Monte Carlo Simulations of Atomic Layer Deposition on 3D Large Surface Area Structures

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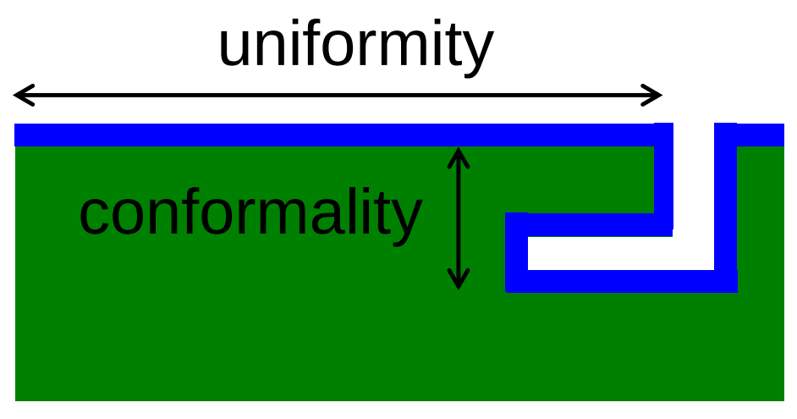
Introduction

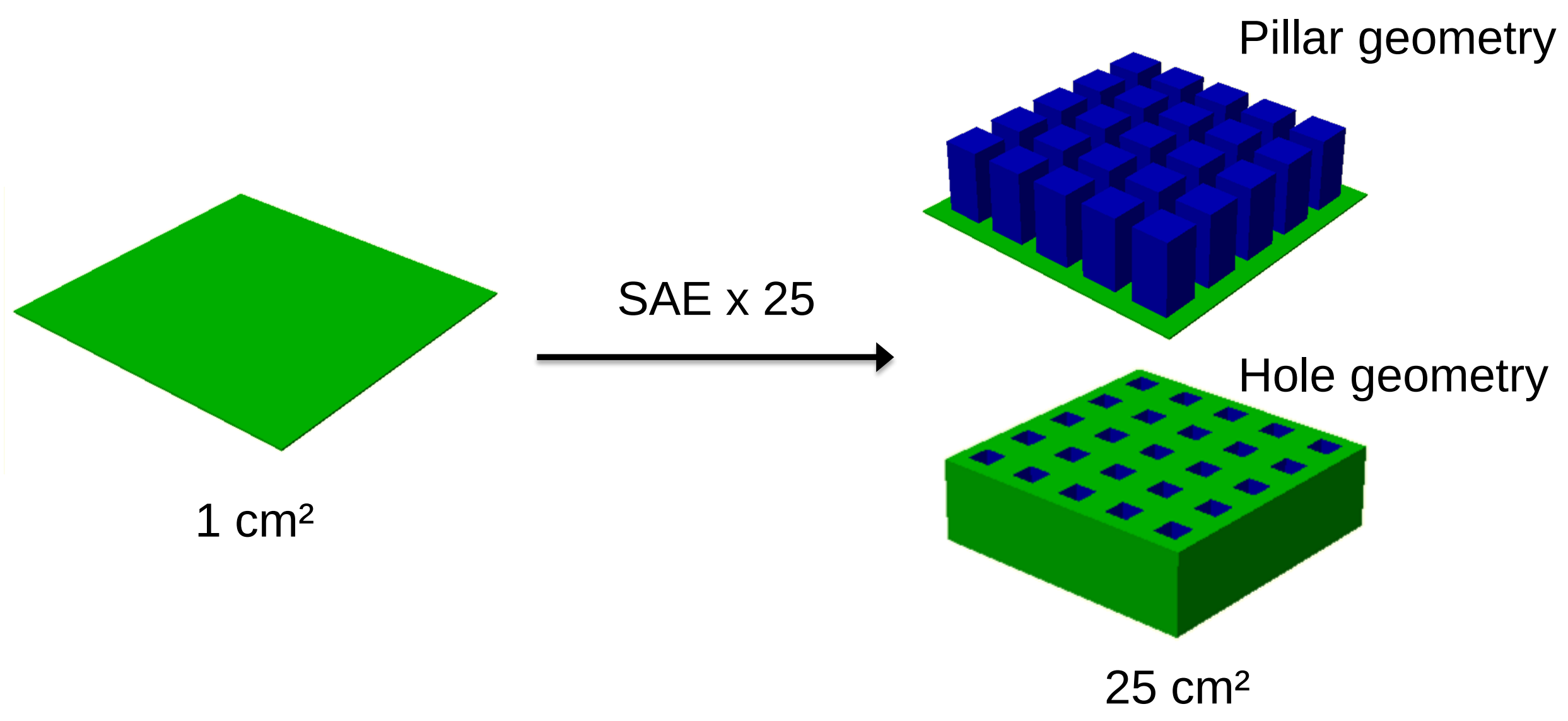
Atomic Layer Deposition (ALD)

ALD is an ultrathin film deposition method based on sequential self-terminating gas-solid surface reactions. Key advantages of ALD are the atomic level thickness control and excellent conformality.

