Computational modelling of nanowire growth

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Introduction

Background

- ➔ Semiconducting nanowires are small crystalline filaments with diameters in the order of a few nanometres.
- ➔ Usually made of type III-V semiconductors, such as GaAs or InP.
- ➔ They are interesting because they show many potential applications.

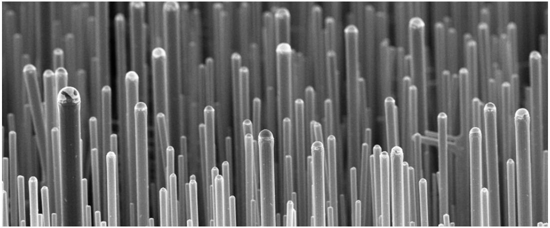


Figure: https://www.cvdequipment.com/portfolio-item/silicon-nanowires-sem-10-k-x/

Application: Majorana zero modes

- ➔ They can be used to implement the Majorana chain.
- ➔ Nanosystem with topological phase that shows applications in topological quantum computing.
- ➔ Solves the decoherence problem by creating topologically-protected qubits.

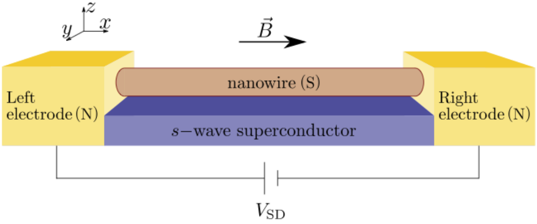


Figure: https://arxiv.org/pdf/1902.05821.pdf

Nanowire growth

- ➔ There are many different procedures for growing semiconducting nanowires.
- ➔ One of them is selective area epitaxy (SAE).

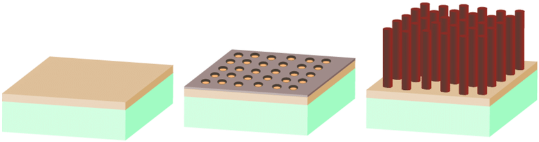
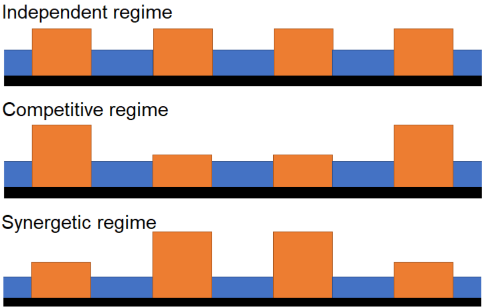


Figure: *https://www.researchgate.net/publication/303682098*

Experimental observations

- ➔ It has been observed experimentally that sometimes nanowires grow unevenly.
- ➔ Three distinct growth regimes can be identified



Experimental observations

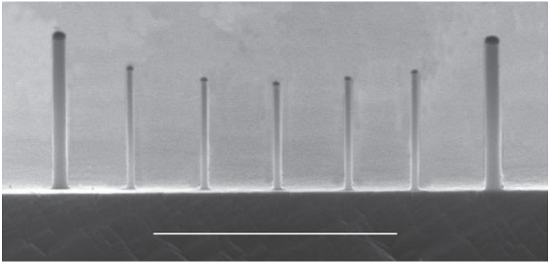


Figure: *Borgstrom, M. et al - Synergetic nanowire growth (Nature nanotechnology)*

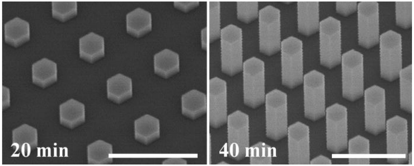


Figure: *https://aip.scitation.org/doi/10.1063/1.4916347*

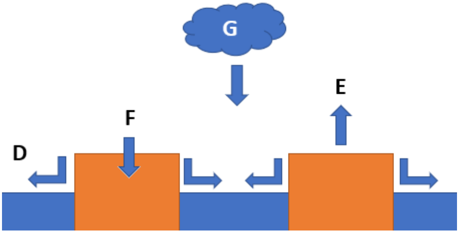
Motivation

- ➔ A simple model for selective area epitaxy may provide qualitative information about the origin of these regimes.
- ➔ Knowing their origin can provide information on the underlying mechanisms for nanowire growth.
- ➔ For example, optimization: How can synergy be effectively suppresed?

