

FROM RESEARCH TO INDUSTRY

cea tech

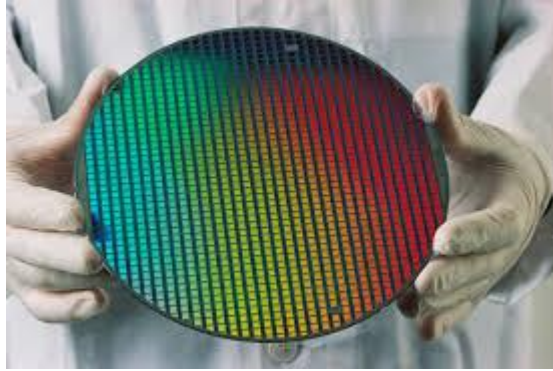
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# Modeling Directed Self-Assembly of Block Copolymers for Lithographic applications

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COMSOL  
CONFERENCE  
2015 GRENOBLE

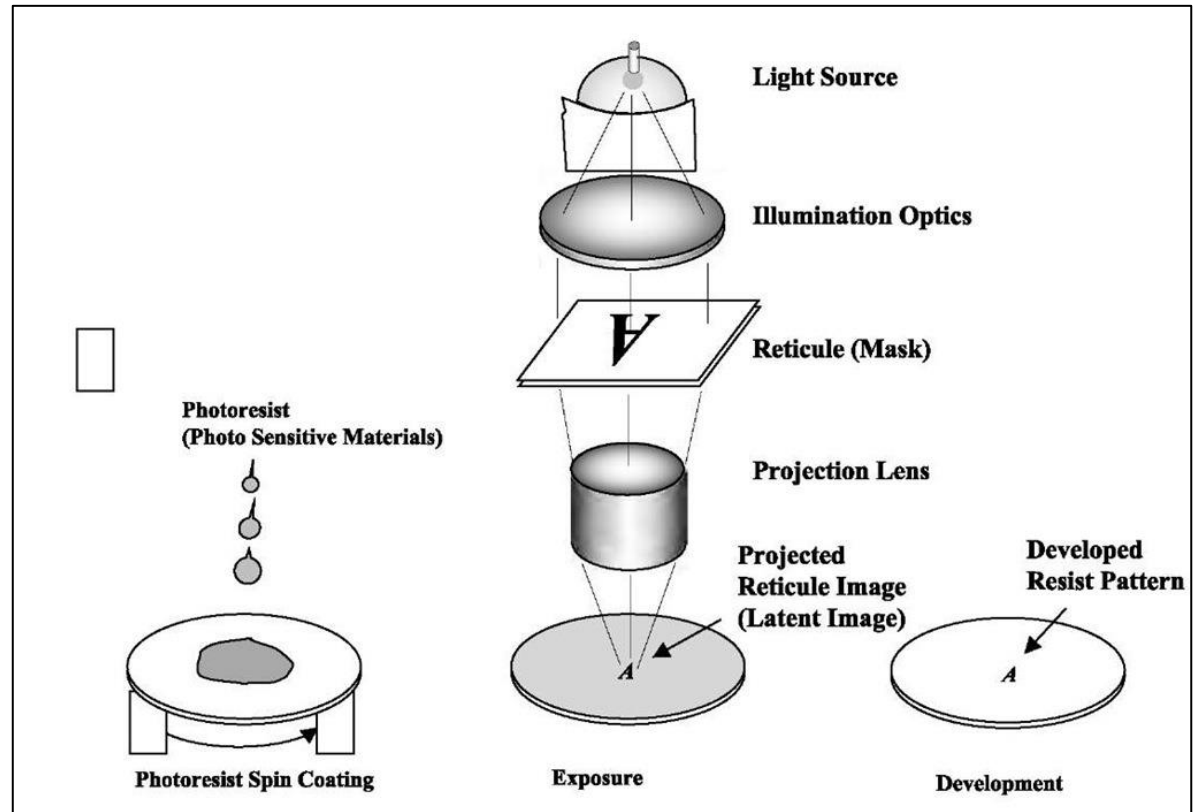
- The DSA technology for nano patterning
- Modeling with Comsol phase field interface
- Some results & applications



