Kinetic Monte-Carlo modelling of SiN:H thin film deposition by PECVD on complex substrates: characterization of air-connected porosity and improvement by ion beam assisted deposition

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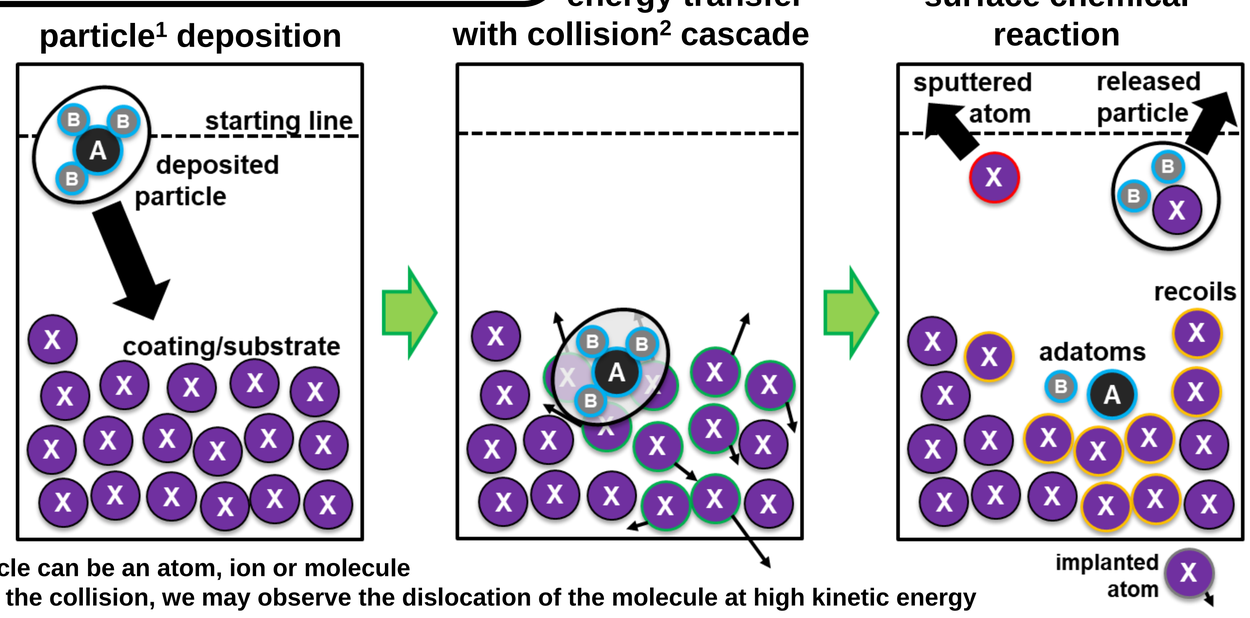
Methodology
Applications

Introduction

In the case of devices sensible to oxidation and/or moisture like OLED (organic light emitting diode), thin film encapsulation is required and it is critical to detect air-connected pores to avoid the deterioration of such device.
The purpose of this work is to simulate the SiN:H encapsulation of complex objects by PECVD using SiH4 as a precursor, in order to predict pores, especially those connected to the surface. To do so, we will first deposit in-silico a 3D SiN:H coating on complex shaped substrate by means of kinetic Monte-Carlo code NASCAM 5 [1]. Then, the porosity is computed to detect critical zones where the substrate can be exposed to moisture and oxidation. Different deposition processes will be investigated to reduce this porosity (rotating source, ion assisted deposition).

[1] R. Tonneau et al. (2021) "Understanding the role of energetic particles during the growth of TiO2 thin films by reactive magnetron sputtering through multi-scale Monte Carlo simulations and experimental deposition". J. Phys. D. Appl. Phys.

1 - Thin film growth modeling

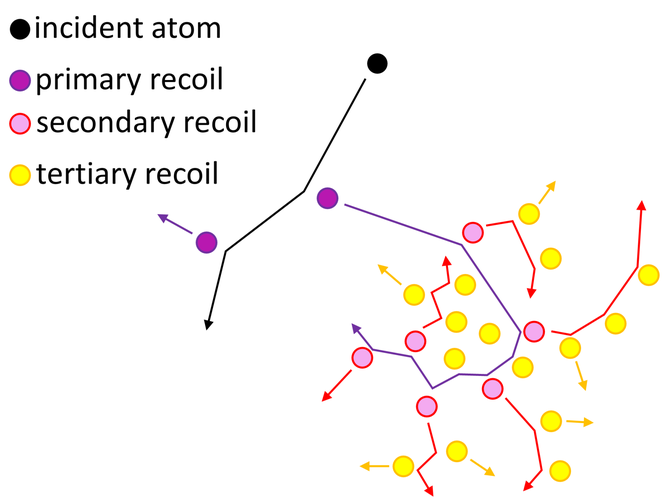


[1] a particle can be an atom, ion or molecule
[2] during the collision, we may observe the dislocation of the molecule at high kinetic energy