The model

MBE

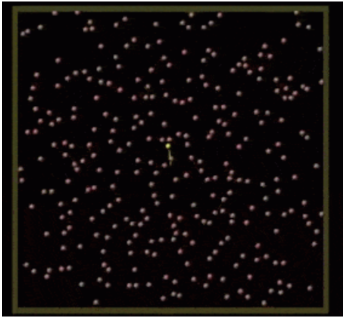
We can highlight some elements when modelling a SAE process:



- ➔ G: Number of particles adsorbing to the system per unit time
- ➔ F: probability of an adatom to nucleate into the semiconductor.
- ➔ E: probability of an adatom to evaporate back.
- ➔ D: tendency of the system to equilibrate concentrations.

Proposed models

➔ We could model the paths of the particles with a random walk;



➔ But it is more practical to postulate and solve a differential equation.

The diffusion equation

- The equations that model particles in diffusion are the Fick laws.

$$J = -D \cdot \nabla c \qquad \text{First Fick law,}$$

$$\frac{\partial c}{\partial t} = \nabla(D \cdot \nabla c) \qquad \text{Second Fick law.}$$

- The most useful equation is the second Fick law in steady-state form.

$$\nabla(D \cdot \nabla c) = 0$$

- Needs the *quasistatic* approximation: equilibrium much faster than growth.

The model

- We can add a source term for the incoming particles and sink terms for the loss of adatoms.

$$\nabla(D \cdot \nabla c) - (E + F) \cdot c + G = 0$$

- Note that the diffusion constant depends on characteristic time and characteristic length.

$$D = \frac{L^2}{4t}$$

- The definition of the characteristic time enables us to redefine the parameters and the equation in a more physically meaningful way.

$$E + F = \frac{1}{t}$$

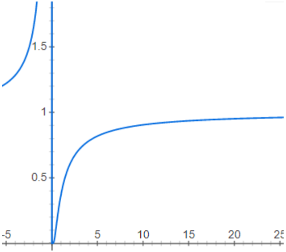
$$\nabla \left(\frac{L^2}{4t} \cdot \nabla c \right) - \frac{c}{t} + G = 0$$

Temperature

- Temperature may be introduced through Arrhenius law.

$$A \to A(T) = A \exp\left(-\frac{E_a}{K_B T}\right)$$

- Should work for D, but what about L, t and G? Values for E_a?
- Observe how $A = A(T \to \infty)$



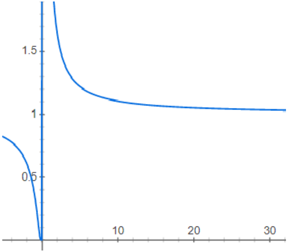
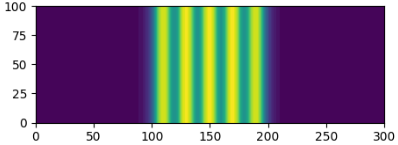


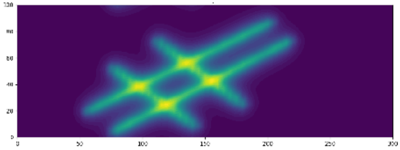
Figure: Plots for $\exp \frac{-1}{x}$ *and* $\exp \frac{1}{x}$

Approach

Solving the equation numerically

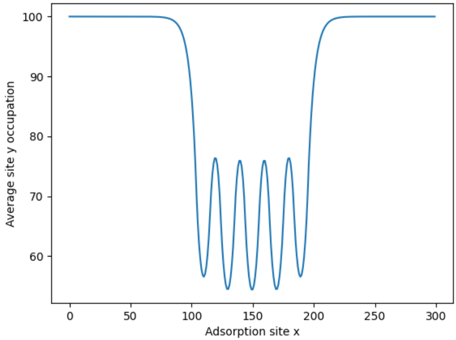
- Use of a finite-element solver with periodic boundary conditions.
- The result of the equation is the steady-state distribution of adatoms in the surface, proportional to the nanowire growth rate.
- The equation can be solved for an arbitrary trench geometry. However, for rectilinear trenches the process is computationally more efficient and more insightful.

