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## 3D kinetic Monte-Carlo simulation of diamond growth

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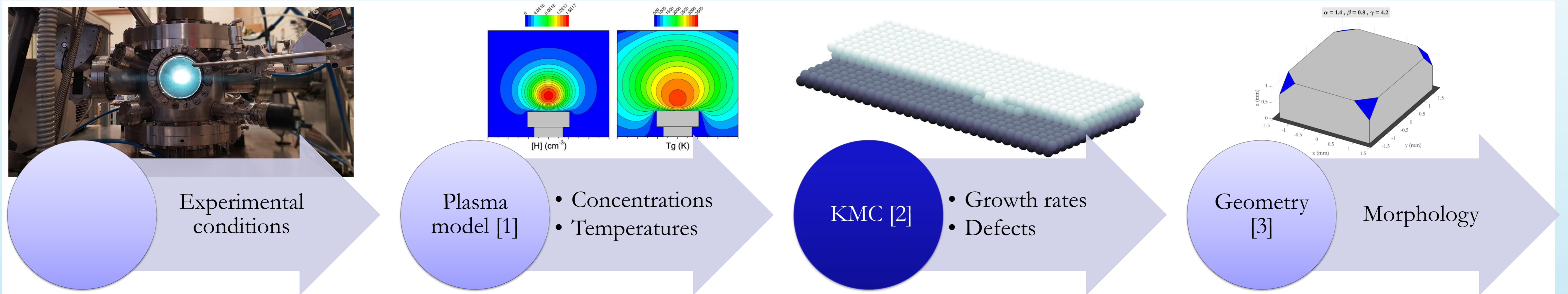
**<https://hal.science/hal-04643844v1>**

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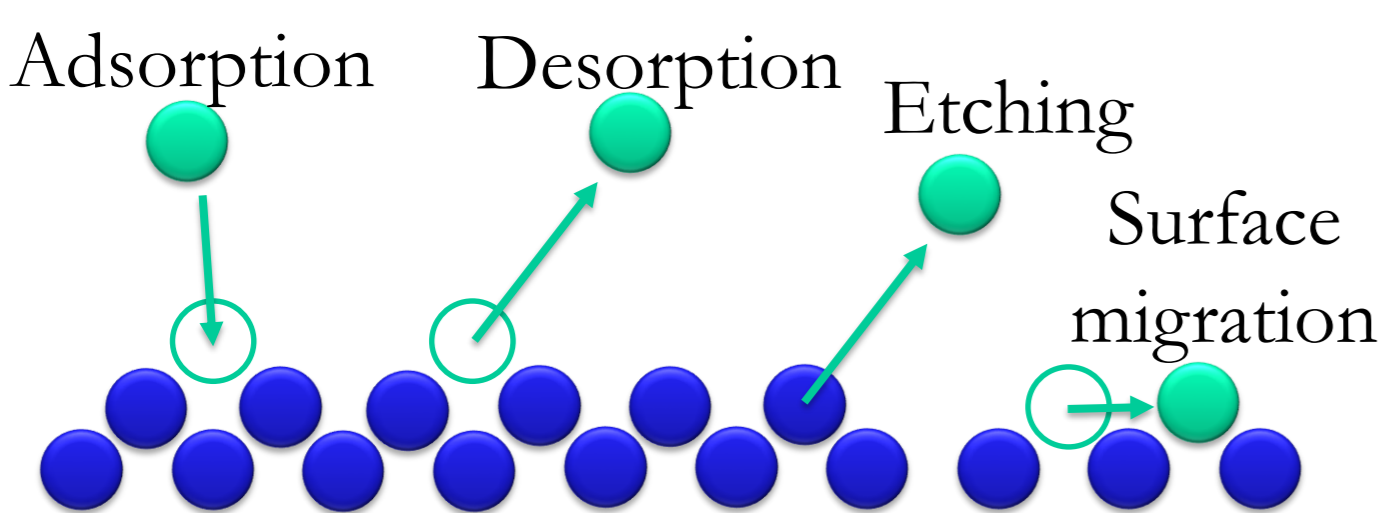
## Context



