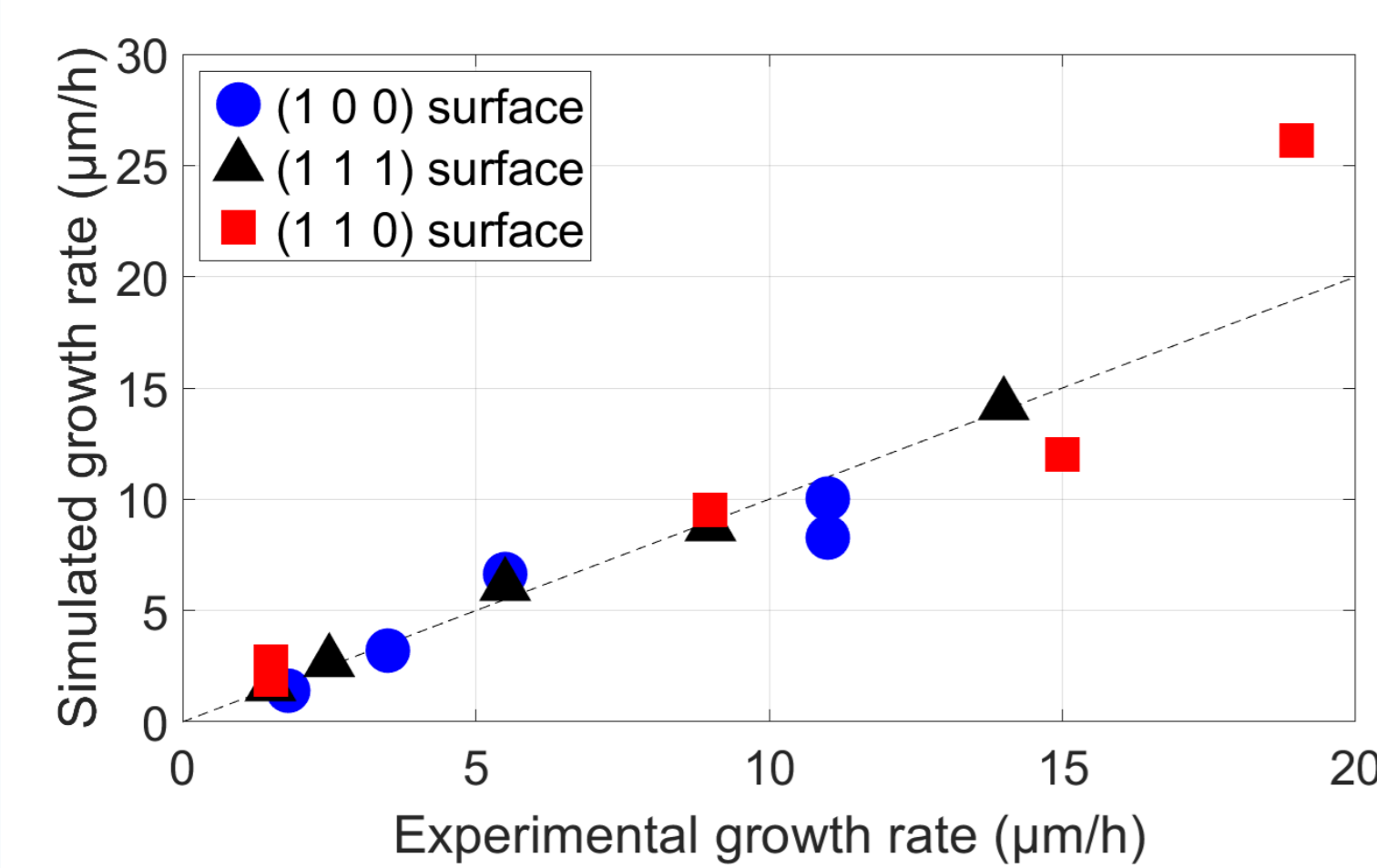
### Computational details [2]