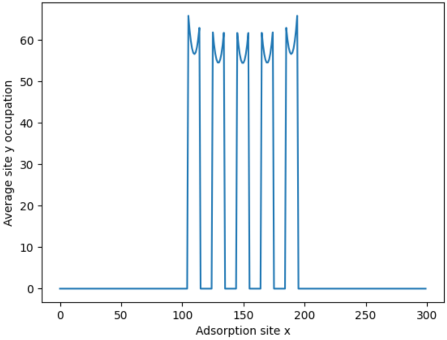




Solving the equation numerically

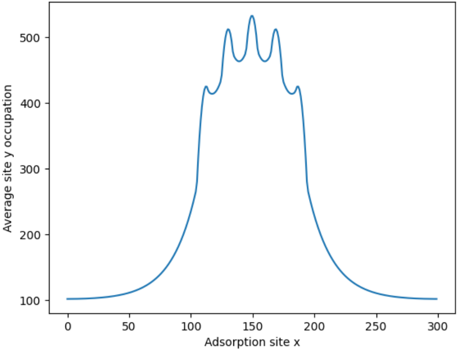
For some parameter values the resulting regime is competitive...

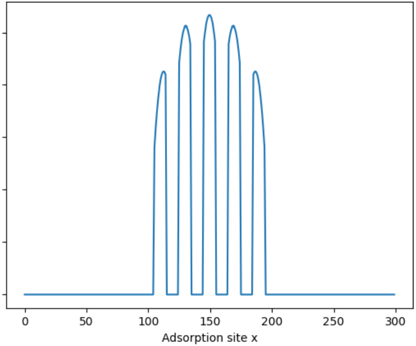




Solving the equation numerically

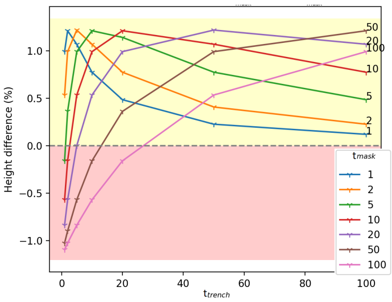
...while for others is synergetic

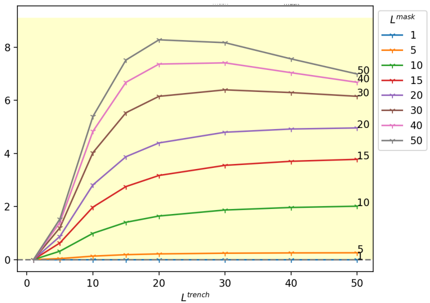




Characterizing the regimes

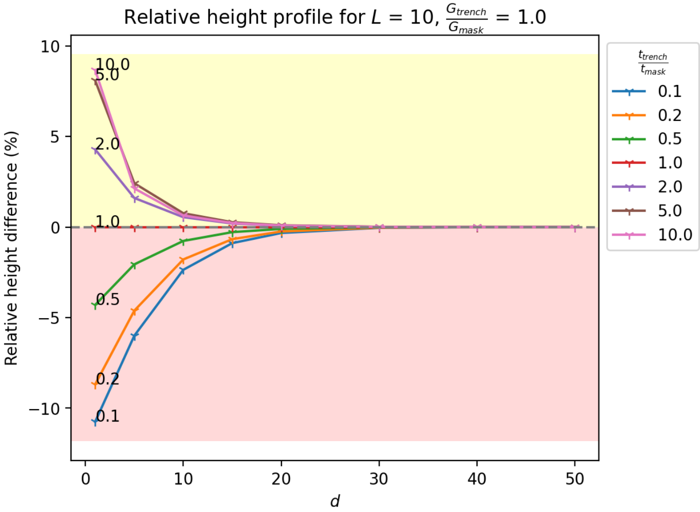
- To characterize the growth regimes, we can use the difference in nanowire heights $r = h_1 - h_0$. Material volume could also be used.
- Plot r for different values of (d, t, L, G), fixing two of them.
- For the parameters t and G we consider the ratios between mask and trenches, while for L and d we consider the values.



