Modeling of InAs nanowire growth using a dual-adatom diffusion-limited approach

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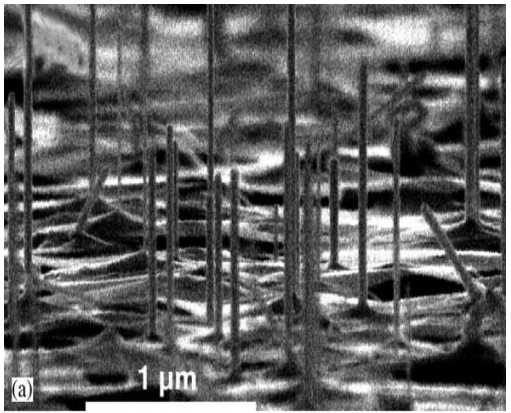
Introduction

Introduction: VLS growth of compound semiconductor nanowires

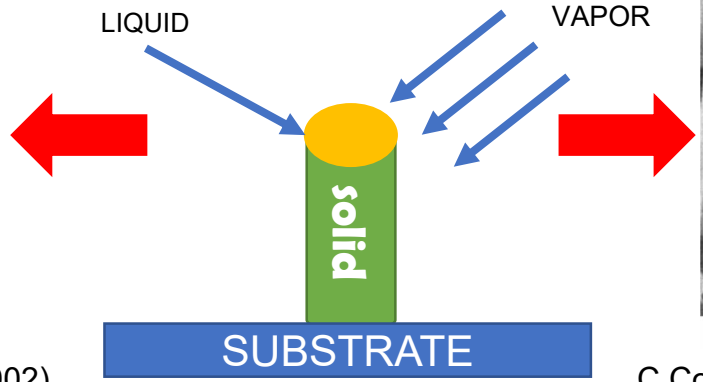
Gold-catalyzed growth

Material: InAs



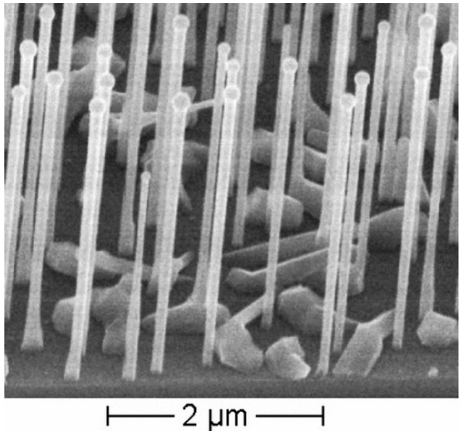
B.J. Ohlsson et al. Physica E 13 (2002)

Vapor-Liquid-Solid growth mechanism



Self-catalyzed growth

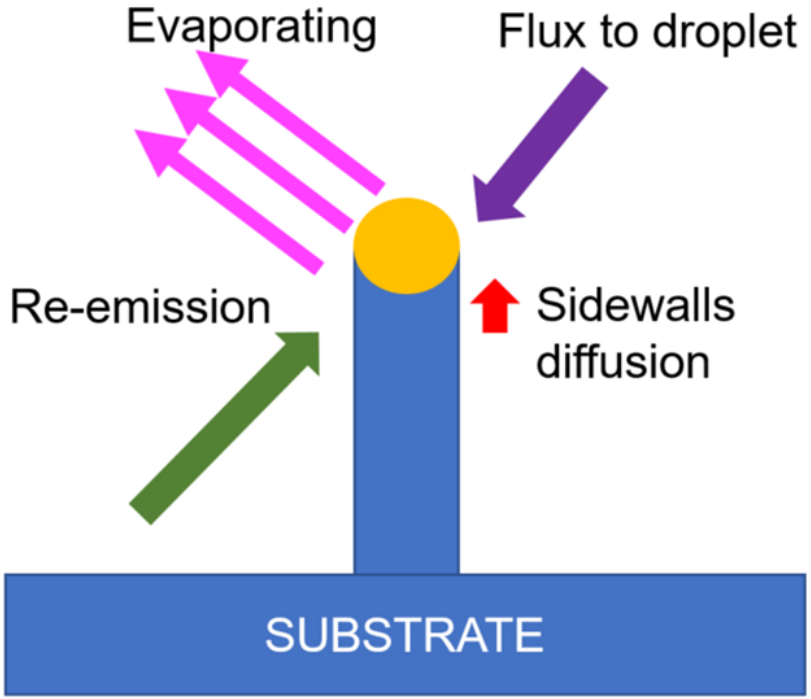
Material: GaAs



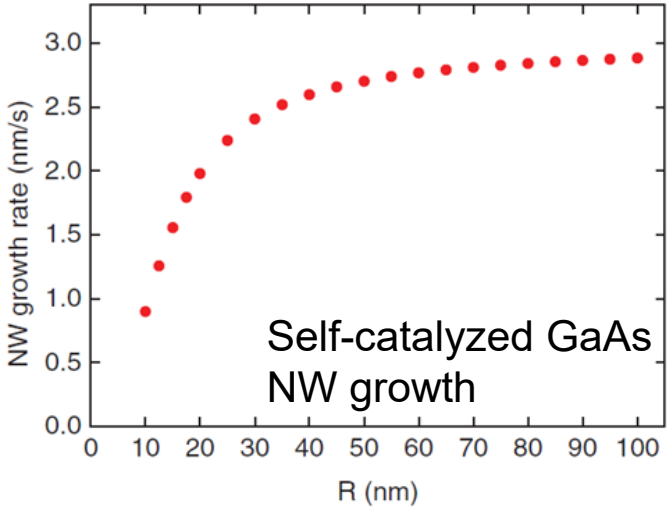
C.Colombo et al. Phys. Rev. B 77, 155326 (2008)

The current of adatoms arriving to the droplet is important!

ARSENIC current



Arsenic-limited growth rate

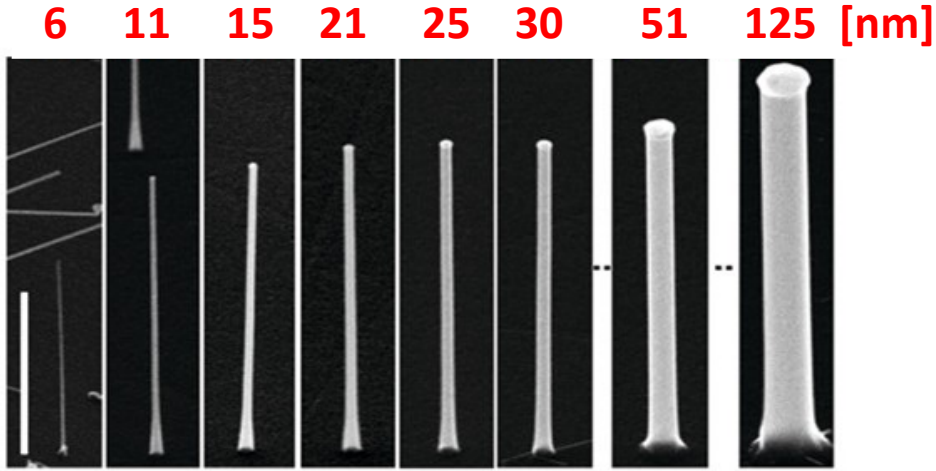


Glas F. et al., Phys. Rev. B 88, 195304 (2013)

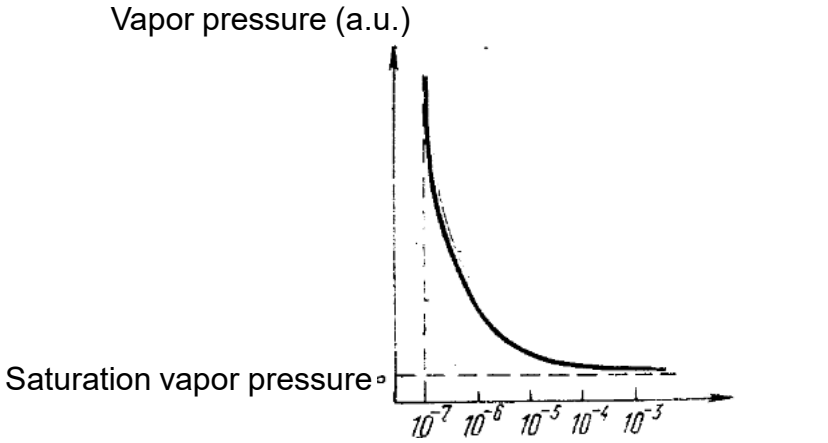
Model of Glas describes growth with excess of Ga