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



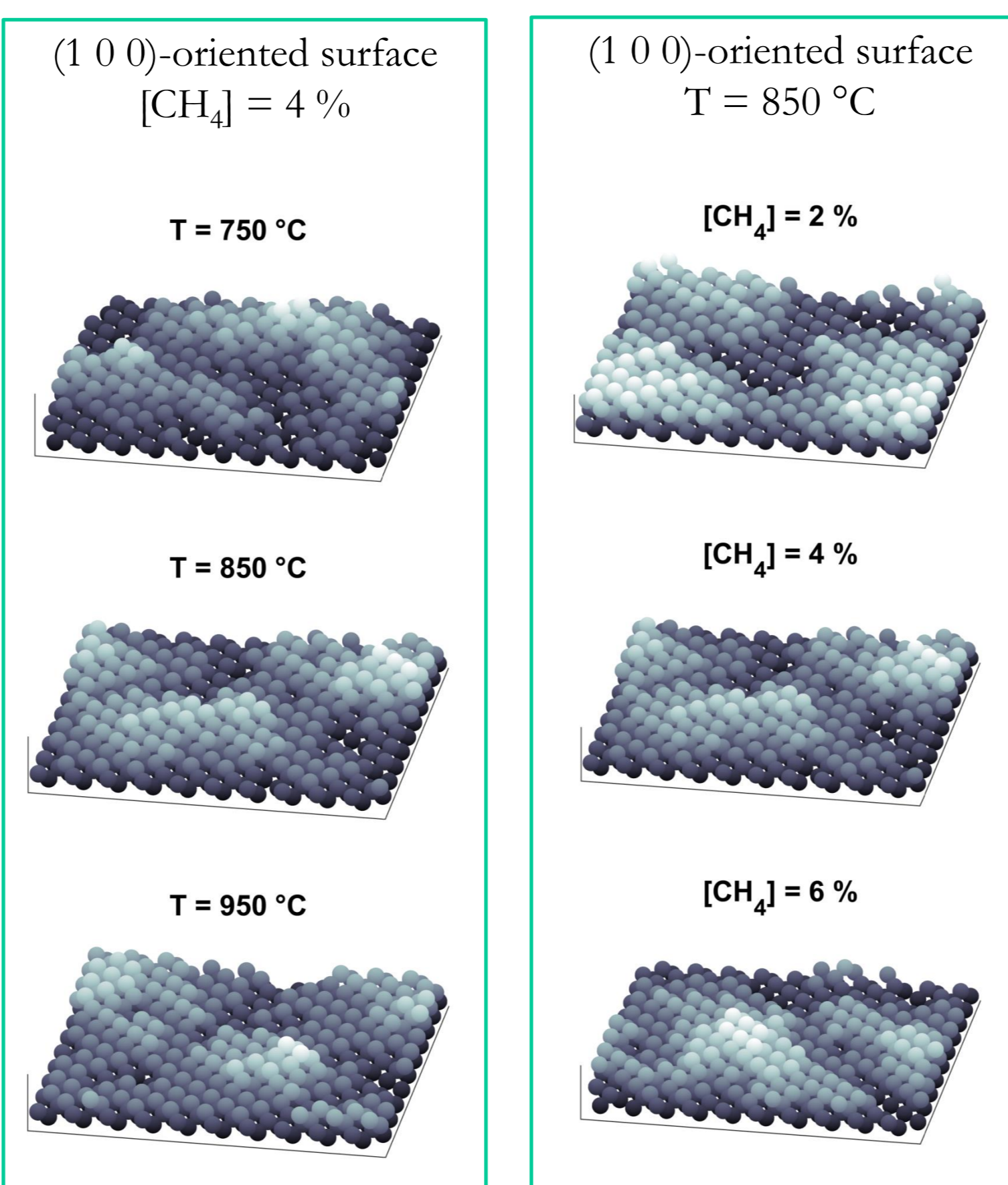
### Growth rates

Comparison to experimental data from [4]