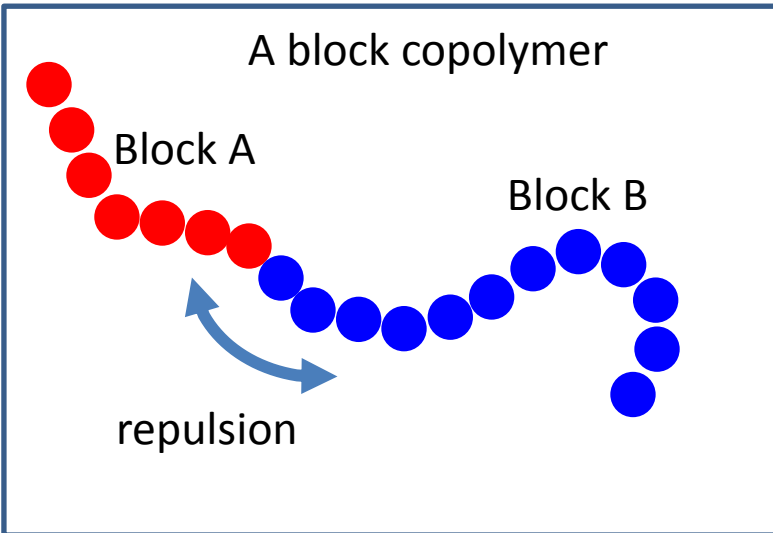
*A full silicium patterned wafer*

## Nano patterning for chip fabrication → Lithography step

**Limitations of  
conventional  
optical lithography  
due to resolution  
( $\lambda=193\text{nm}$ )**



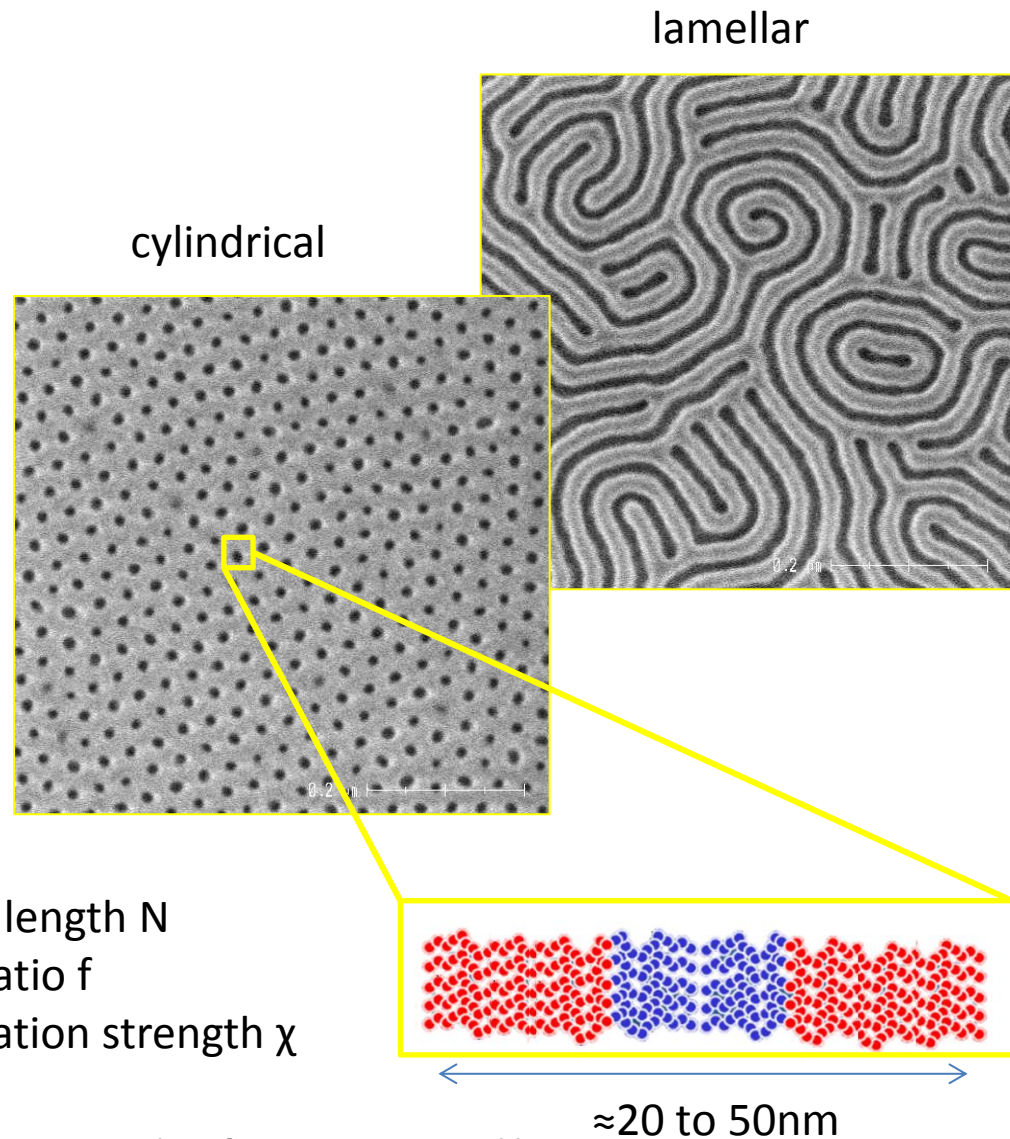
*Optical lithography : principle schematic*