Kelvin effect

Material: Ge



Shadi A. Dayeh. et al., Nano Lett. 2010

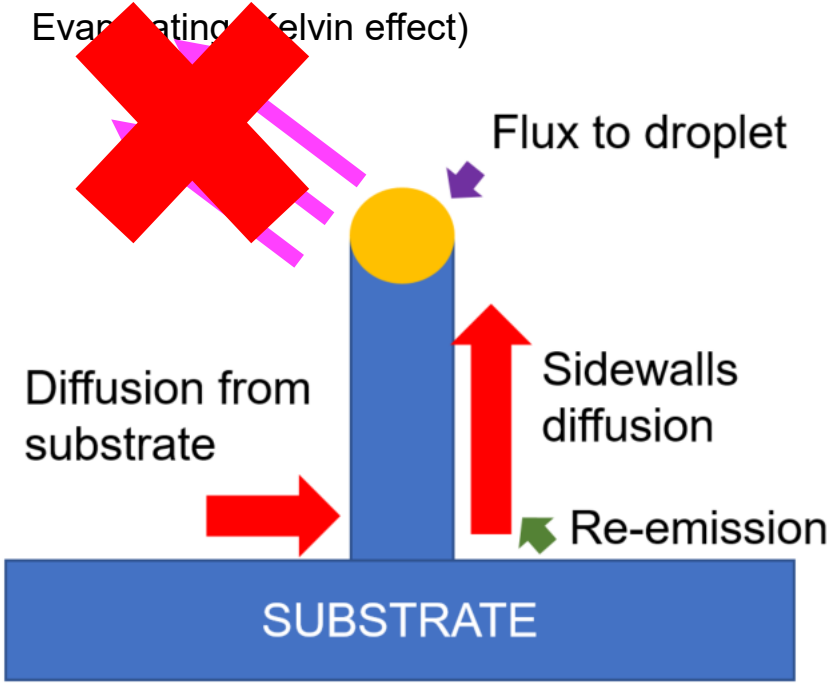


Meyer K., Physikalisch-chemische Kristallographie (1968)

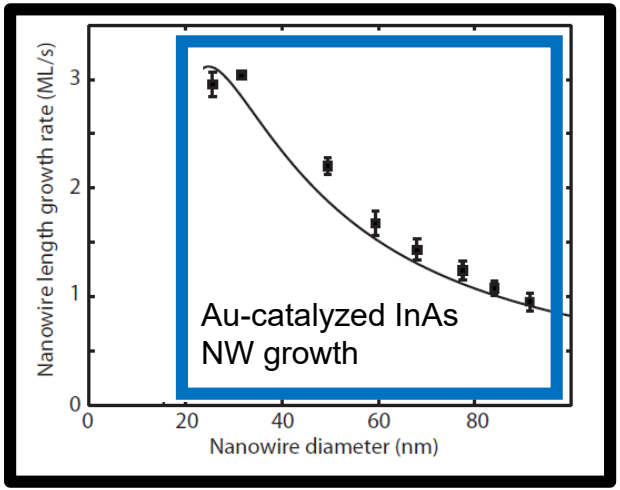
The surface energy becomes crucial at small radius

INDIUM current

Evap ating (Kelvin effect)



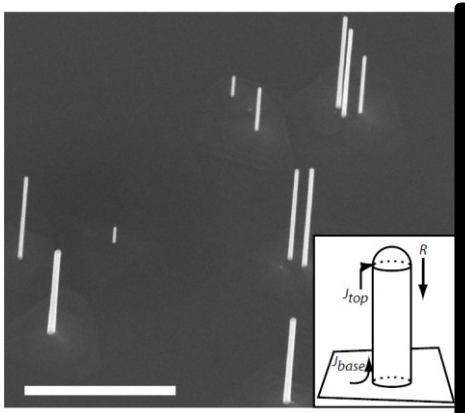
Diffusion-limited growth rate

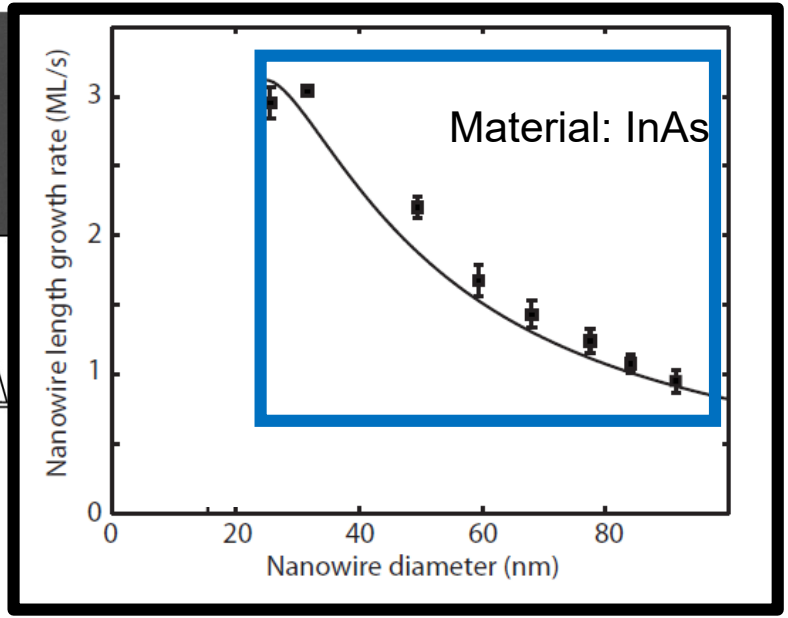


Fröberg, et al. Phys. Rev. B 2007, 76, 153401.

Main current of Indium reaches the droplet via diffusion

Fröberg's growth model





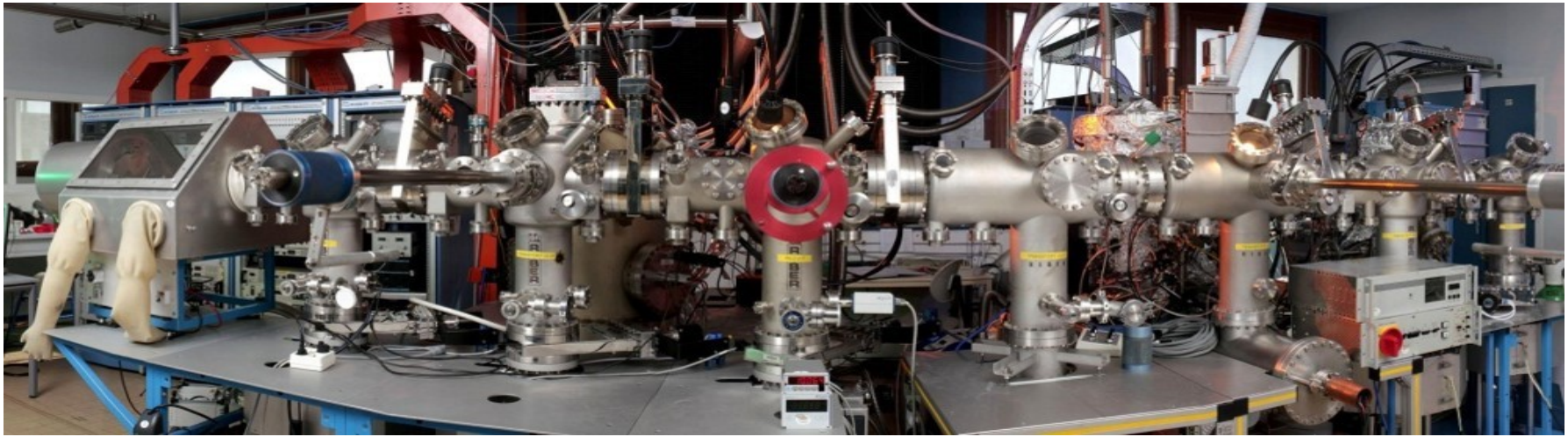
- **Diffusion**
- **Kelvin effect**

Fröberg, et al. Diameter-dependent growth rate of InAs nanowires. Phys. Rev. B 2007, 76, 153401.

Model of Fröberg based on In diffusion and Kelvin effect

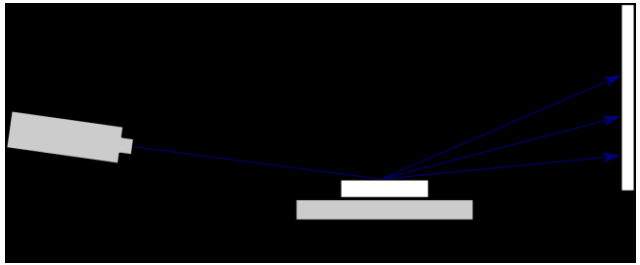
Nanowires growth

Molecular Beam Epitaxy

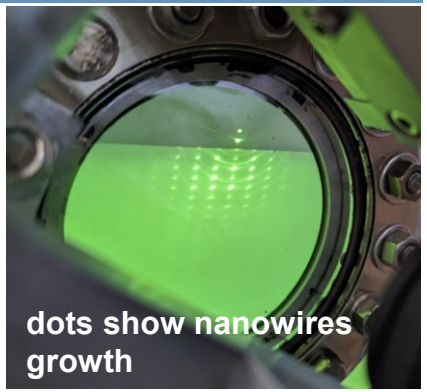


We are using the MBE technic for nanowire growth

RHEED (reflection high-energy electron diffraction)

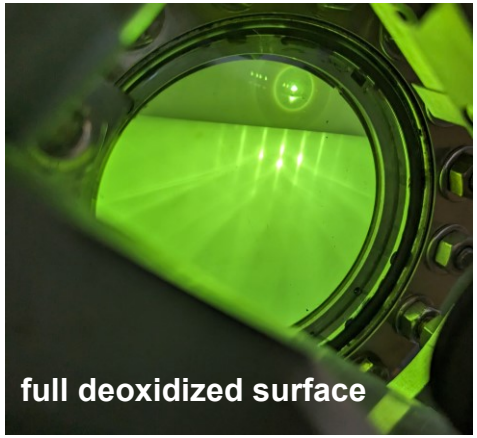


Functional scheme of RHEED
(picture from Wikipedia)