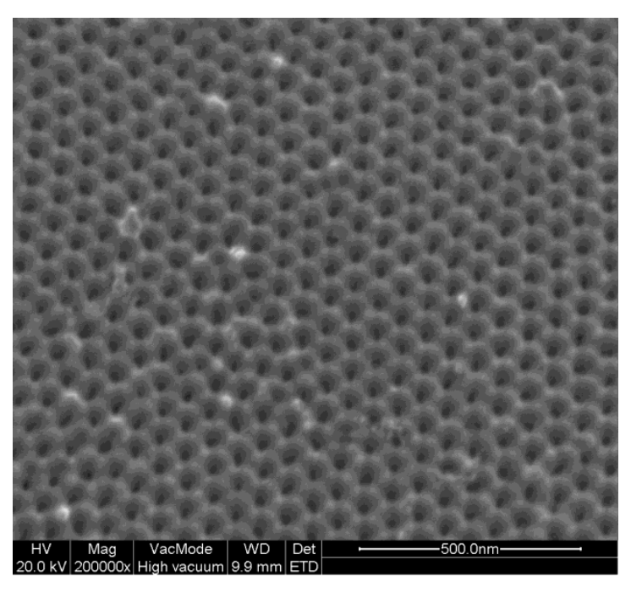


Surface Area Enhanced (SAE) structures

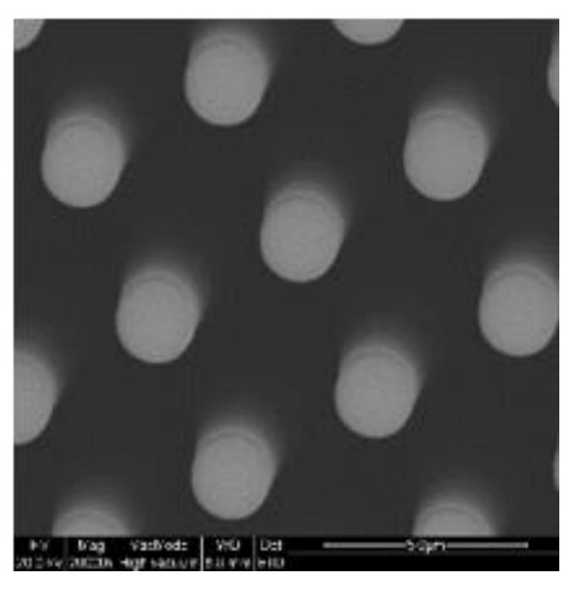
SAE structures are used to increase the active area, for example, in fuel cells, batteries, sensitized solar cells and photocatalytic surfaces.



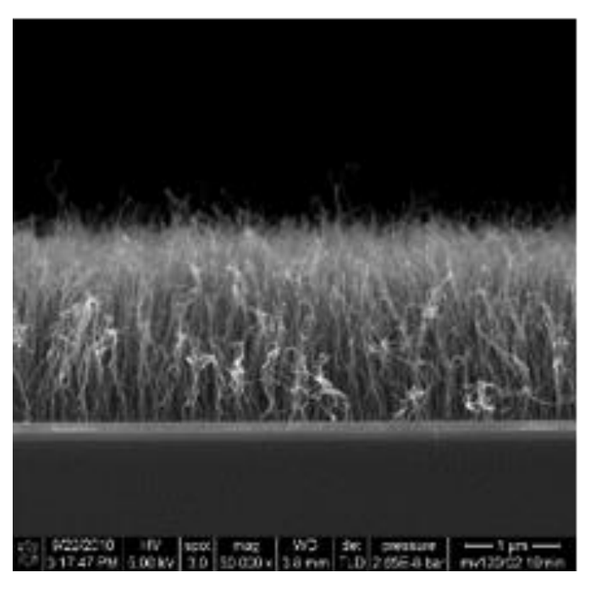
Examples of frequently used SAE structures:



anodic aluminum oxide (AAO) with cylindrical pores



silicon pillars



carbon nanotubes (CNT)