## The KMC model

### Processes taken into account

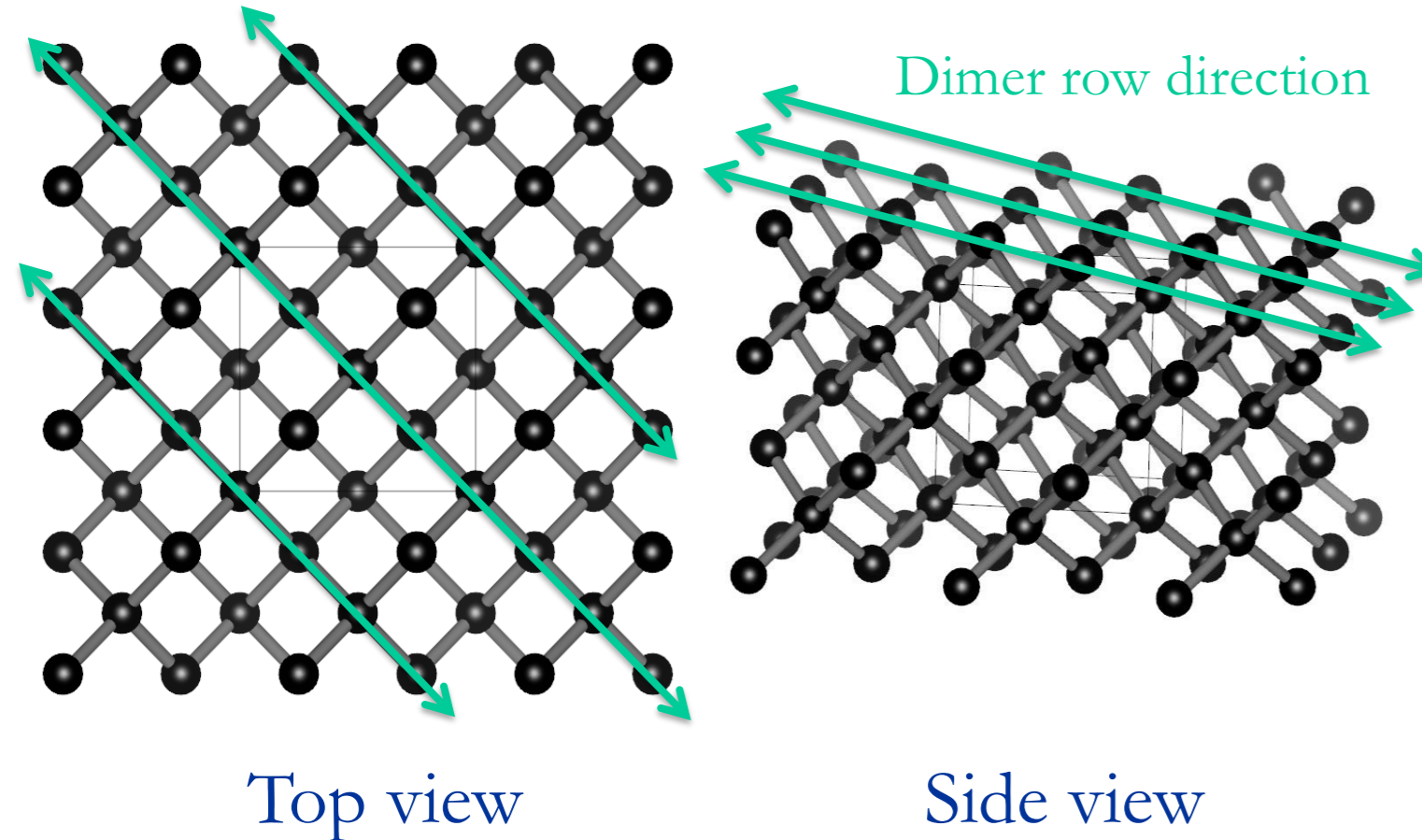
[CH<sub>3</sub>] and T taken from [6]