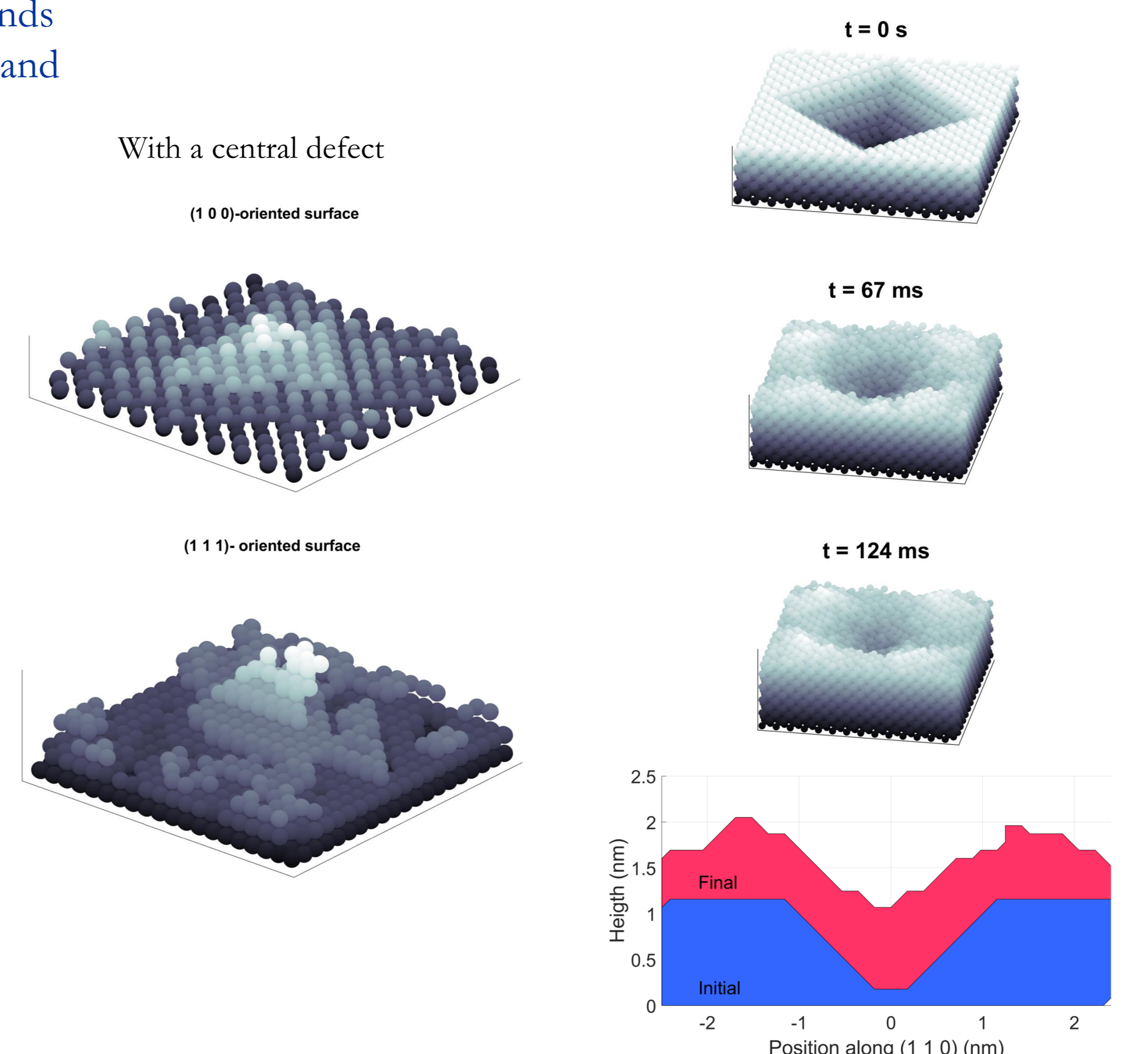
### Surface morphologies

- 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

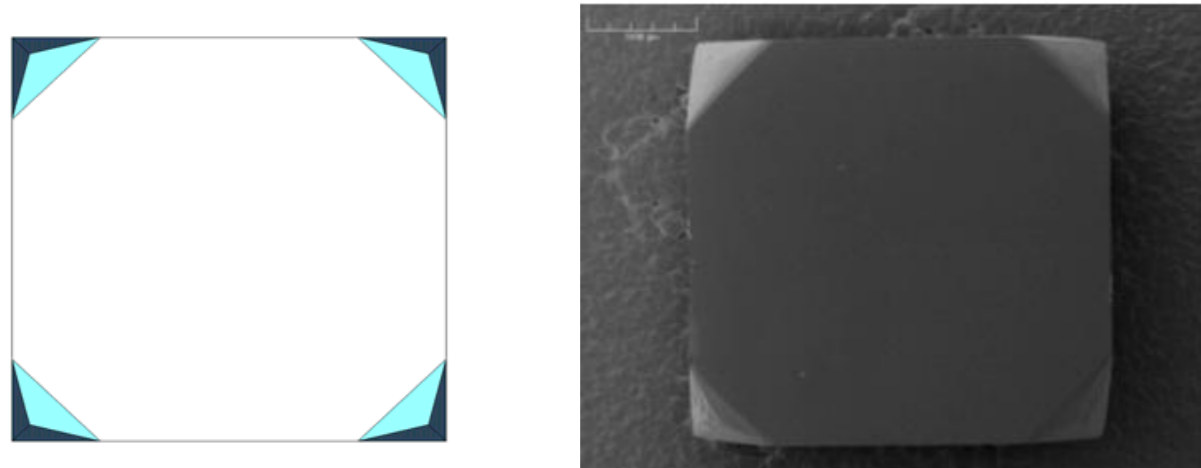
- Flat bottom
- (1 1 1) faces only



## The geometric model

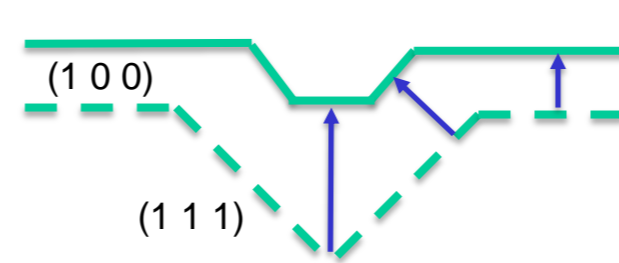