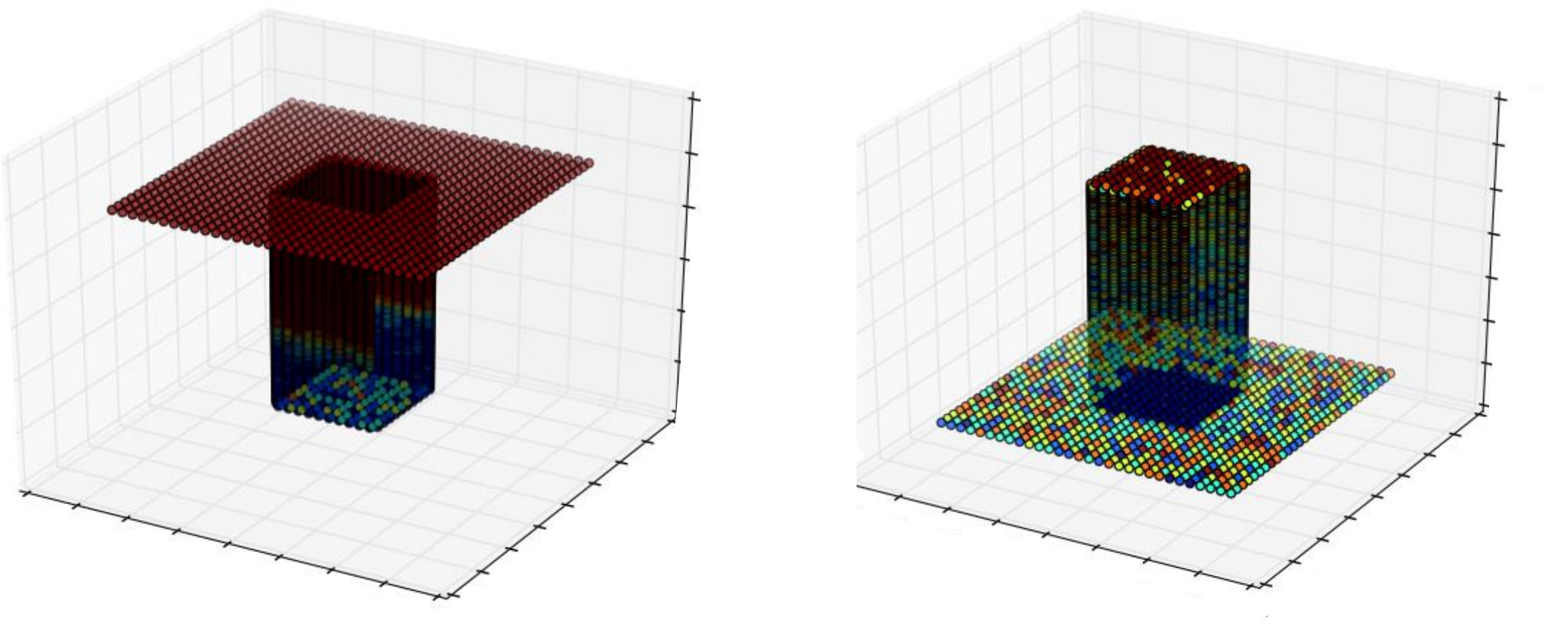
Simulations

Model

A **3D Monte Carlo** simulation model was developed to optimize the ALD process parameters to achieve conformal coverage of 3D substrates.