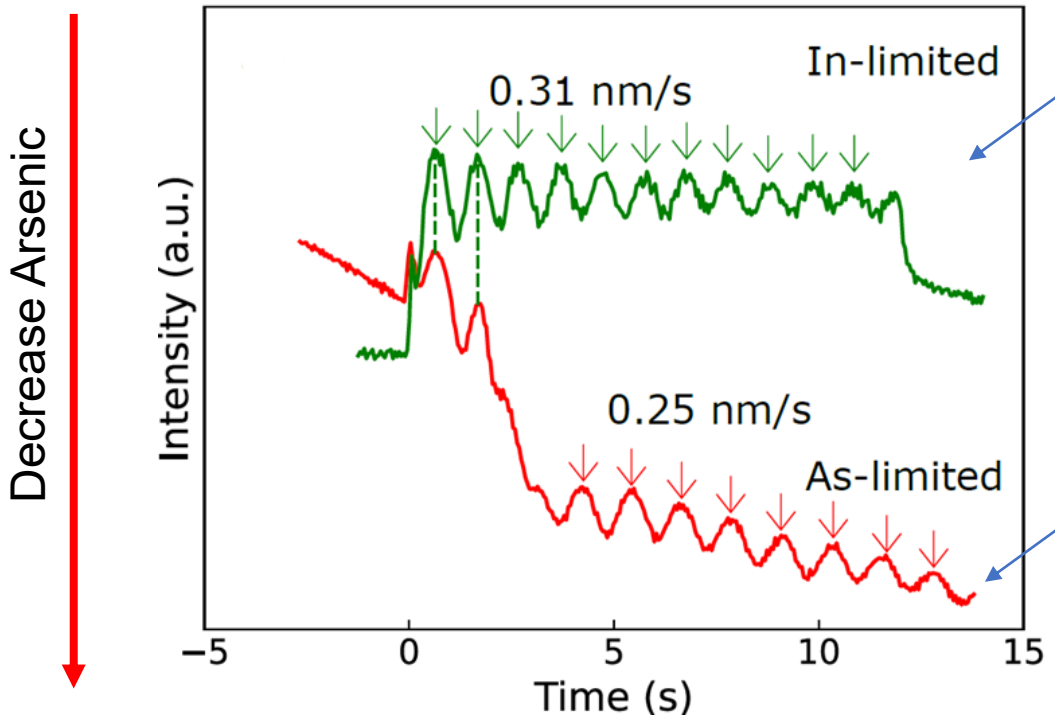
RHEED helps :