Process	Frequency	Ref
Adsorption	$\frac{v_{CH_3}}{4} [CH_3] \times \rho \times S \times R_H$	
Desorption	$\frac{k_B T}{h} \exp\left(-\frac{E_a}{RT}\right)$ , $E_a = 200 \text{ kJ/mol}$	[4]
Etching	$\frac{k_B T}{h} \exp\left(-\frac{E_a}{RT}\right) \exp\left(-\frac{\varepsilon N_N E_a}{RT}\right)$ , $\varepsilon = 0.365$	
Surface migration	$6.13 \times 10^{13} \times \exp\left(-\frac{18269}{T}\right) \times R_H$	[5]

### Lattice geometry

- (1 0 0) surfaces
- Dimer rows (in green) taken into account

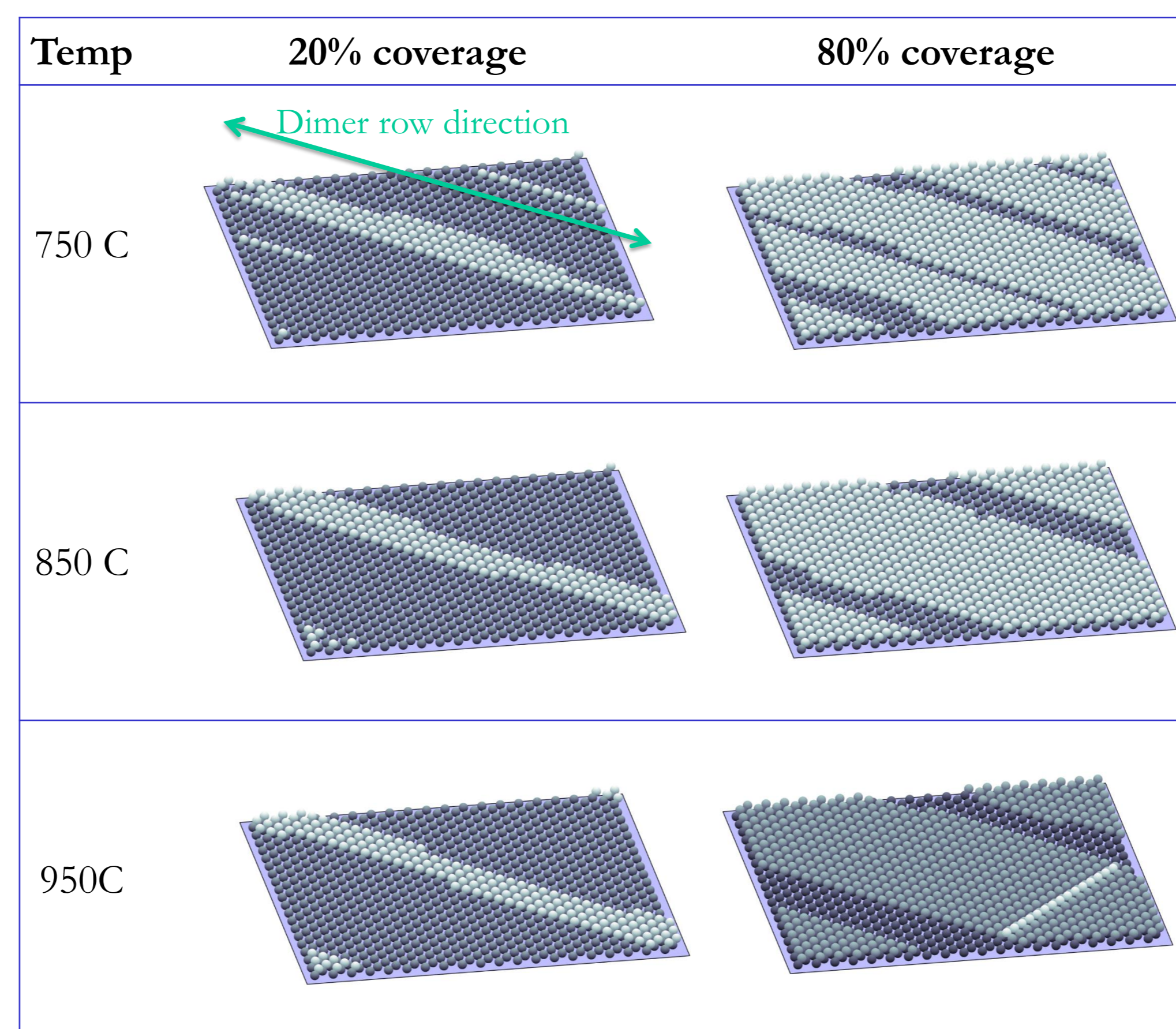


## Growth of a single layer

### Effect of temperature

[CH<sub>4</sub>] = 4%

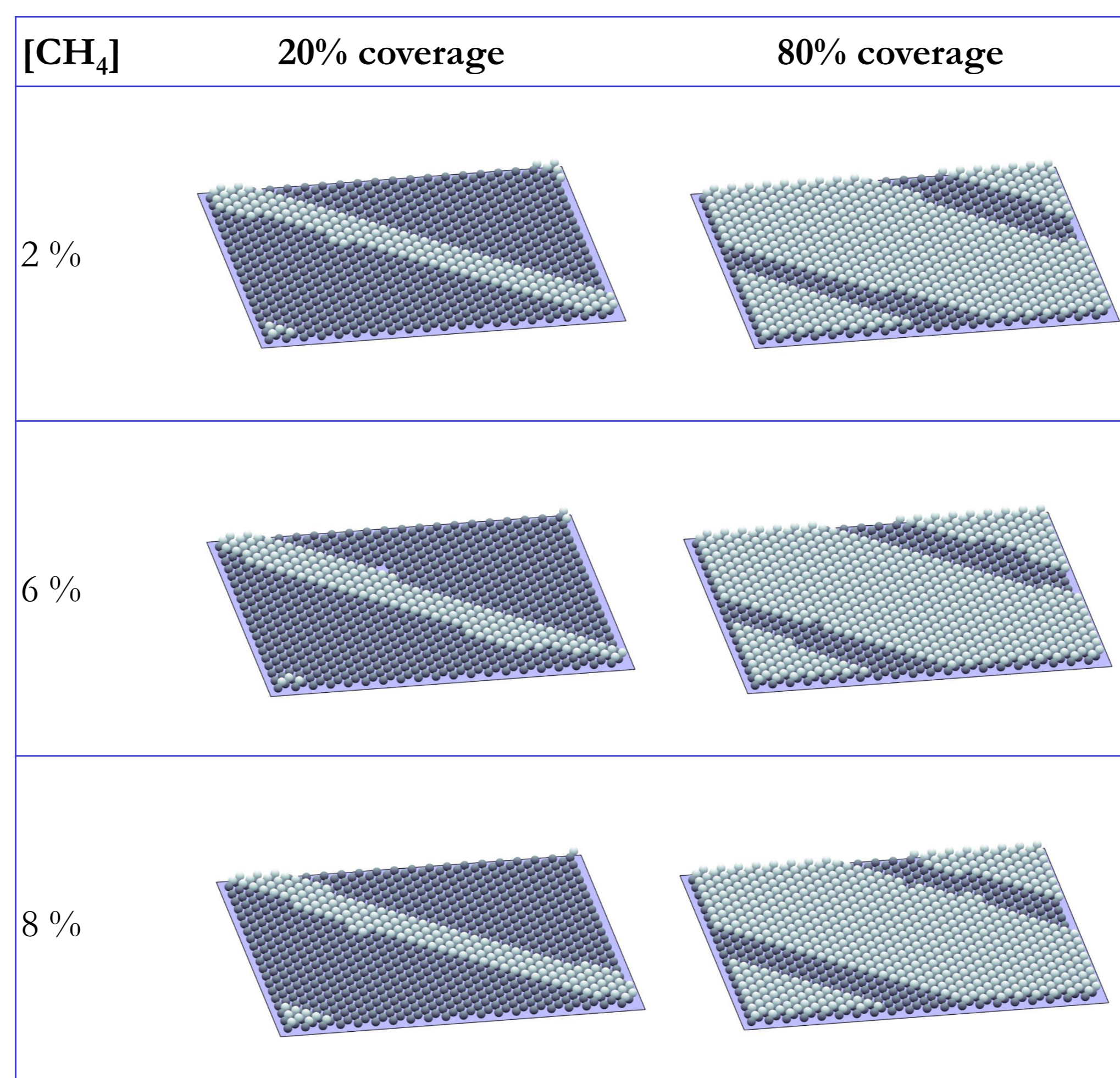
- Long islands due to dimer rows
- Germination at low and high temperature