exposure = P . t ~ precursor cost

P = partial precursor pressure
t = precursor pulse time



Colour ~ degree of coverage

Blue: uncovered
Red: completely covered

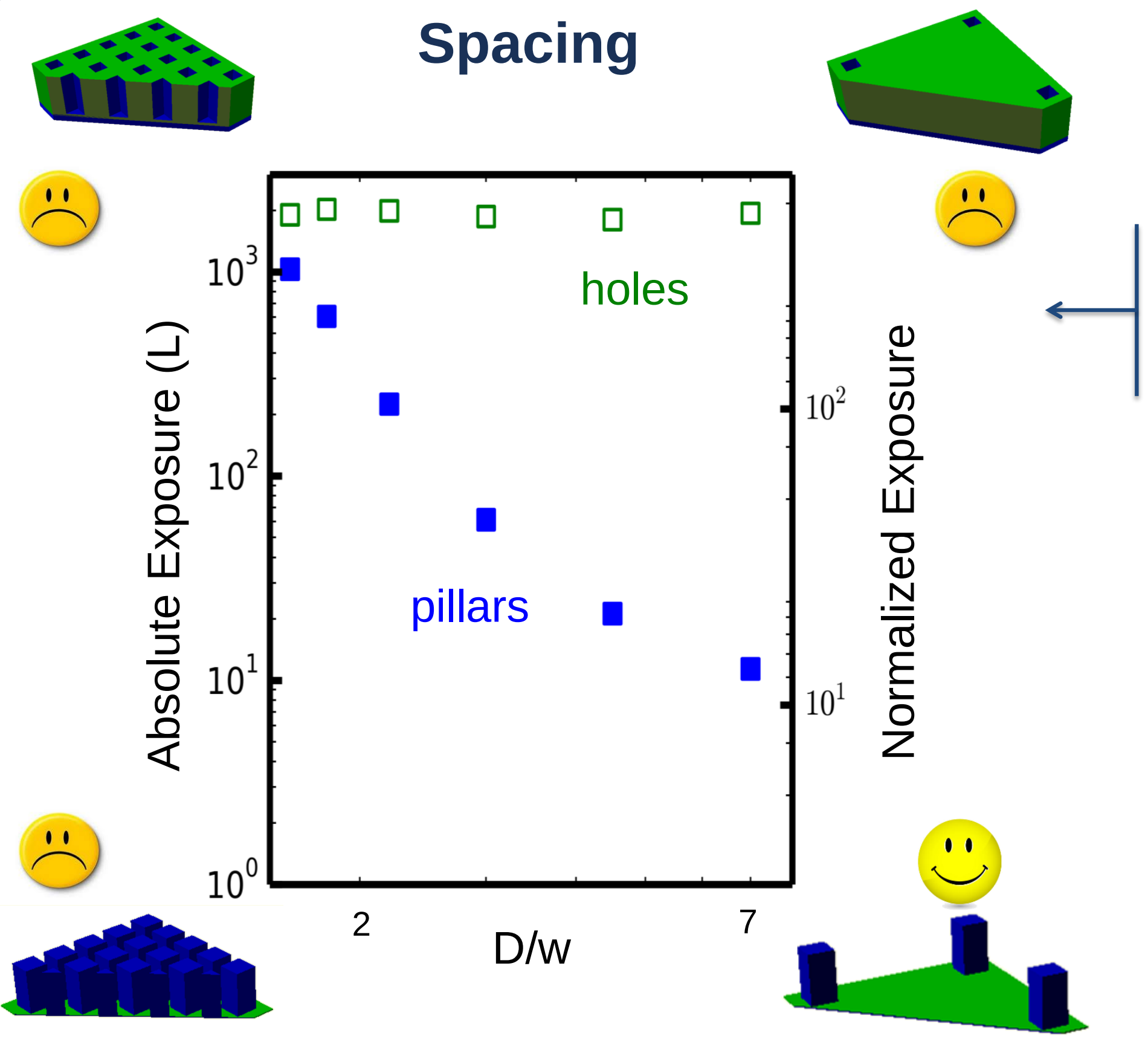
Objective

To compare the exposure needed to conformally coat an array of pillars or holes with equal surface area. → Which geometry requires the lowest precursor cost?