- **determining the surface state**
- **measuring the growth rate**



Growth rate calibration

Flux calibration using RHEED oscillations

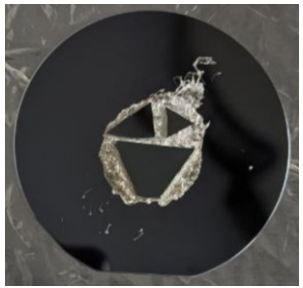


In BEP: $7.7*10^{-7}$ Torr
As BEP: $42*10^{-7}$ Torr

In BEP: $7.7*10^{-7}$ Torr
As BEP: $22*10^{-7}$ Torr

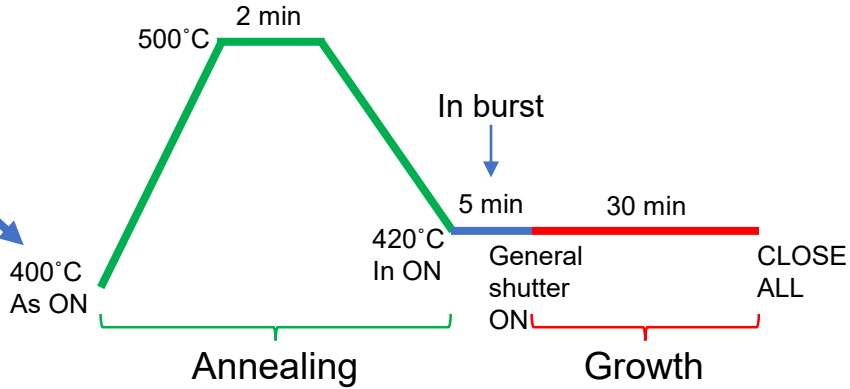
Sample preparation and growth process

Colloid bottle

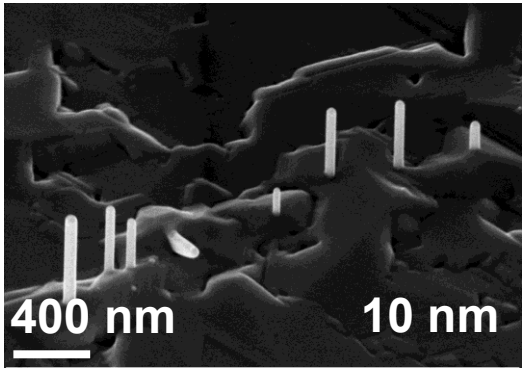


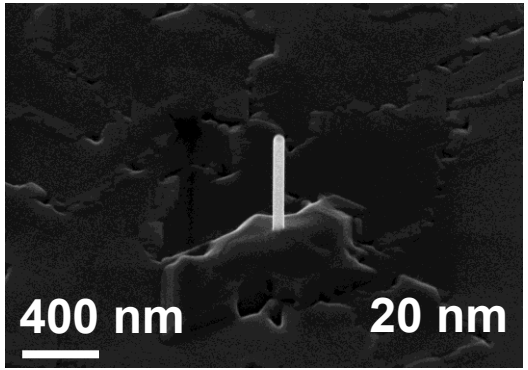
Samples

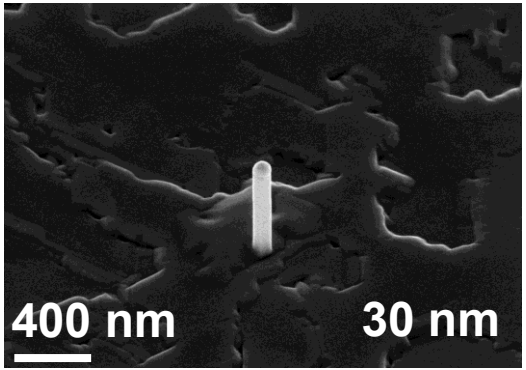
Degassing at 250˚C

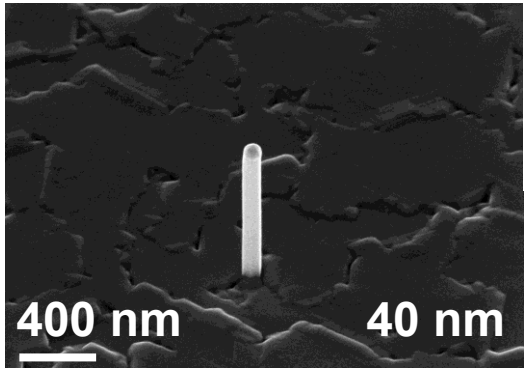


Example of InAs wires grown @NPSC

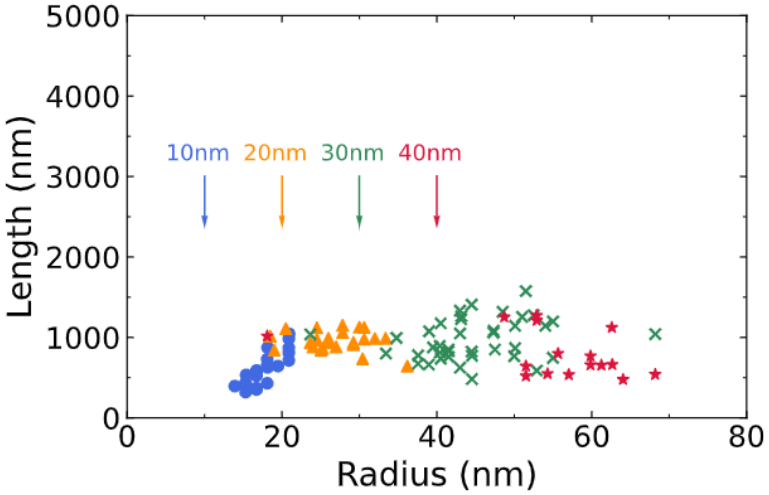






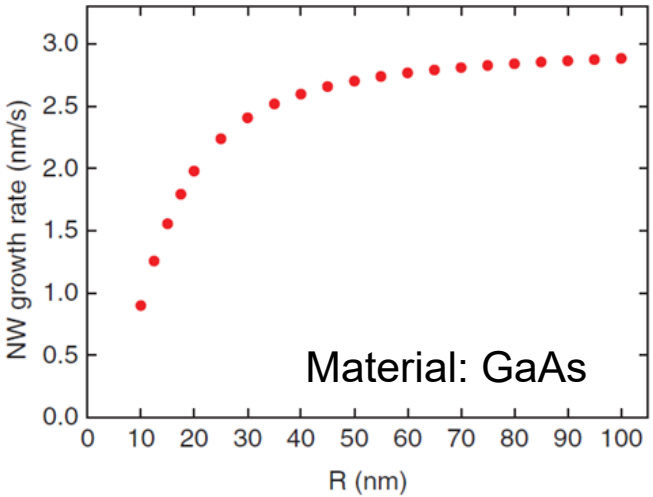


NW901 V/III flux ratio = 0.9

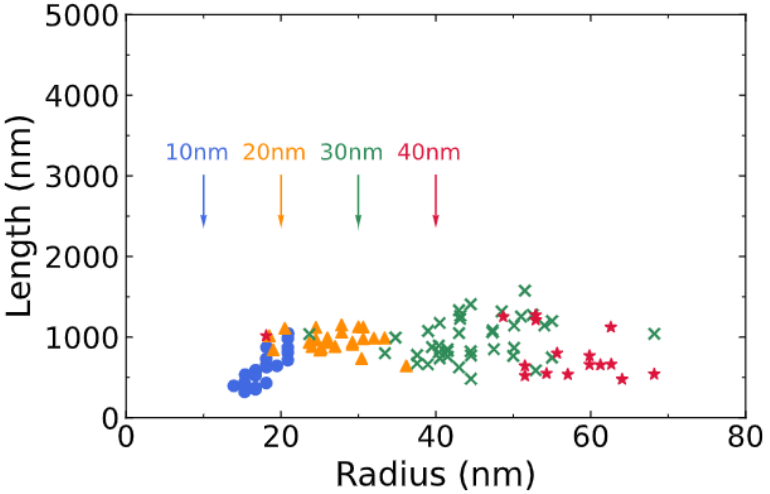


Growth modeling NW901

Model of Glas et al.

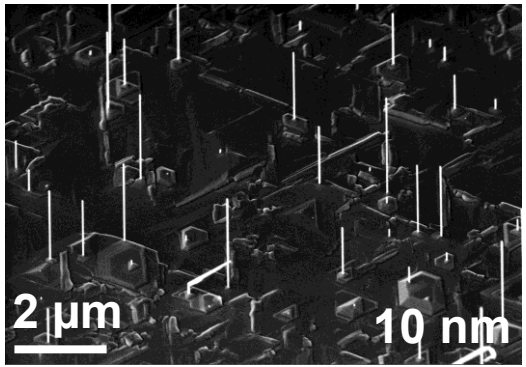


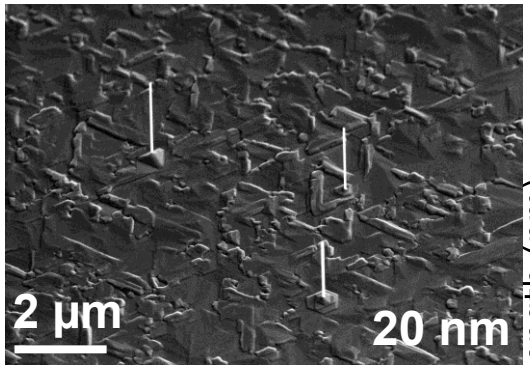
V/III ratio = 0.9

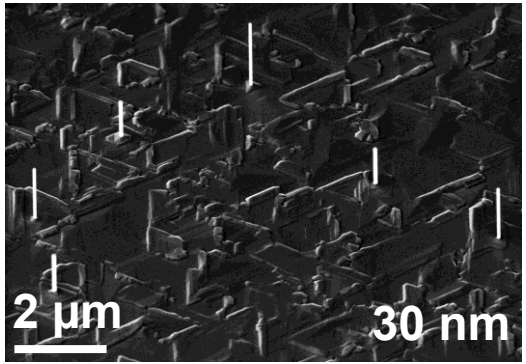


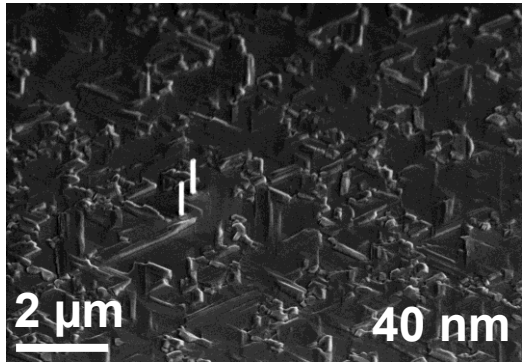
Here we will use the model of F.Glas with the As current

Example of InAs wires grown @NPSC

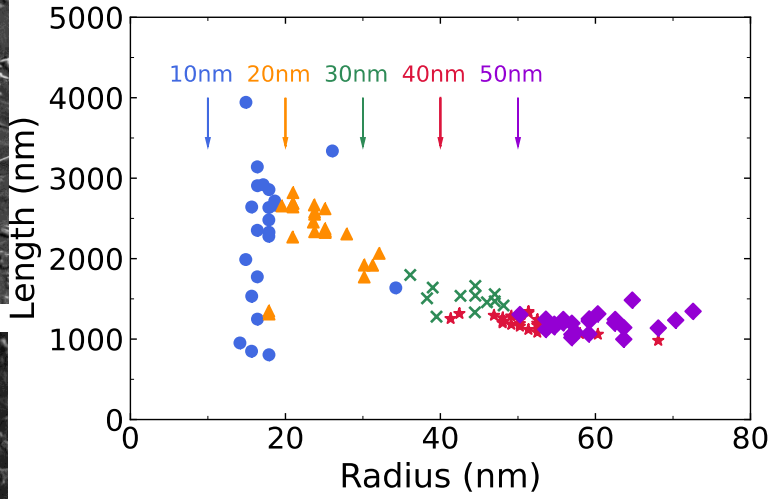






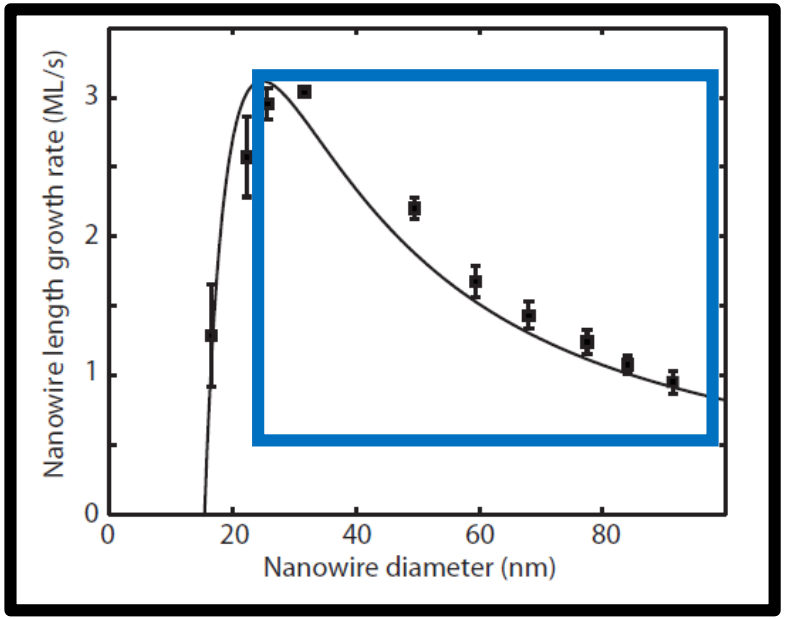


NW898 V/III flux ratio = 10.6

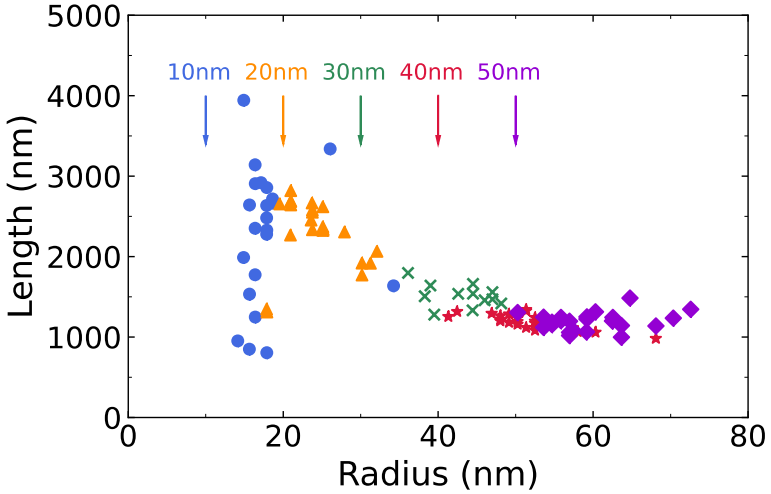


Growth modeling NW898

Model of Froberg



V/III ratio = 10.6



In diffusion explains the large diameter part and we can determine the In current