### Effect of methane concentration

T = 850 C

- Effect of methane concentration is not visible
- Germination expected at high concentration



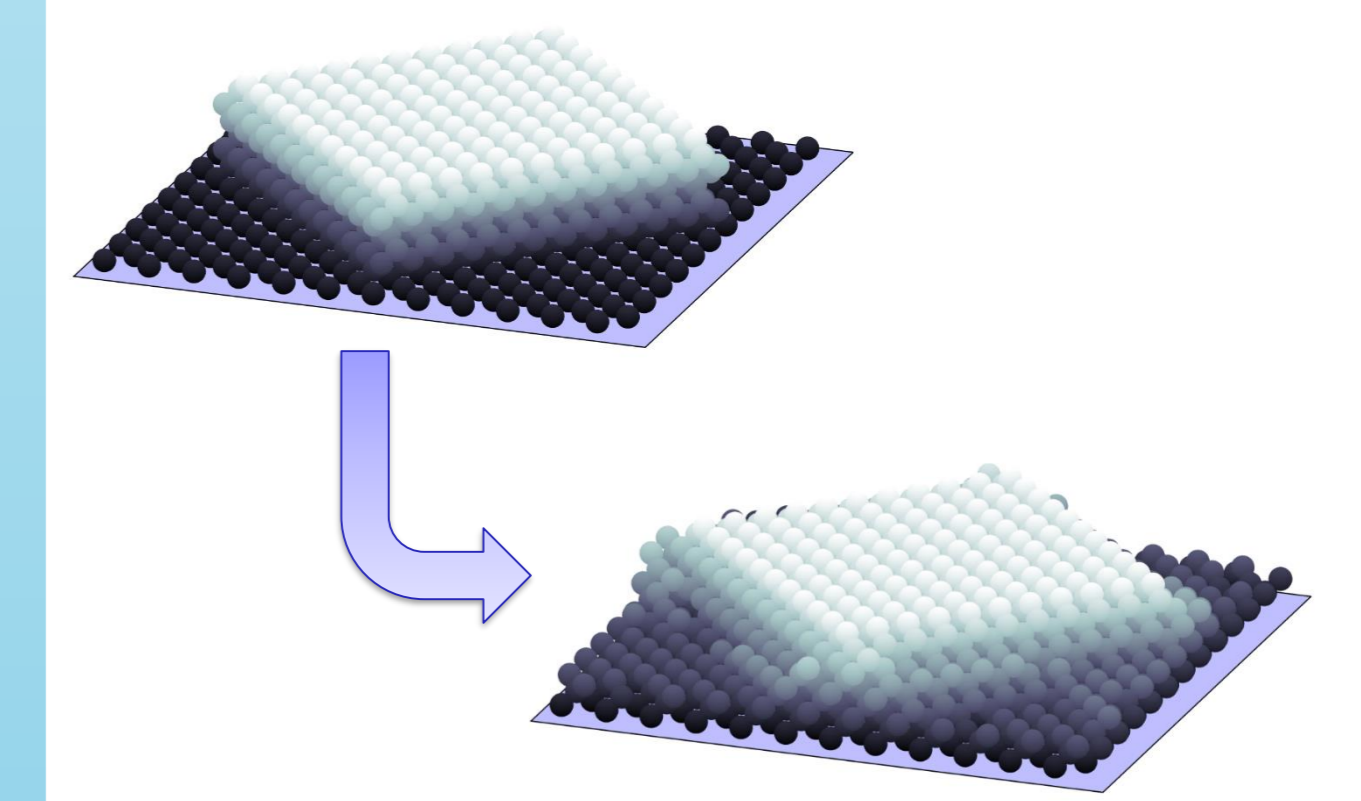
## Growth on nanostructures

All simulation below performed with:

- [CH<sub>4</sub>] = 4% and T = 850 C
- (1 0 0) growth model: new faces appear but their growth is not treated

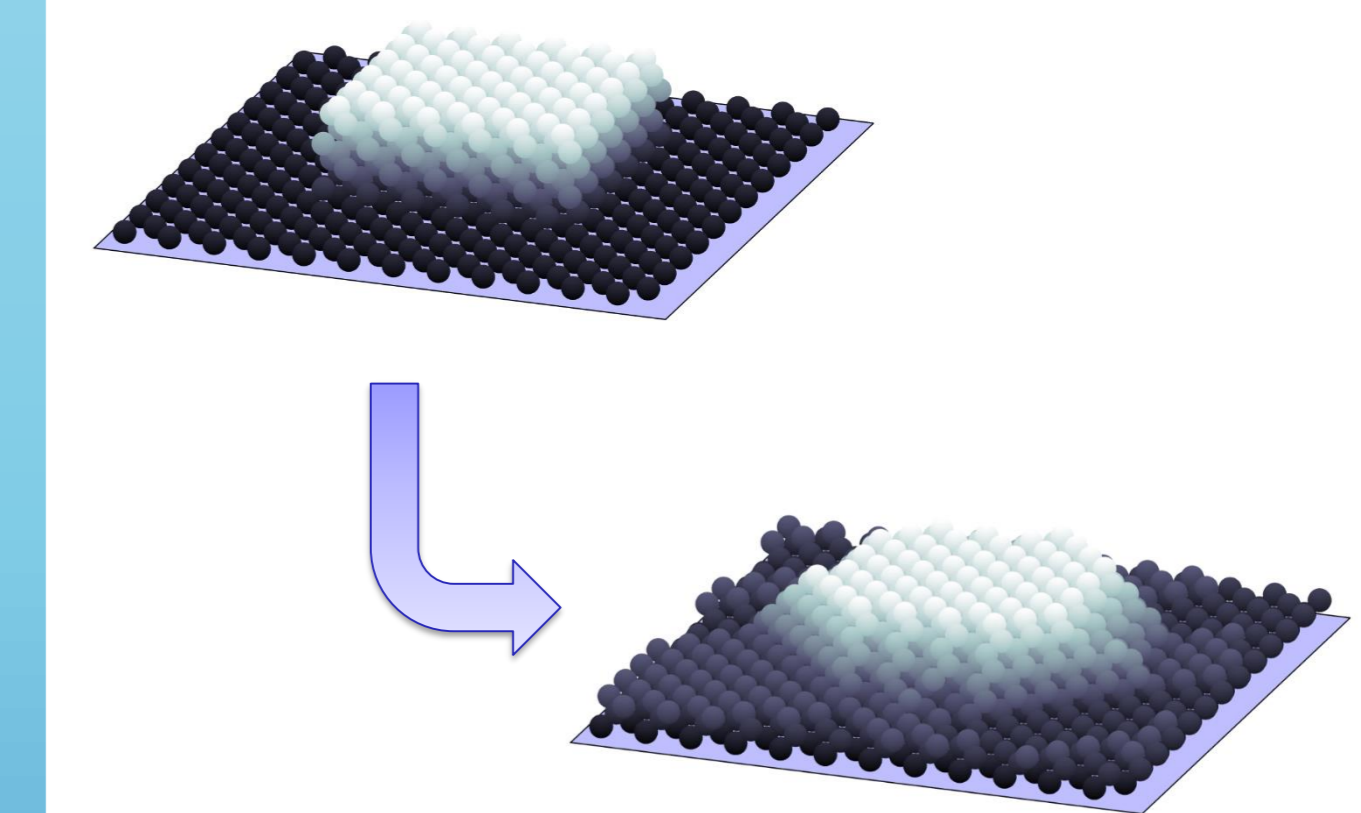
### (1 1 0)-oriented pillars

Appearance of (1 1 1) and (1 1 0) faces



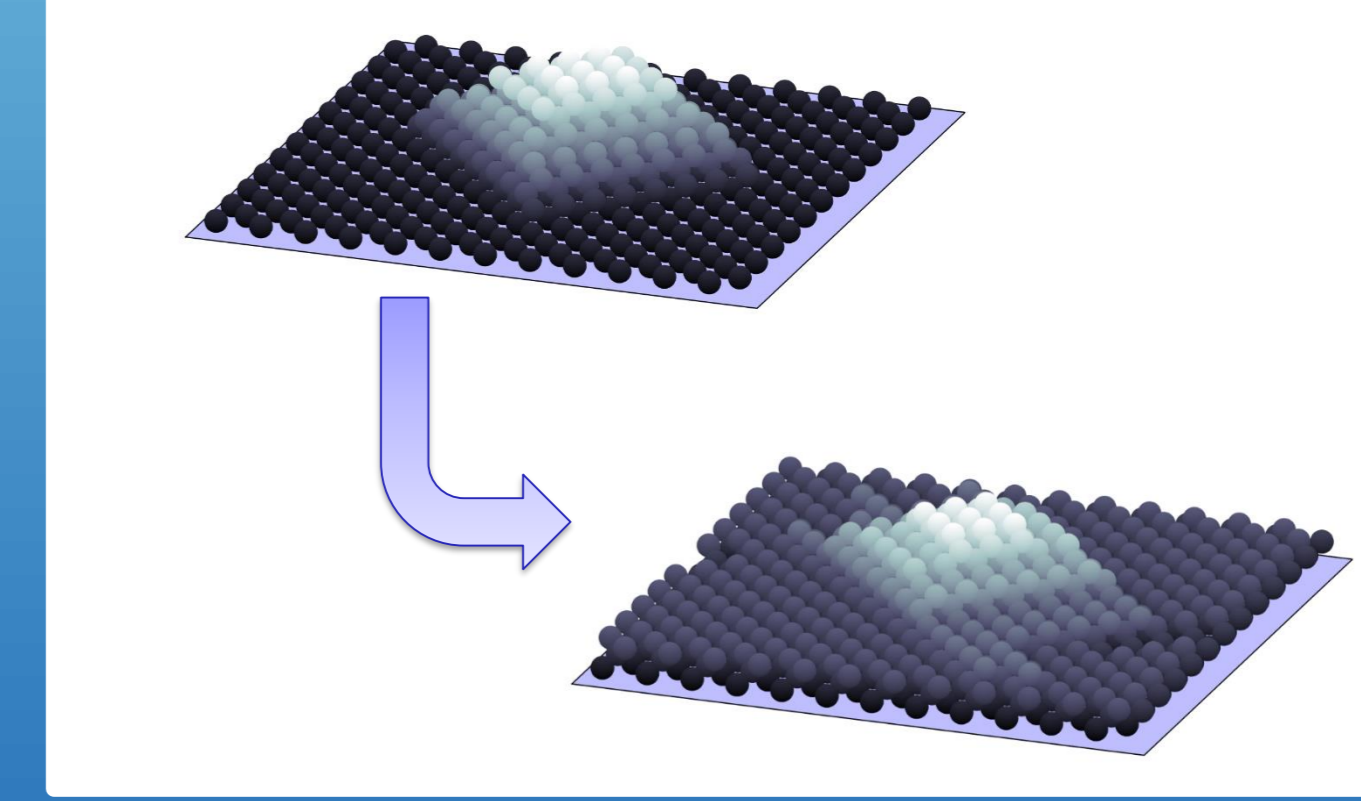
### (1 0 0)-oriented pillars

Appearance of (1 1 1) faces