H = height
w = width
D = center-to-center distance = spacing

Results

Spacing

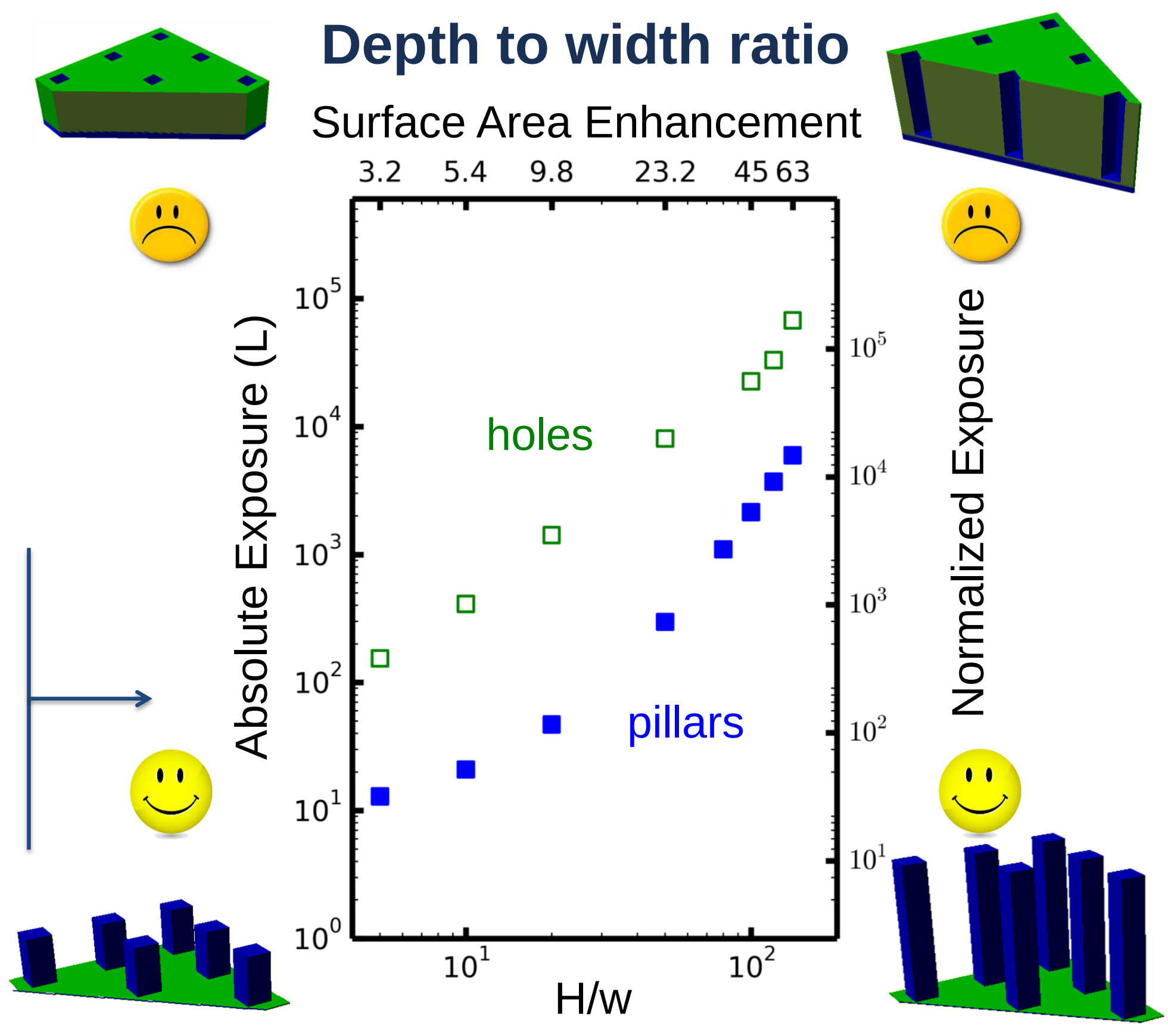


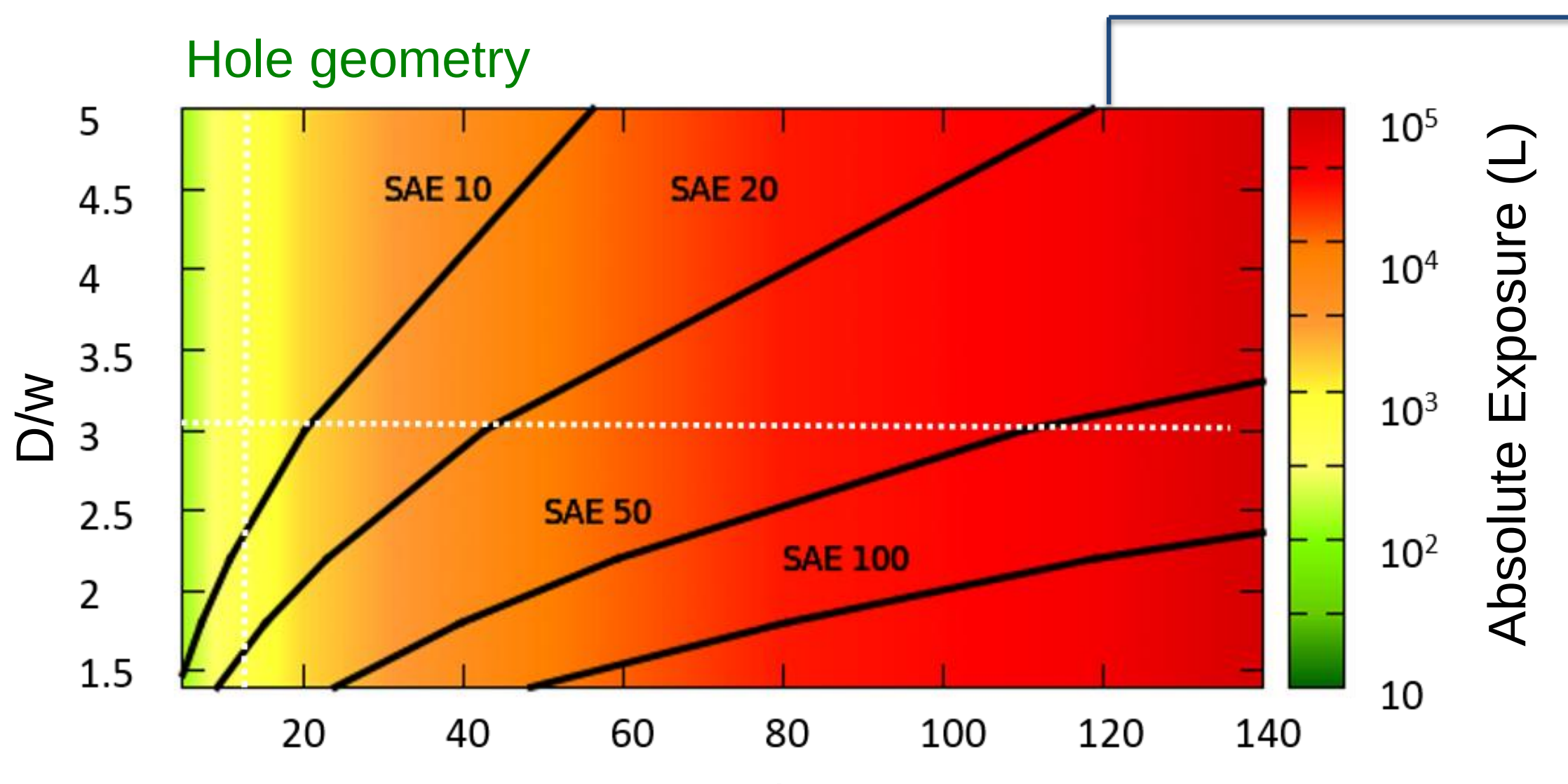
The **spacing** of the **holes** has **no influence** on the exposure. For the **pillars**, the exposure **increases with decreasing spacing** and converges in the limit to the exposure of the holes.