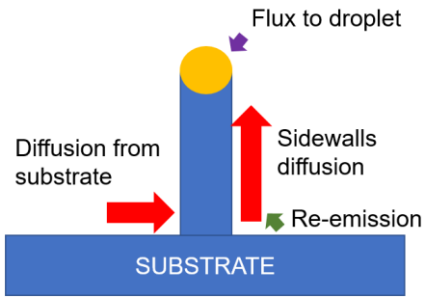
Modeling

Dual-adatom model

Case of InAs nanowires: In and As have very different physical properties

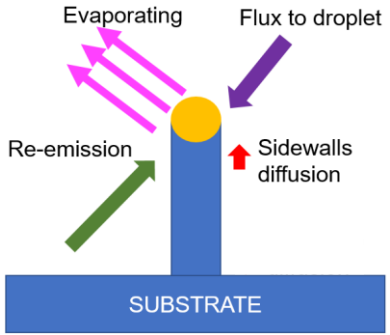
In

- Low evaporation rate
- Long diffusion length
- Low surface re-emission



As

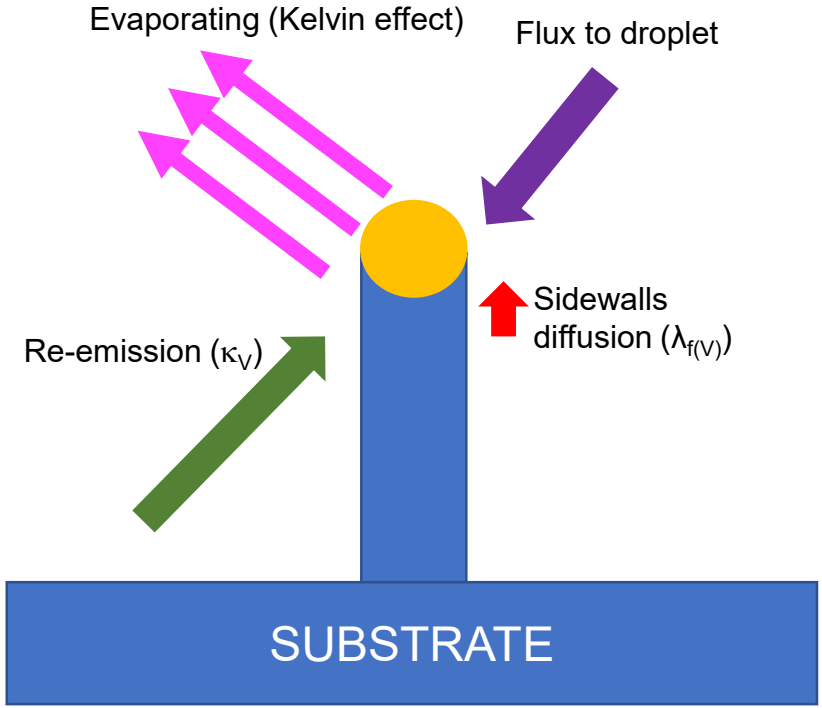
- High evaporation rate
- Suffers from Kelvin effect
- Small diffusion length
- High surface re-emission

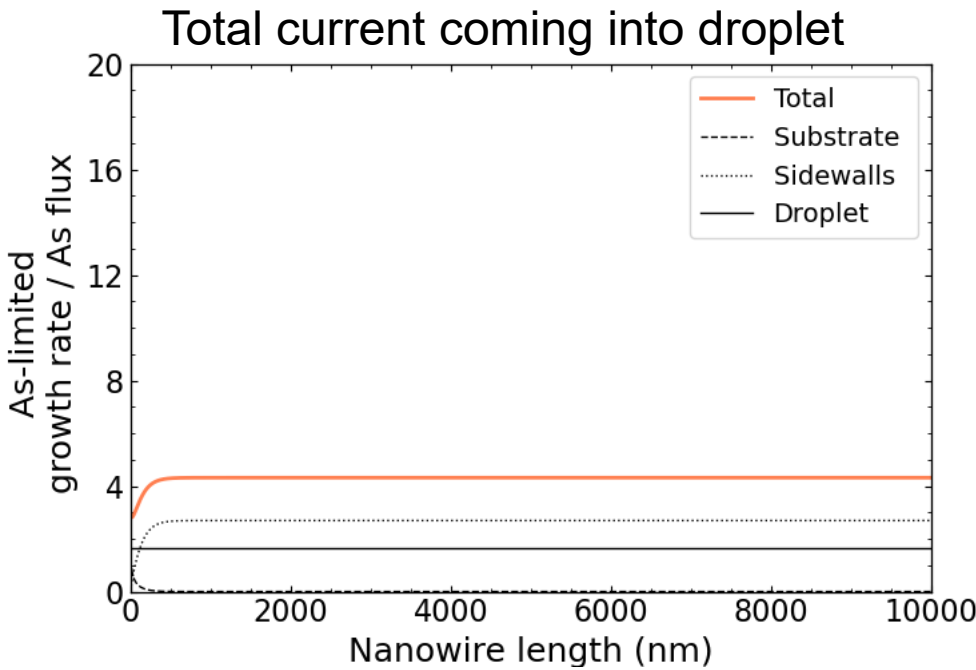


Proposition: develop a model for growth taking into account two species, In and As