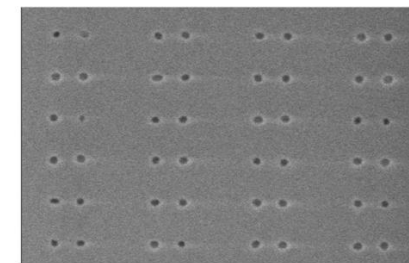
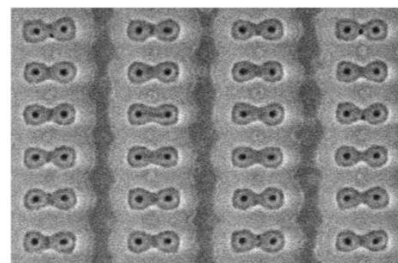
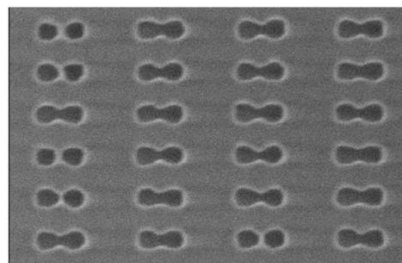
**Annealing → Self-assembly in ordered 2-phases structures**

Change morphology by tuning material's properties

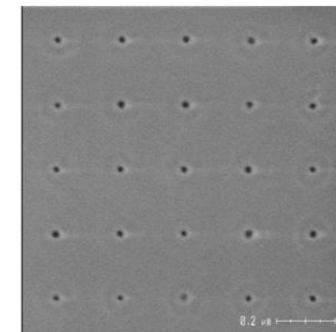
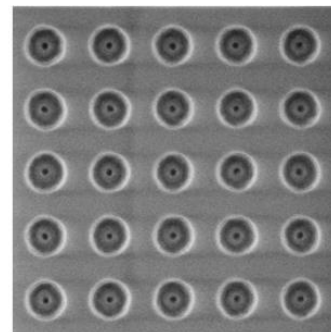
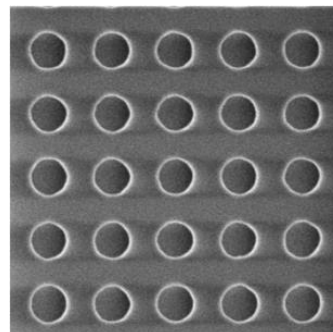
- chain's length  $N$
- Block ratio  $f$
- Segregation strength  $\chi$