For a certain SAE factor, **10 to 30 times less exposures** are required to cover **well-spaced pillars** instead of holes.

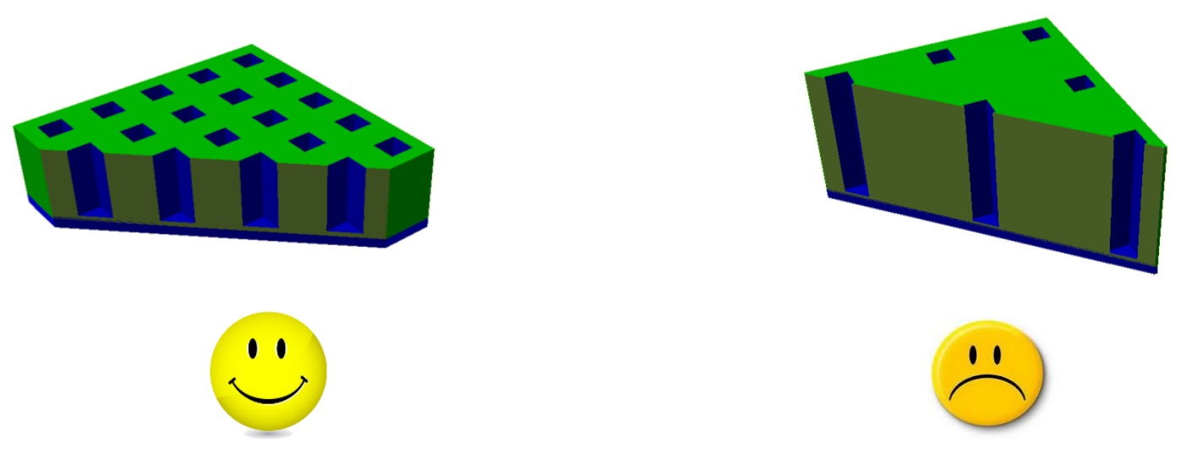
If one needs structures with a **larger SAE**, one can **increase** the **height of well-spaced pillars**. The exposure will increase but will still be smaller than the exposure of the holes.