### Computational details [3]

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

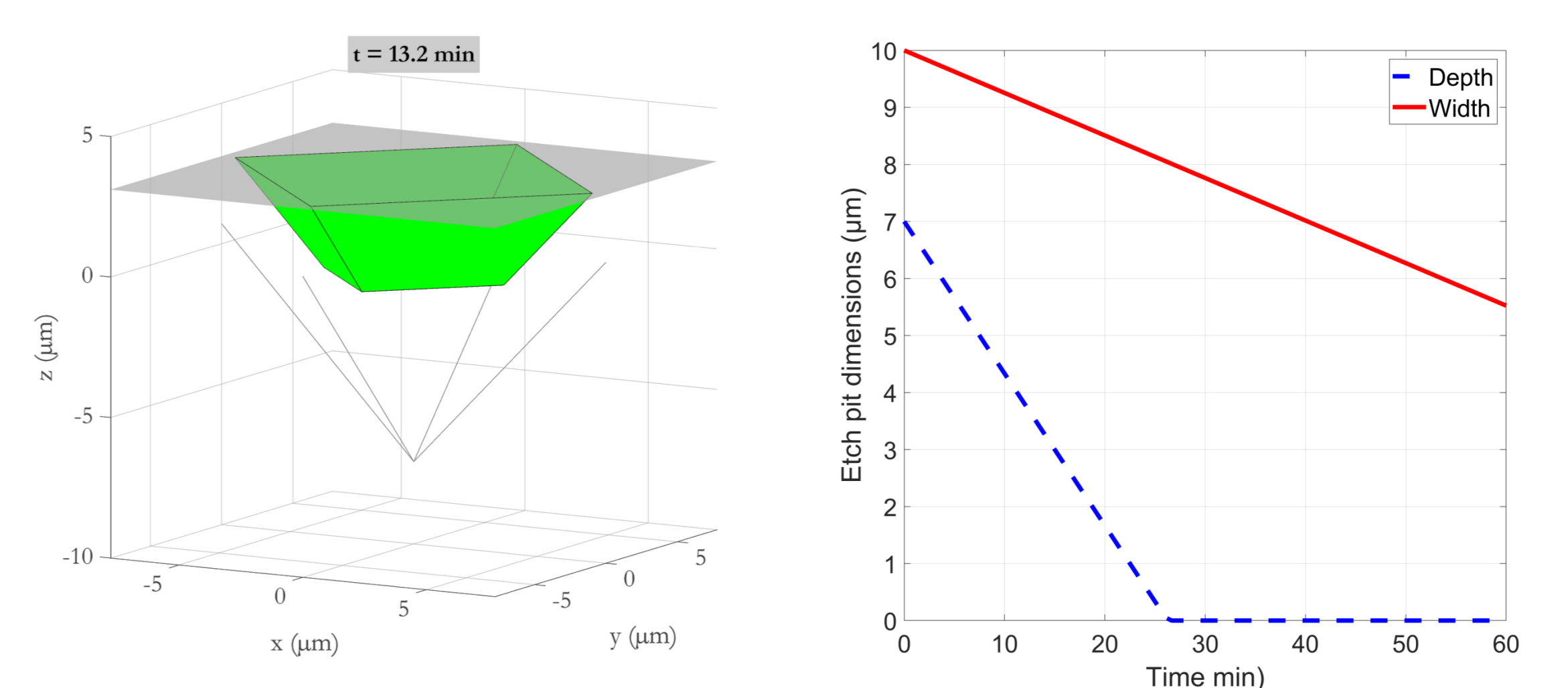


### Growth in a micrometric etch pit

- 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

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