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# Tailoring zigzag and kinked silicon nanowires with metal assisted chemical etching

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# Outline

- Metal assisted chemical etching [MACE]
  - Description
  - 2D Model
- Kinked Si nanowires
  - Tailored structures
  - Model
- Conclusions

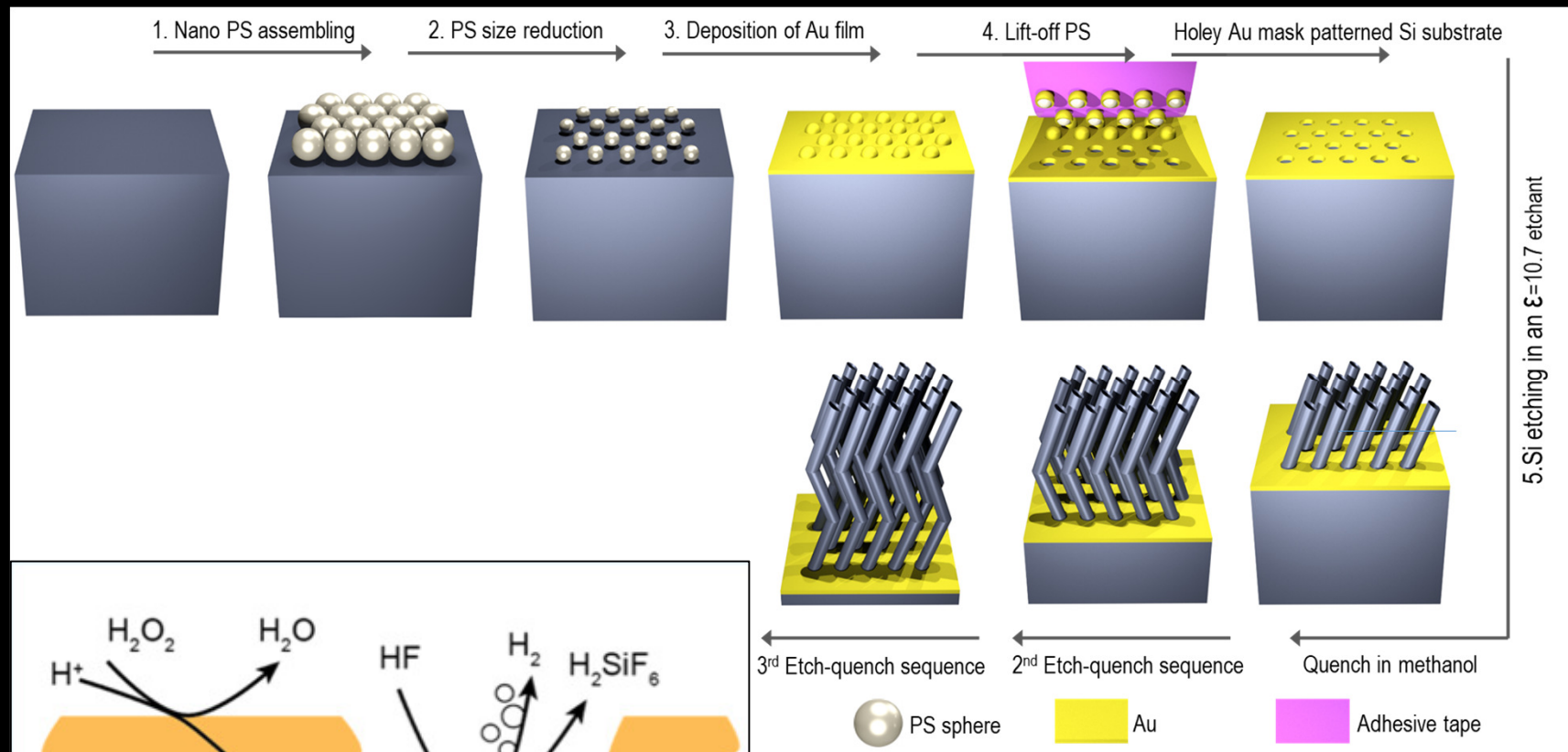


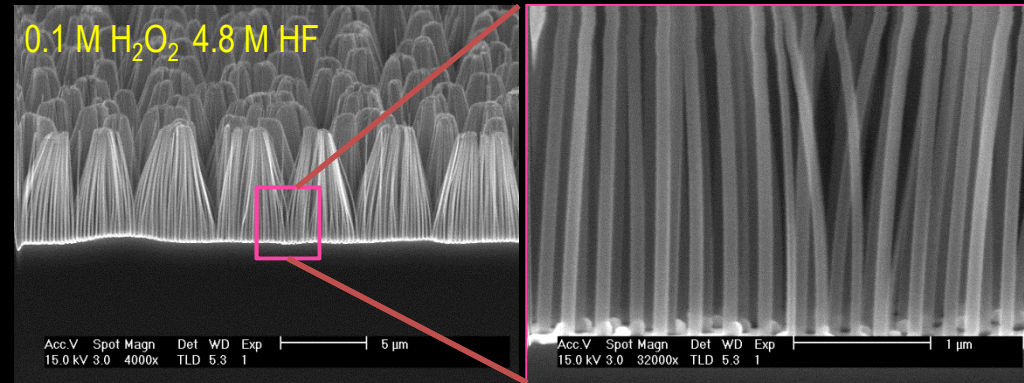
FIG. 1: Etching mechanism model diagram

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FIG. 2: Patterned MACE diagram