As species

$J_{total\ (As)} = J_{facets} + J_{direct} + J_{reemission} - J_{evaporation}$

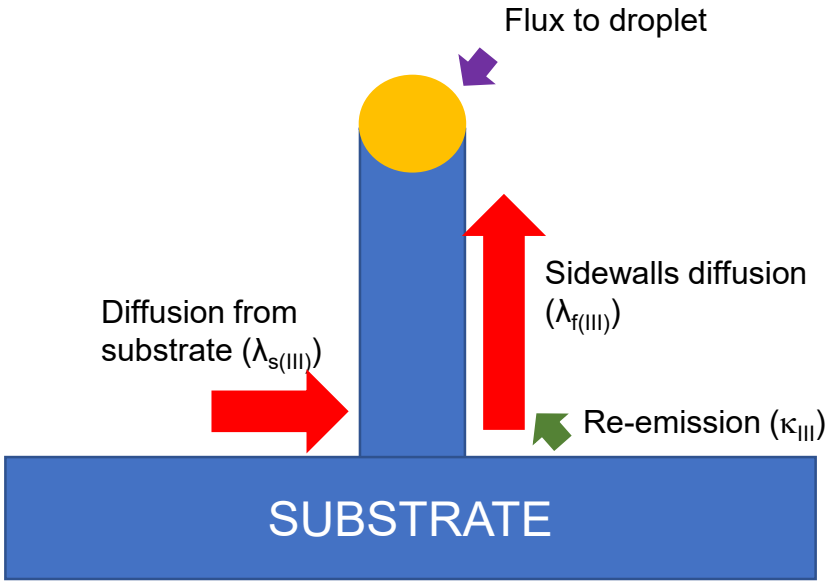




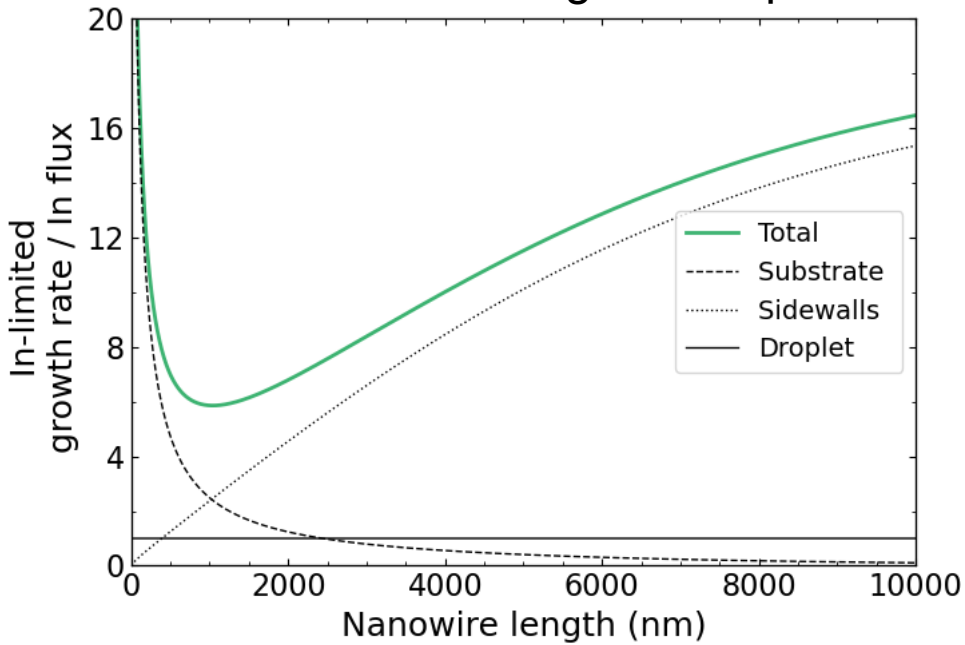
R= 20 nm

In species

$J_{total(In)} = J_{sub} + J_{facets} + J_{direct}$



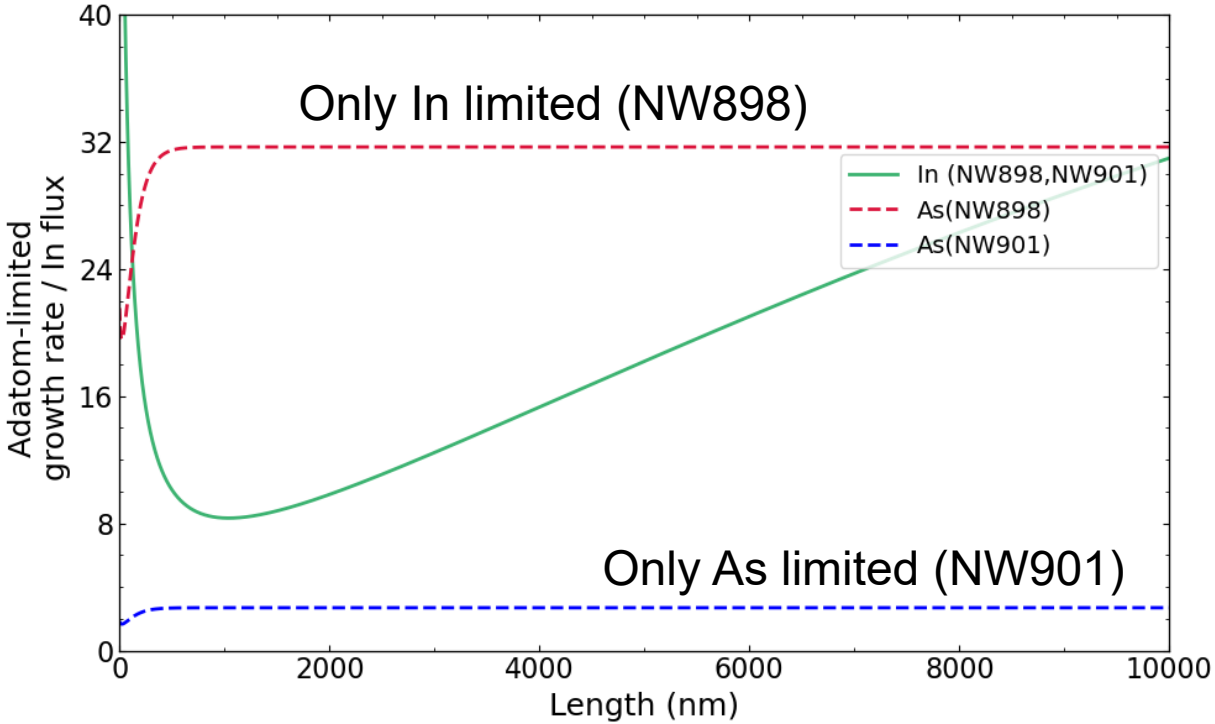
Total current coming into droplet



Evolution of the current versus NW length

As current change → curve shifts up and down

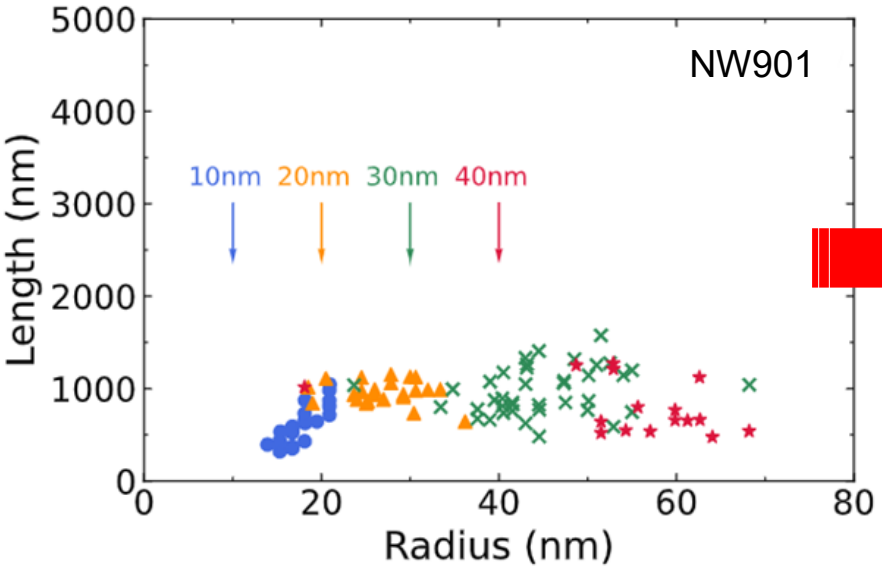
Growth always limited by smallest current