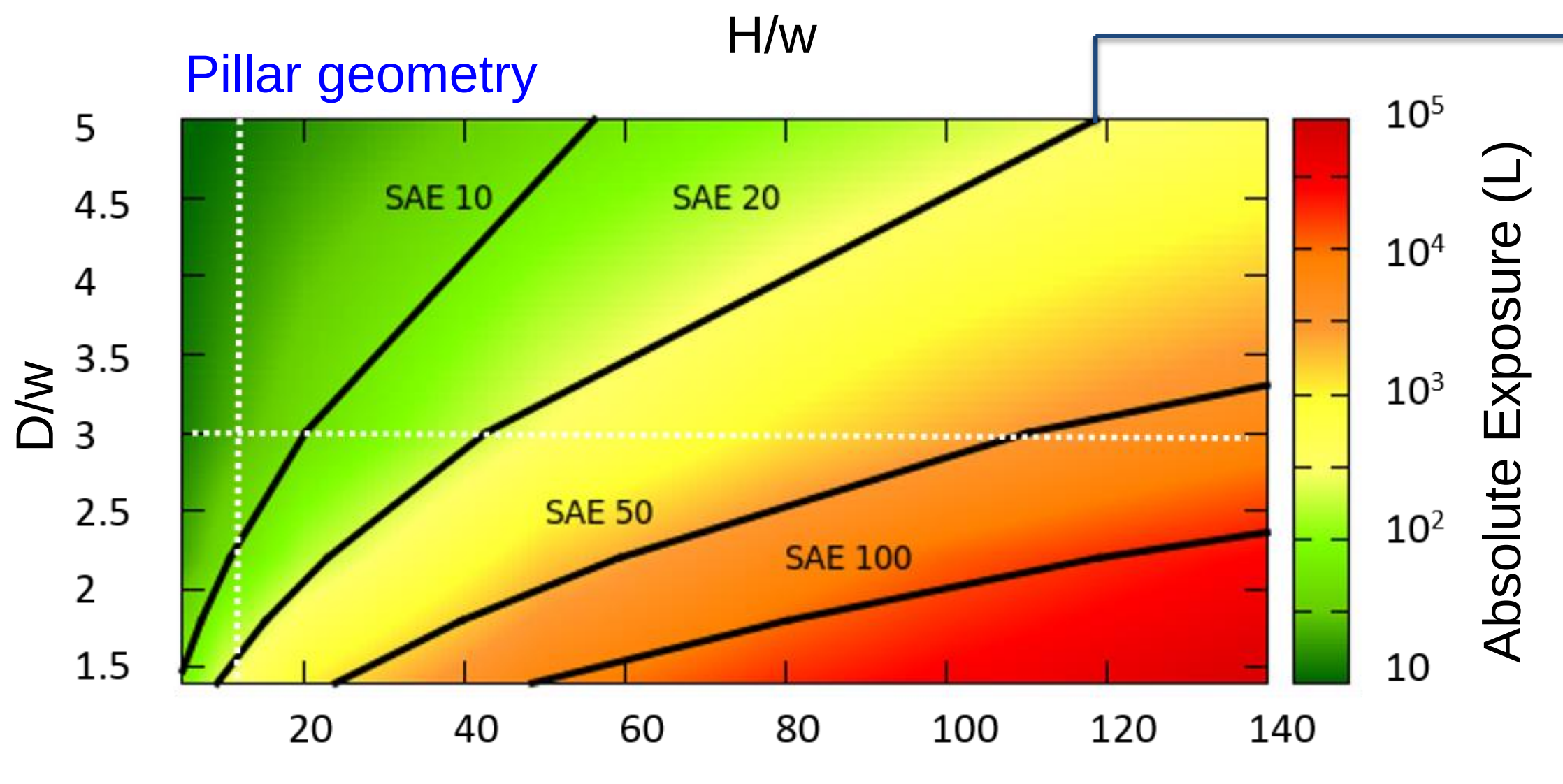
Depth to width ratio



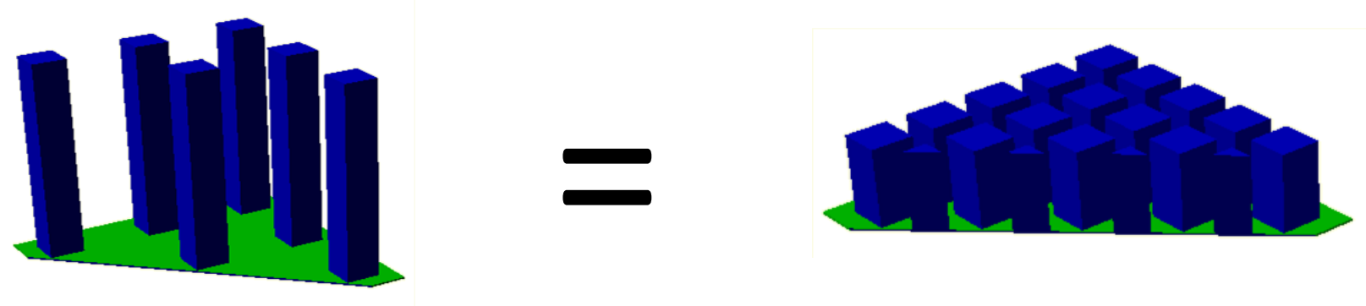


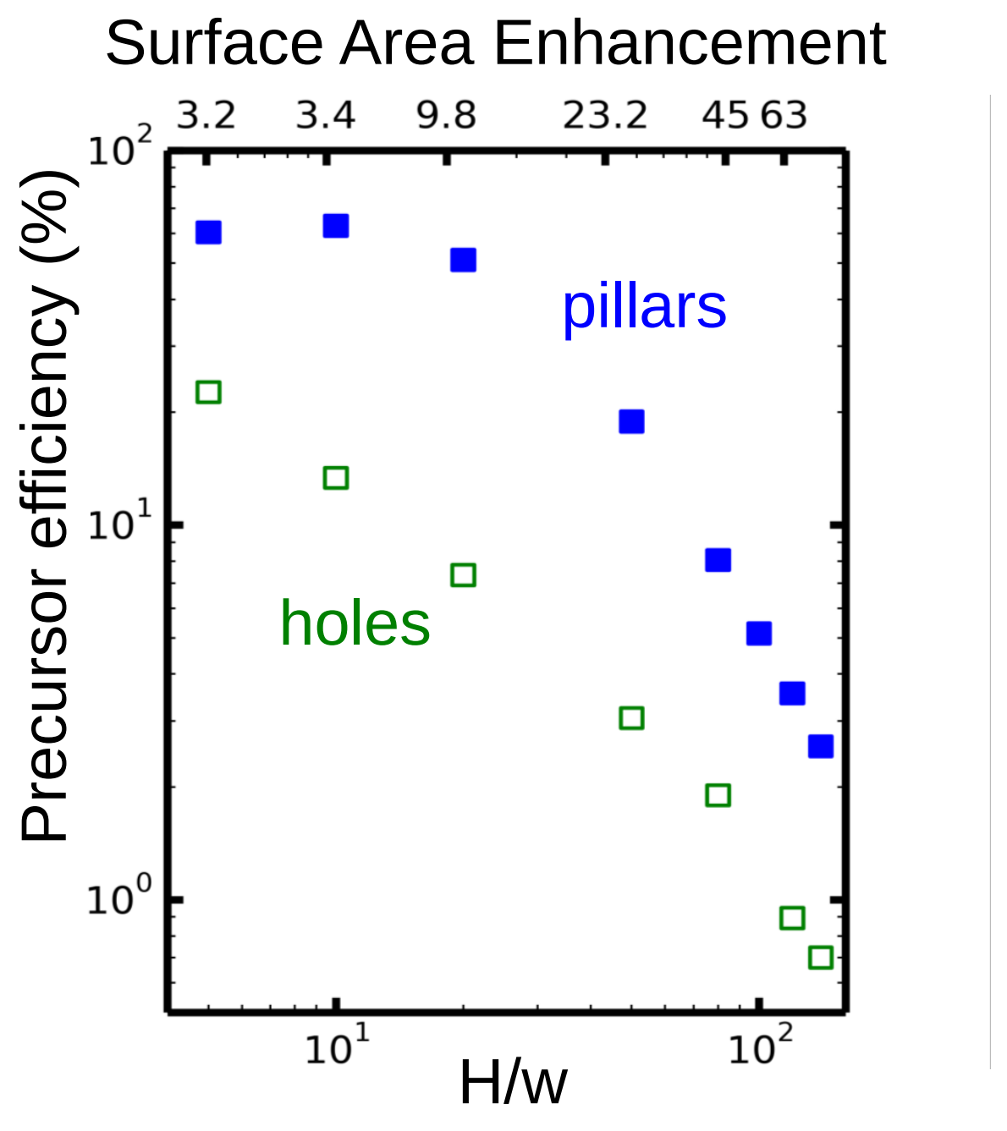
For a certain SAE factor, e.g. 20, it is easier to coat undeep holes with a small spacing than deep holes with a large spacing.





For a certain SAE factor, e.g. 20, the required exposure to cover pillars is independent of the exact geometry (H, w, D).