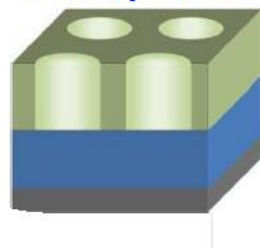
« Contact doubling »



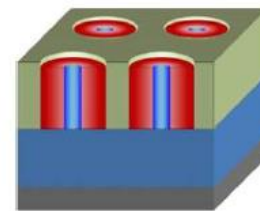
« Contact shrink »



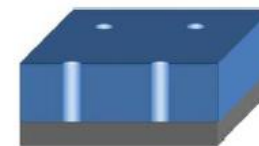
193nm or e-beam litho pattern



BCP self-assembly



BCP pattern transfer

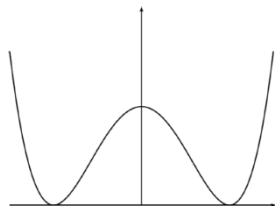


- Purpose:
    - Metrology not sufficient (lack of resolution)
    - Development cost
  - Requirements:
    - Good runtime, especially for 3D for parametric studies
    - Proper boundary conditions for dealing w/ interfaces
  - Choice of the model:
    - not atomistic or particle model (too slow)
    - phase field model :
- ➔ describe system through order parameter

- Cahn-Hilliard equation  
→ phase separation of a binary mixture
- Free energy

$$E = \underbrace{\int_{\Omega} \left( \frac{\phi^4}{4} - \frac{\phi^2}{2} \right) d\mathbf{r}}_{\text{Mixing energy}} - \underbrace{\int_{\Omega} \epsilon^2 \|\nabla\phi\|^2 d\mathbf{r}}_{\text{Interfacial energy}} + \underbrace{\int_{\Omega} \int_{\Omega} \alpha(\phi(\mathbf{r}) - \phi_0)(\phi(\mathbf{r}') - \phi_0)G(\mathbf{r}, \mathbf{r}') d\mathbf{r}' d\mathbf{r}}_{\text{Long range interactions}}$$

Mixing energy



Interfacial energy

Long range interactions



Added in weak formulation

- Fick's law

$$\frac{\partial \phi}{\partial t} = \Delta \mu \quad \text{with} \quad \mu = \frac{\delta E}{\delta \phi} \quad \text{the chemical potential}$$

- Finally 
$$\frac{\partial \phi}{\partial t} = \Delta (\phi^3 - \phi - \epsilon^2 \Delta \phi) - \alpha(\phi - \phi_0)$$

- Boundary conditions 
$$\left\{ \begin{array}{l} \mathbf{n} \cdot \nabla \mu = 0 \\ \mathbf{n} \cdot \nabla \phi = -\cos(\theta) \end{array} \right.$$

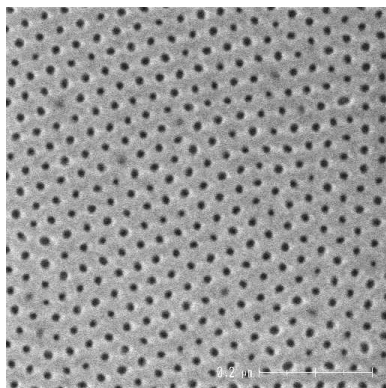
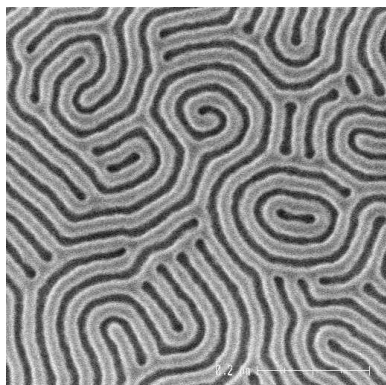
Contact angle