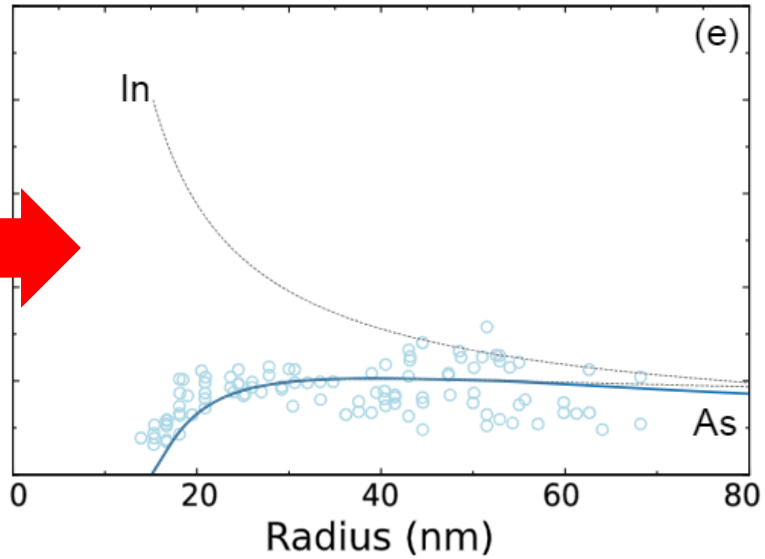
Modeling for our samples for R=20 nm

Fit for the growth results

V/III ratio = 0.9



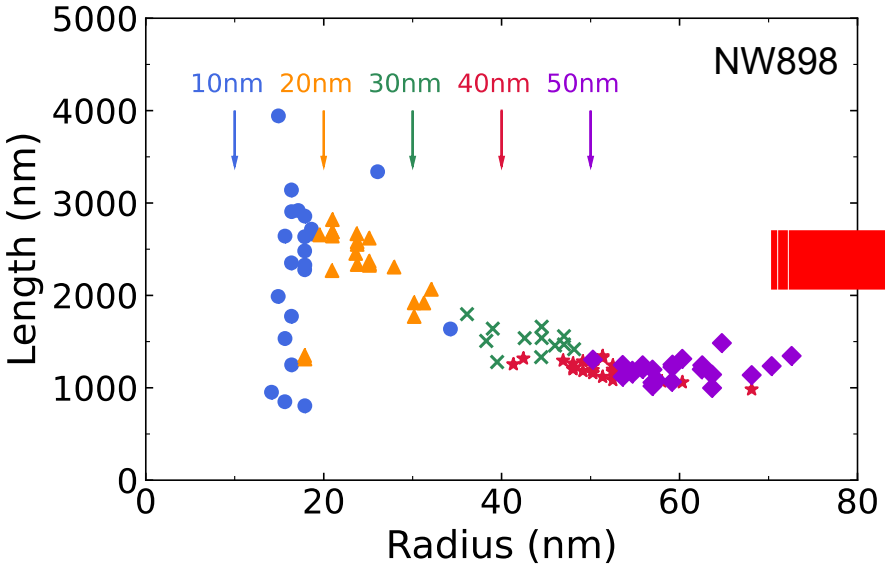
Example of fit



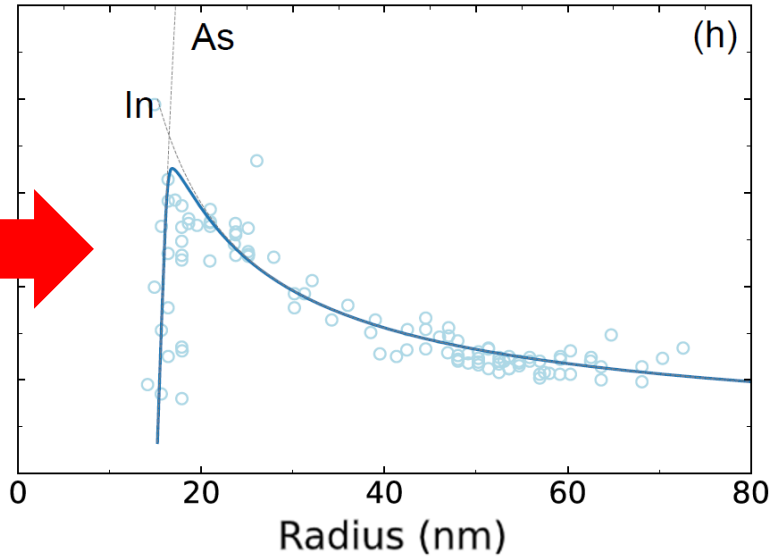
Full As-limited growth

Fit for the growth results

V/III ratio = 10.6

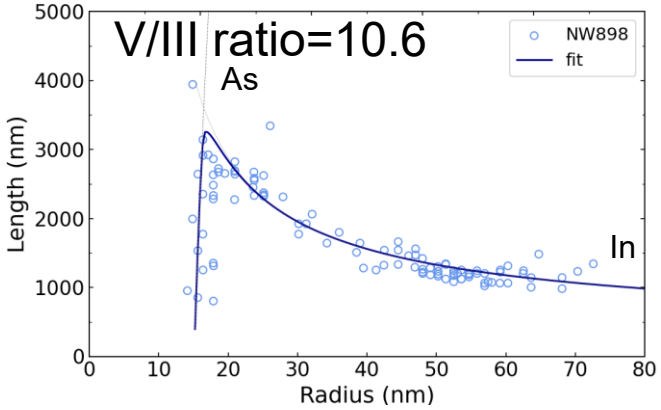


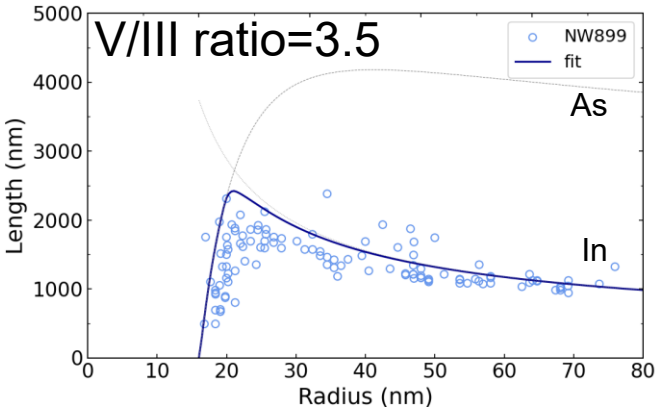
Example of fit

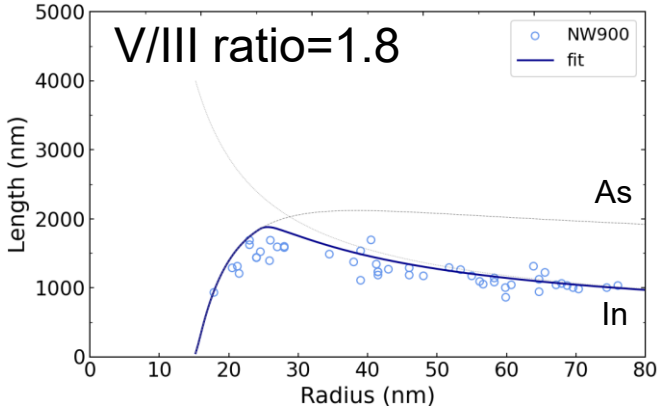


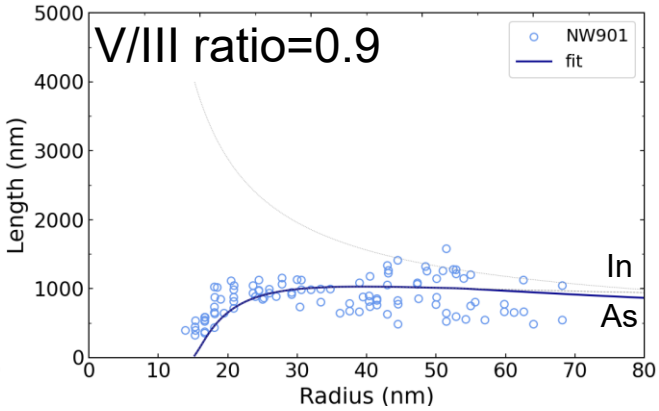
In-limited for radius > 18 nm
As-limited for radius <18 nm
Alternates around 18 nm

Fit of a series of V/III ratios









Fitting parameters for As:

$\lambda_V(s)$ = 50 nm

$\lambda_V(f)$ =100 nm

κ_V=6

Fitting parameters for In:

$\lambda_{III}(s)$ = 200 nm

$\lambda_{III}(f)$ =7500 nm

κ_{III}=0

R_K=8

The model works with different V/III ratios

Conclusions and perspectives

Conclusions:

- Model based on 2 species works, data can be fitted
- NW growth alternates between In and As limited regimes
- Growth regimes depend on the diameter, the height and the V/III ratio can be different: In-limited, As-limited, Mixed

Perspectives:

- Study of the dispersion in length-diameter dependence
- Dependence on growth temperature
- Impact on the structural quality?

PAPER: D.Mosiiets et al. Crystal Growth & Design 2024 24 (9), 3888-3898

Thank you for attention!
Any questions?

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Parameters of the model

Experimental parameters:

- Cell angle (In, As)
- Flux (In, As)

Fitting parameters:

- $\lambda_{substrate(III)}$, $\lambda_{substrate(V)}$
- $\lambda_{facets(III)}$, $\lambda_{facets(V)}$
- κ_{III}, κ_V
- R_K

Paper: D.Mosiiets et al. Crystal Growth & Design 2024 24 (9), 3888-3898
DOI: 10.1021/acs.cgd.4c00186

Current to the droplet from substrate

Current to the droplet from facets

Direct current +re-emission to the droplet

$$dL_V = \left[\frac{2}{R}\frac{1}{U'(\frac{L}{\lambda_{f,V}})}\lambda_{s,V}\frac{K_1(\frac{R}{\lambda_{s,V}})}{K_0(\frac{R}{\lambda_{s,V}})} + \frac{2}{R}\frac{U(\frac{L}{\lambda_{f,V}})}{U'(\frac{L}{\lambda_{f,V}})}\frac{\tan\alpha_V}{\pi}\lambda_{f,V}(1+\kappa'_V) + (1+\kappa_V)\right] \times \left[1-\theta^{in}_{evap}\exp(\frac{R_0}{R})\right] dH_V$$

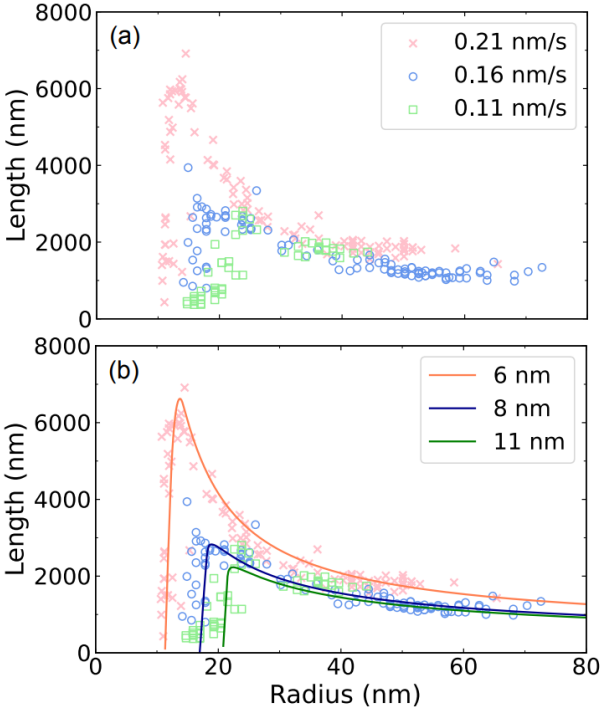
$$dL_{III} = \left[\frac{2}{R}\frac{1}{U'(\frac{L}{\lambda_{f,III}})}\lambda_{s,III}\frac{K_1(\frac{R}{\lambda_{s,III}})}{K_0(\frac{R}{\lambda_{s,III}})} + \frac{2}{R}\frac{U(\frac{L}{\lambda_{f,III}})}{U'(\frac{L}{\lambda_{f,III}})}\frac{\tan\alpha_{III}}{\pi}\lambda_{f,III} + (1+\kappa_{III})\right] dH_{III}$$