### (1 1 1)-oriented pyramids

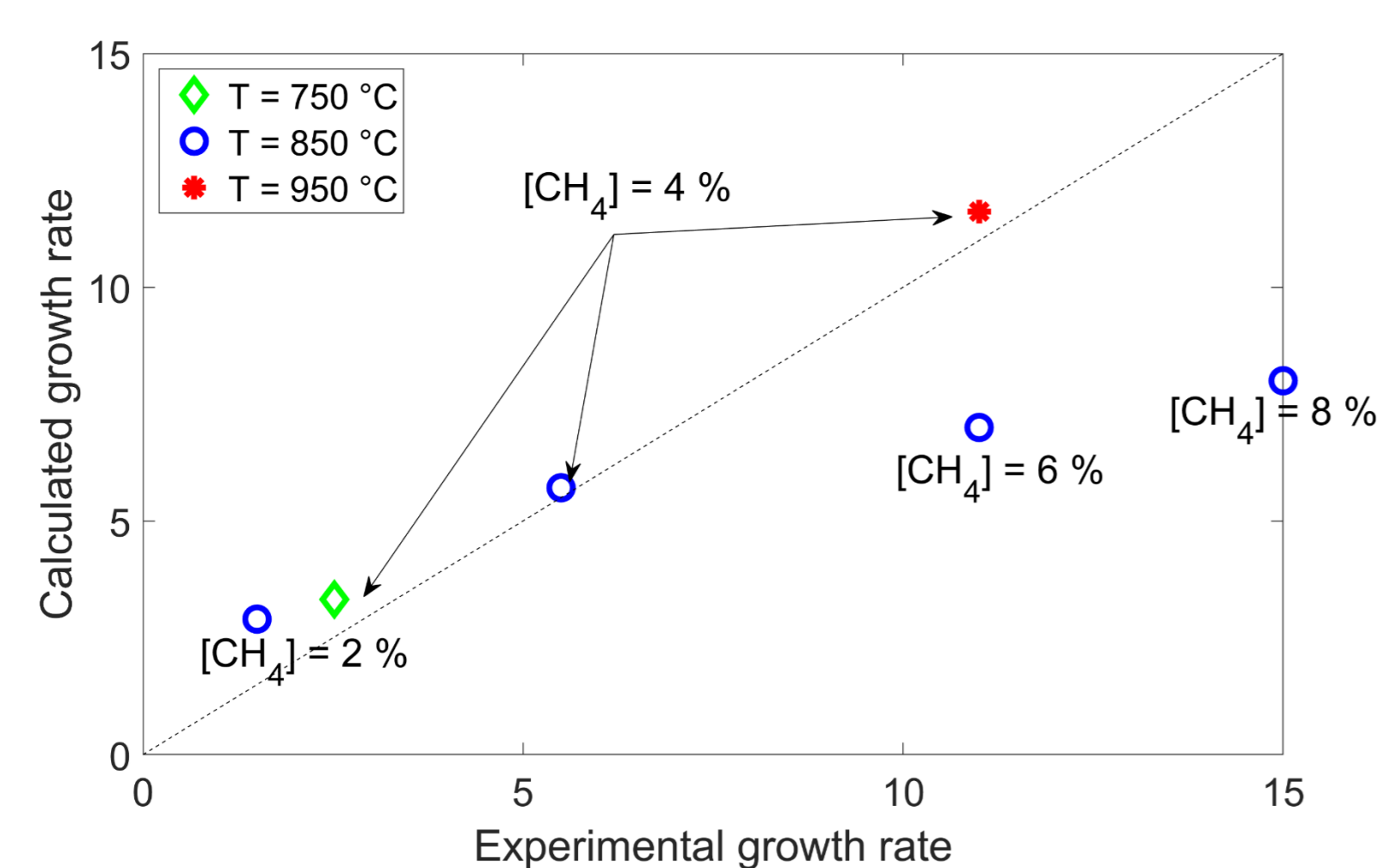
Two atomic layers high steps



## Calculated growth rates

### Comparison to experimental data [7]

- Good reproduction at low methane concentration
- Unrelevant modeling of germination?



## Conclusion & perspectives

Highlights

Growth rates close to experimental data at low methane concentration.  
Step-flow growth of (1 0 0) surfaces  
Crystal morphology

To be added

Germination model improvement  
Extended defects  
Impurities  
(1 1 1), (1 1 0) and (1 1 3) oriented substrates

Perspectives

Growth rates on pillars and holes  
Use in geometric model  
Study of etching

## References

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