2 - Energy transfer

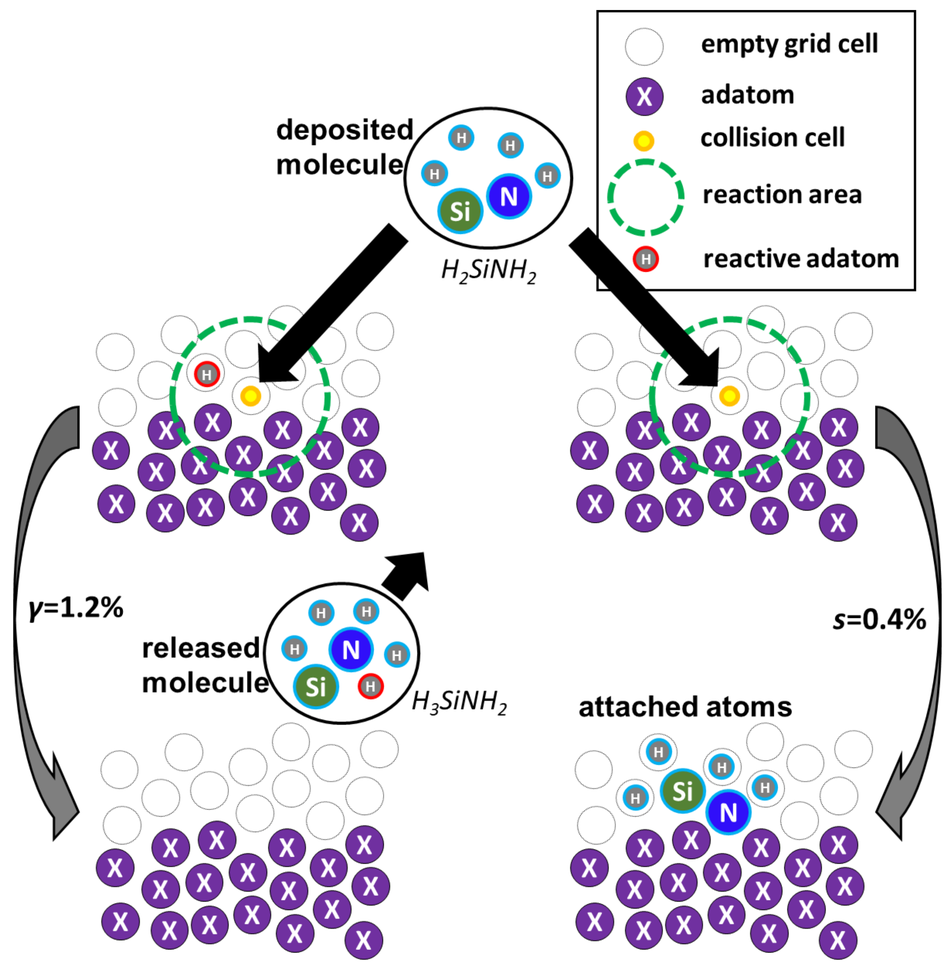
Model:
- binary collision approximation
- full collision cascade

Modelled features:
- recoils
- sputtering (sputtering yield)
- ion implantation
- ion beam mixing



doi.org/10.1088/1361-6463/abd72a

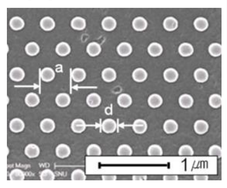
3 - Surface Chemical Reactions



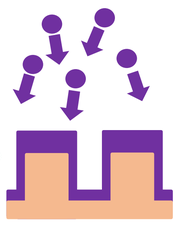
List of deposited molecules and their possible reactions (with recombination *γ* and sticking probabilities *s*) :
- doi.org/10.1088/0268-1242/23/9/095023
- doi.org/10.1039/C6CP05395E
- doi.org/10.1016/S0009-2509(97)84656-8

4 - Simulations and Results

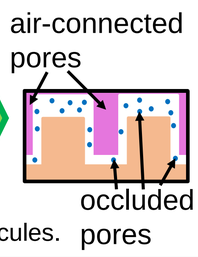
Polymer nanostructure for OLED application[1]