Kelvin effect

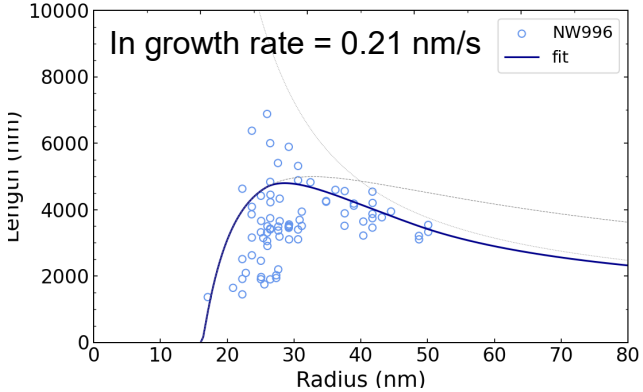
As

In

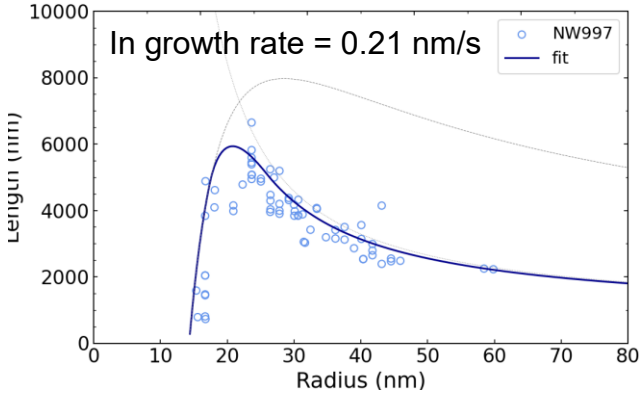
R_{GT} (R_0) phenomena



R_{GT}=8.5

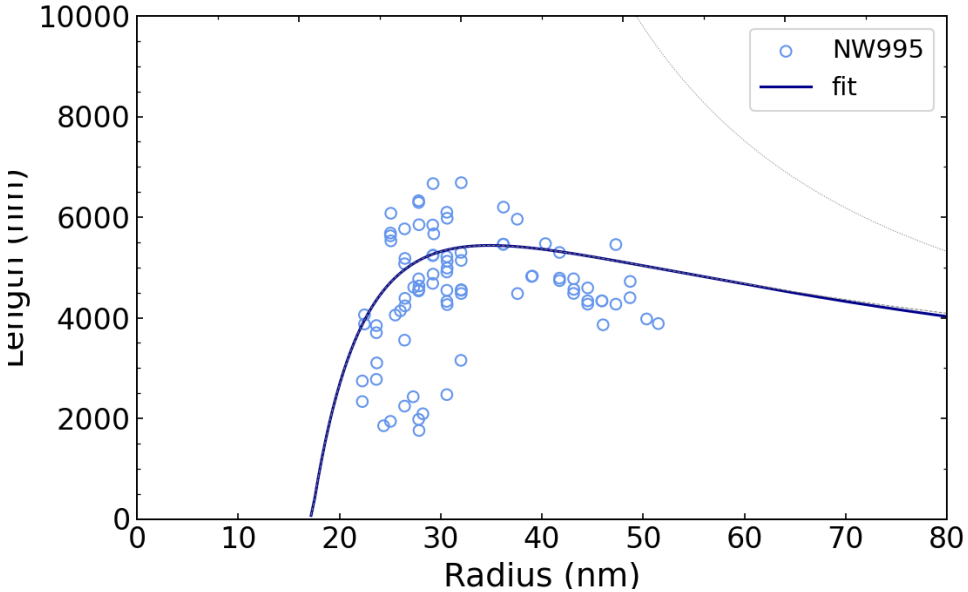


R_{GT}=7.5

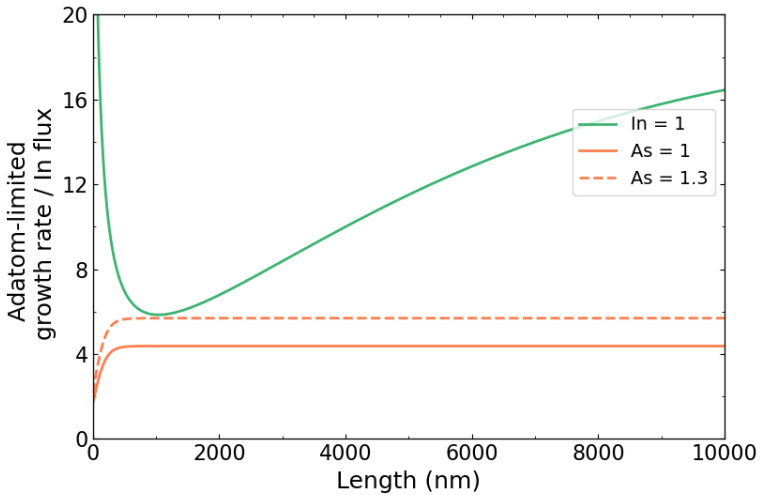


→ In flux is not only factor to define R_{GT}?

Examples of different types of the growth

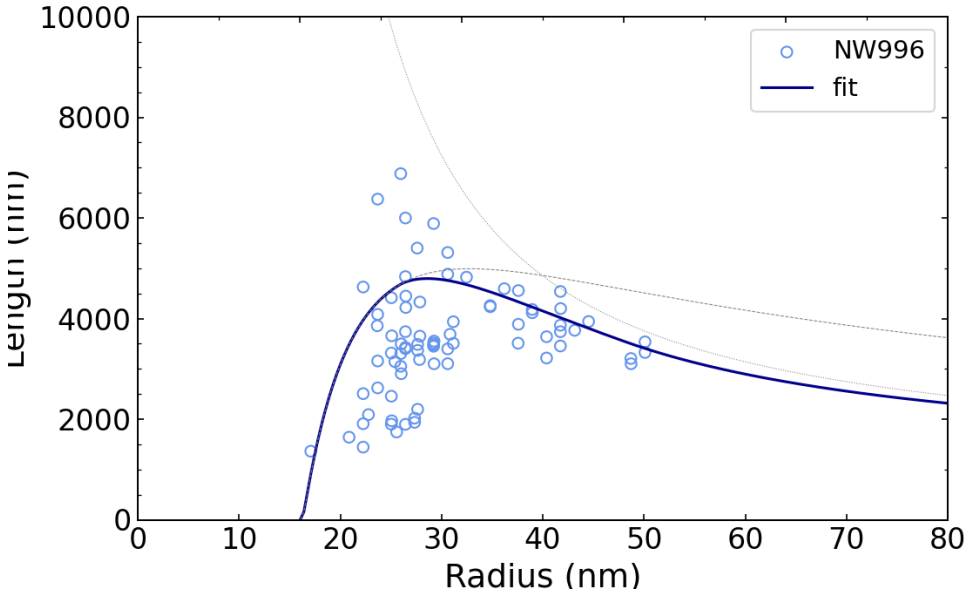


As-limited regime of the growth

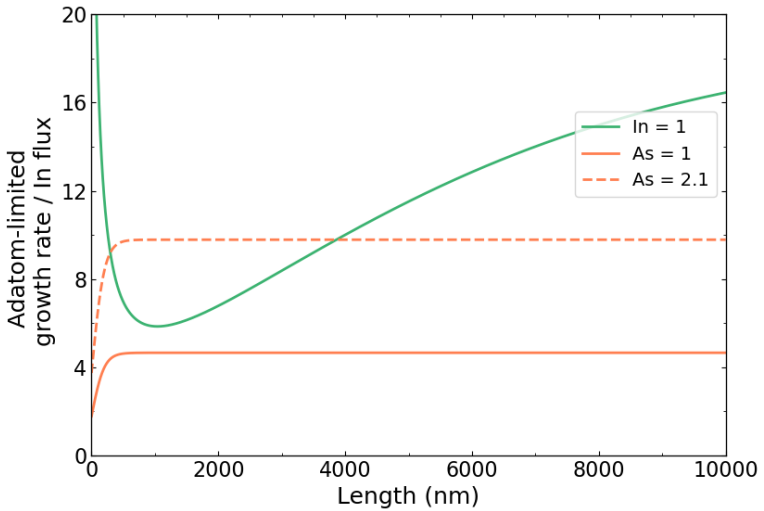


*calculated for nanowire radius=30 nm

Examples of different types of the growth

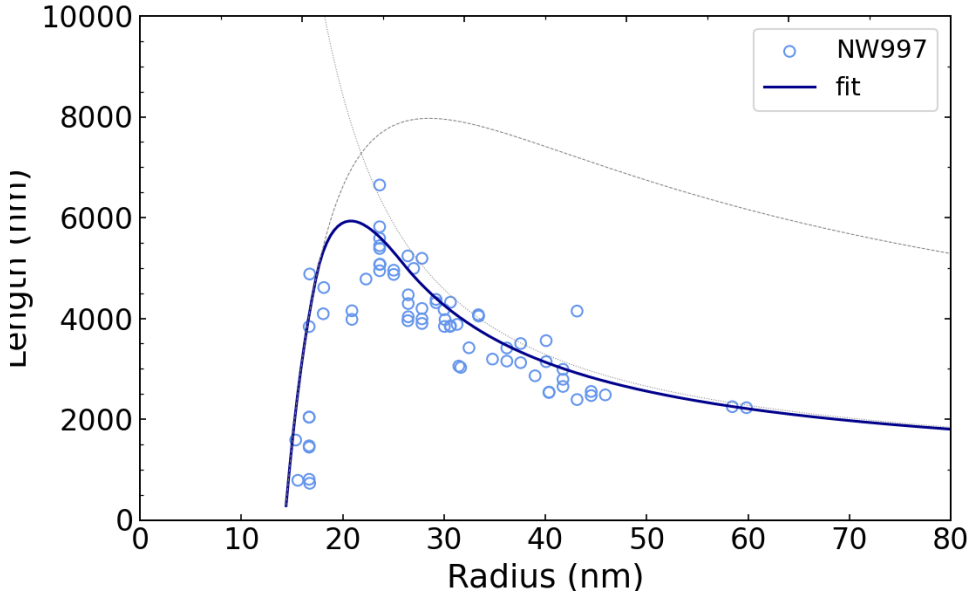


Mixed regime of the growth

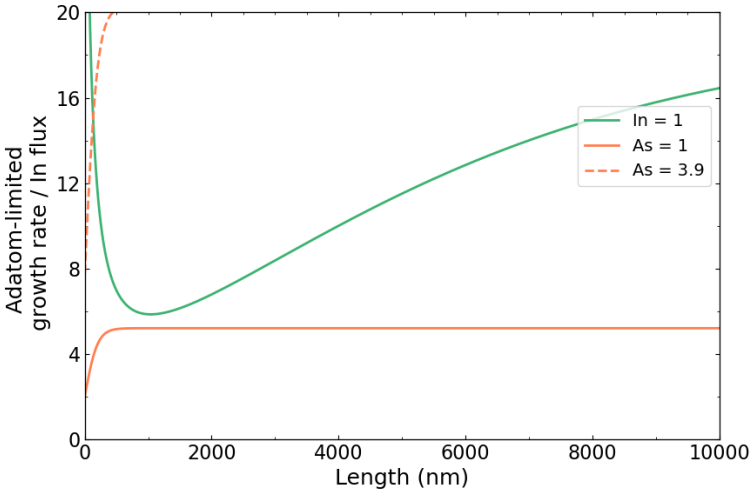


*calculated for nanowire radius=30 nm

Examples of different types of the growth



In-limited regime of the growth



*calculated for nanowire radius=30 nm