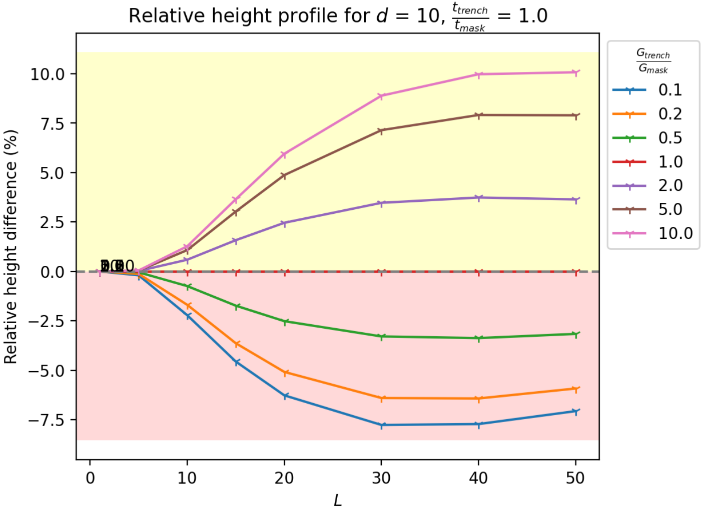


Results

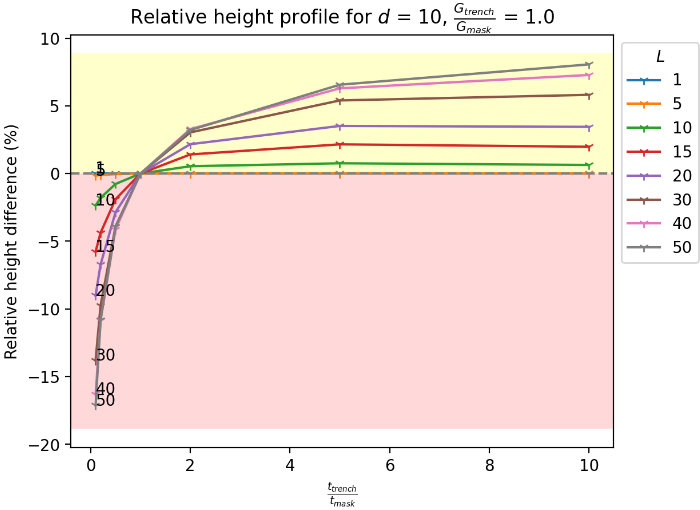
The role of the nanowire separation



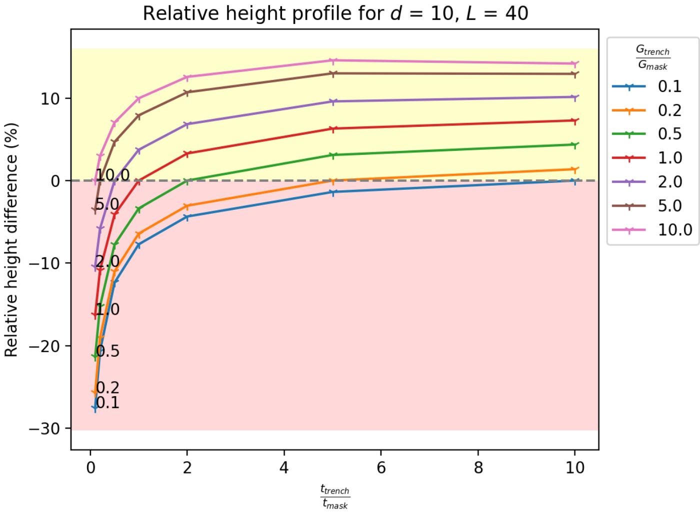
The role of the characteristic length



The role of the characteristic time



The role of the input flux



Conclusions

Conclusions

- ➔ The simple model apparently captures the three regimes depending on two factors.
- ➔ On the one hand: relative adatom density. Characterized by t and G.
- ➔ On the other hand: adatom diffusion. Characterized by L and d.
- ➔ Many potential generalizations (temperature, geometries, more complex model...).

- ➔ **Is this numerical characterization useful for a real process?**
- ➔ **With the right parameters, does it reflect experiment?**

Questions?