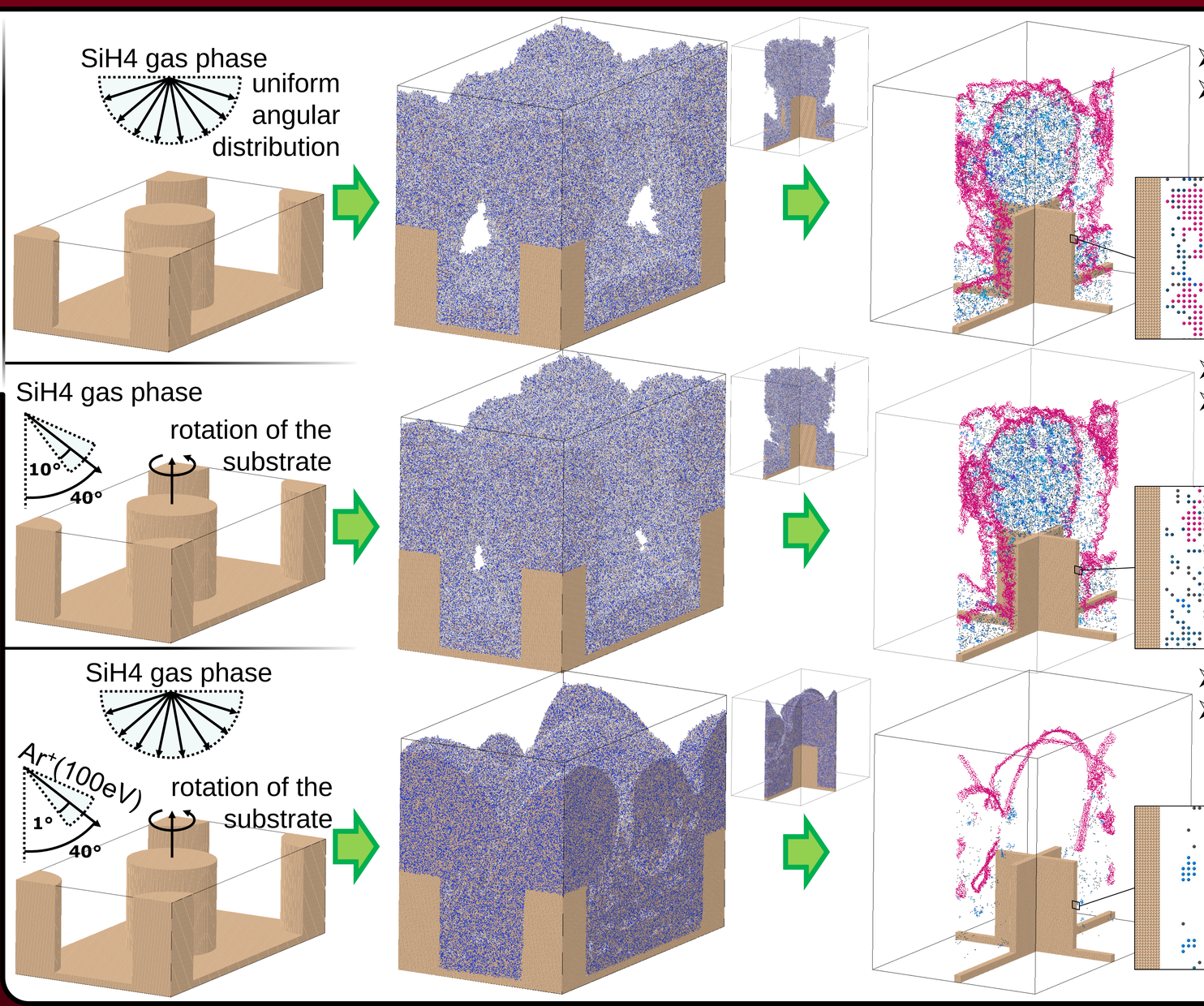
Modelling of SiN:H PECVD deposition[2]



Porosity: scan by a 10Å diameter probe



[1] doi.org/10.1063/1.2939554
[2] up to 500M deposited atoms, ions and molecules.



- high porosity
- air-connected pores connected to substrate
- high porosity
- no air-connected pores connected to substrate
- low porosity
- no air-connected pores connected to substrate

Conclusion

In this work, we modelled the SiN:H encapsulation of 3D nanostructures for OLED application by PECVD using SiH4 as a precursor. We have observed a high porosity due to shadowing, with pores connecting the substrate to the surface. This air-connected porosity can be reduced by using a rotating source. Moreover, we have shown that the density of the coating can be drastically enhanced by mean of an ion (Ar^+) assisted deposition.

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