Less precursor loss in pillar geometry than in hole geometry.

Conclusion

Lower required exposure, ~precursor cost, for **pillar** geometries makes them **much more suit**able for functionalization by **ALD**.

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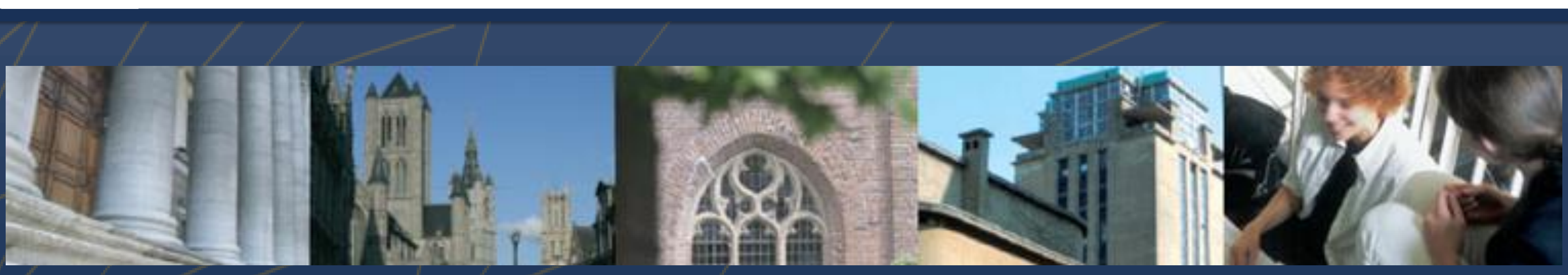

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