- Initial conditions : small fluctuations around  $\phi_0$

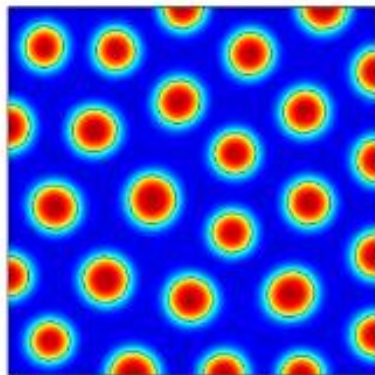
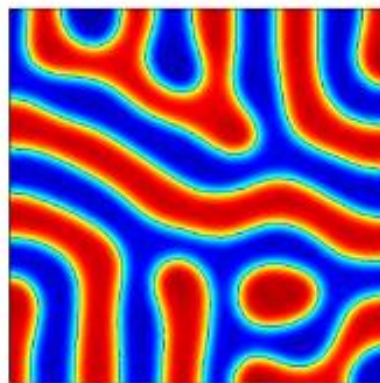


## Free surface simulations

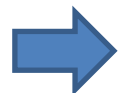
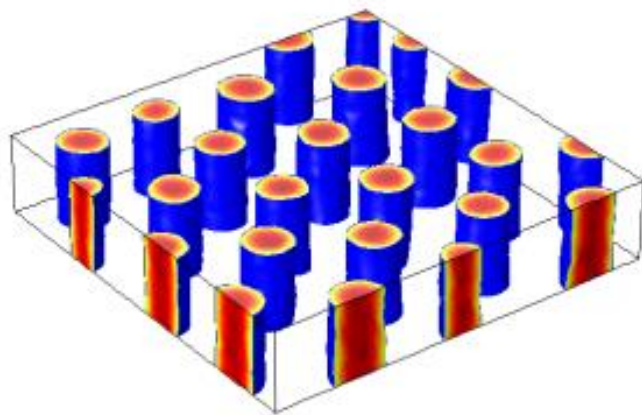
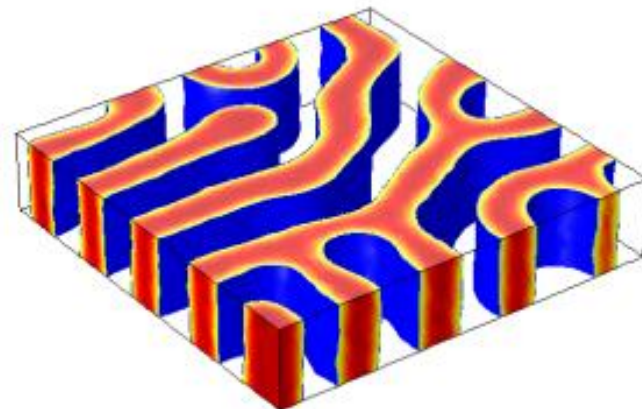
SEM images



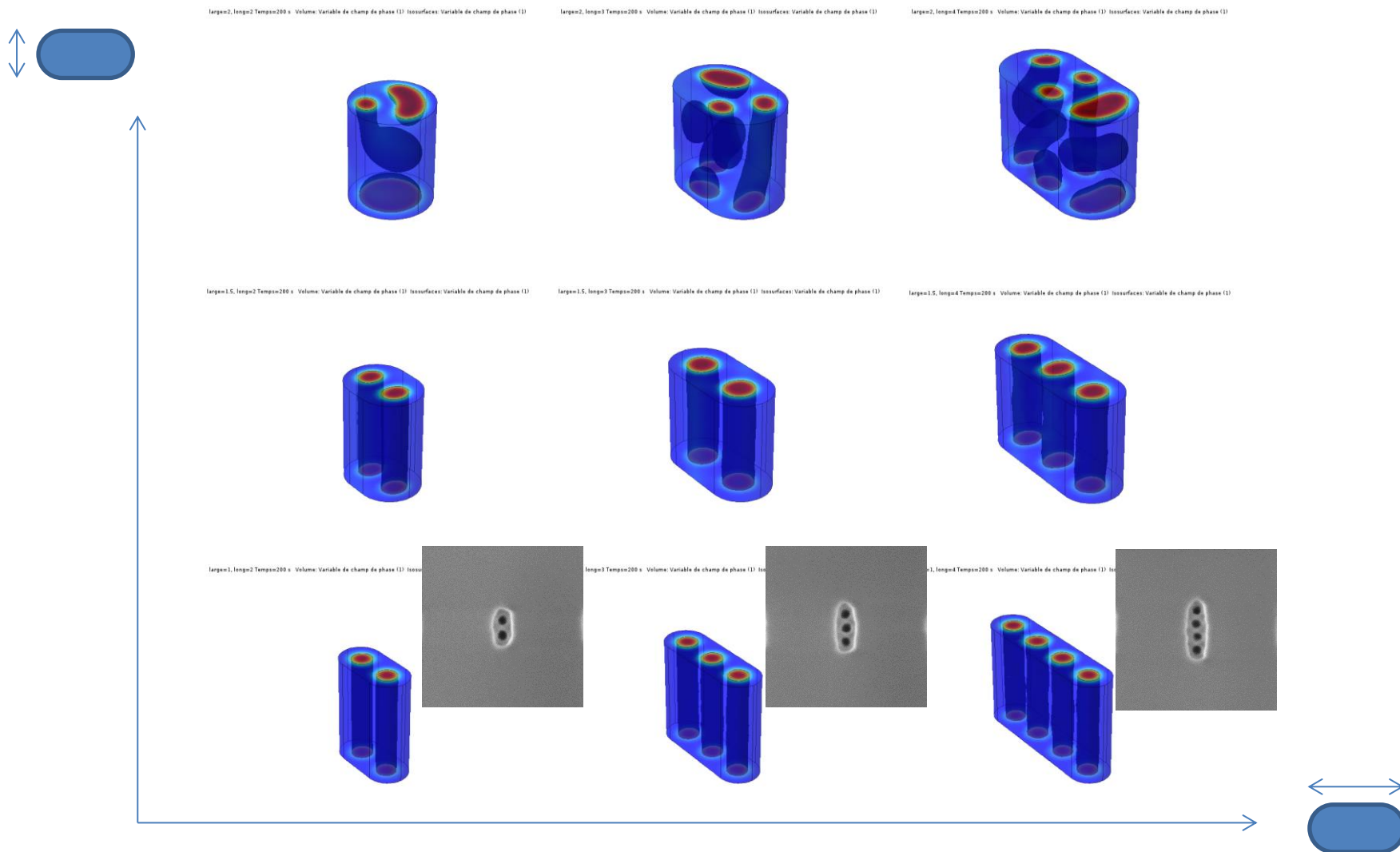
2D



3D



**Good agreement !**



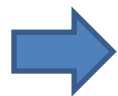
By changing contact angle  $\theta$  we can change the affinity of interfaces



neutral

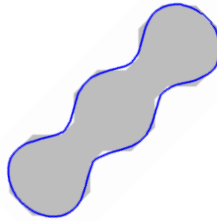


Preferential affinity

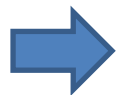
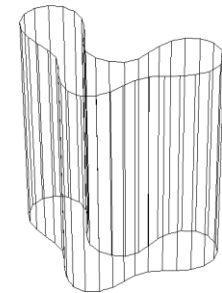
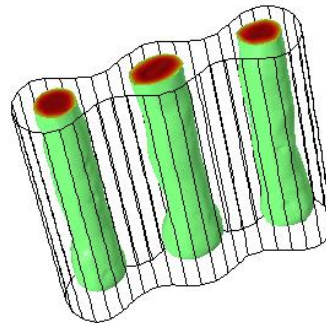
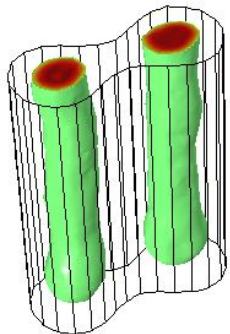


Study impact of a different surface energy

## OPC simulated patterns

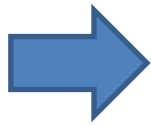


## Corresponding 3D simulations



**Pattern optimization**

- Good qualitative agreement



**Comsol phase field interface is suitable for modeling DSA**

- Perspectives
  - Full Calibration
  - More interesting studies !