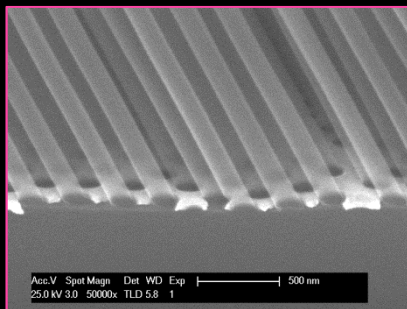
# MACE. I

# MACE. II

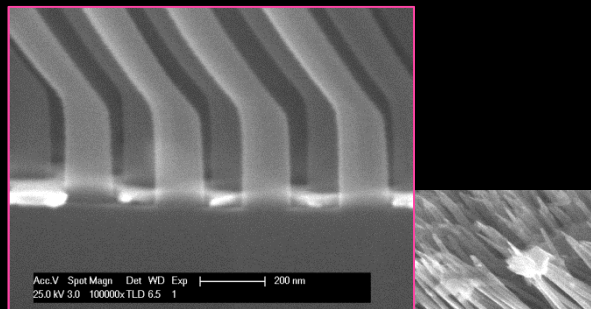


a

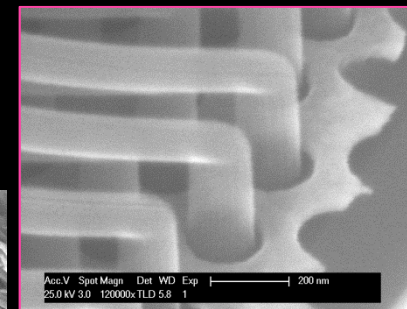
b



c



d



e

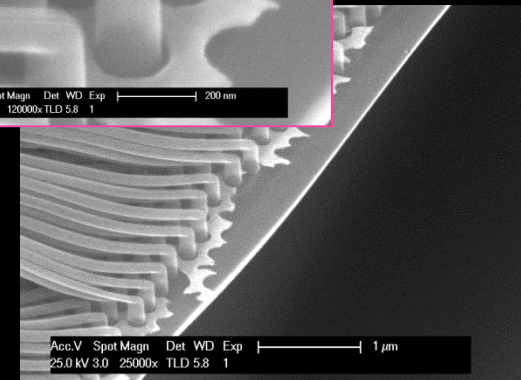
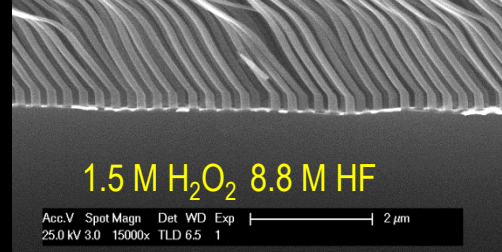
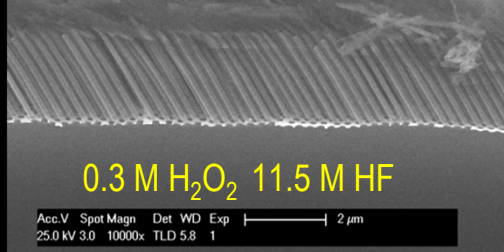
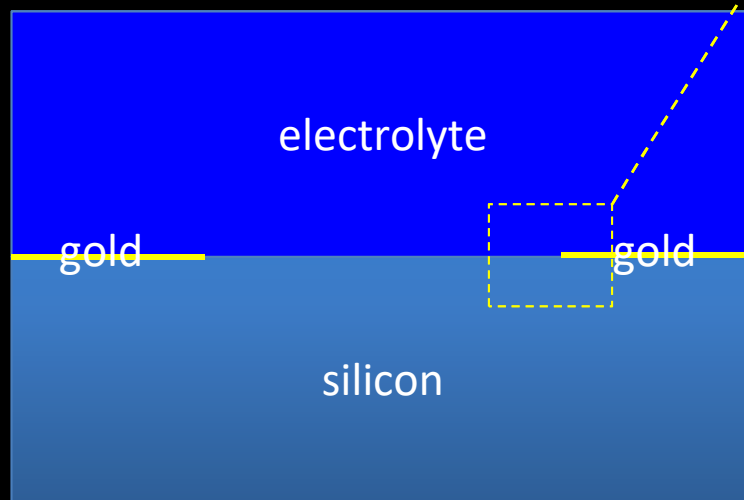
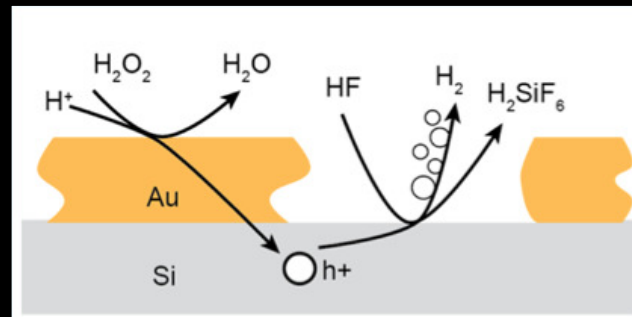


FIG. 3: Different nanowires structures obtained by MACE patterning, on  $p$ -type Si  $\langle 100 \rangle$

# MACE. 2D model

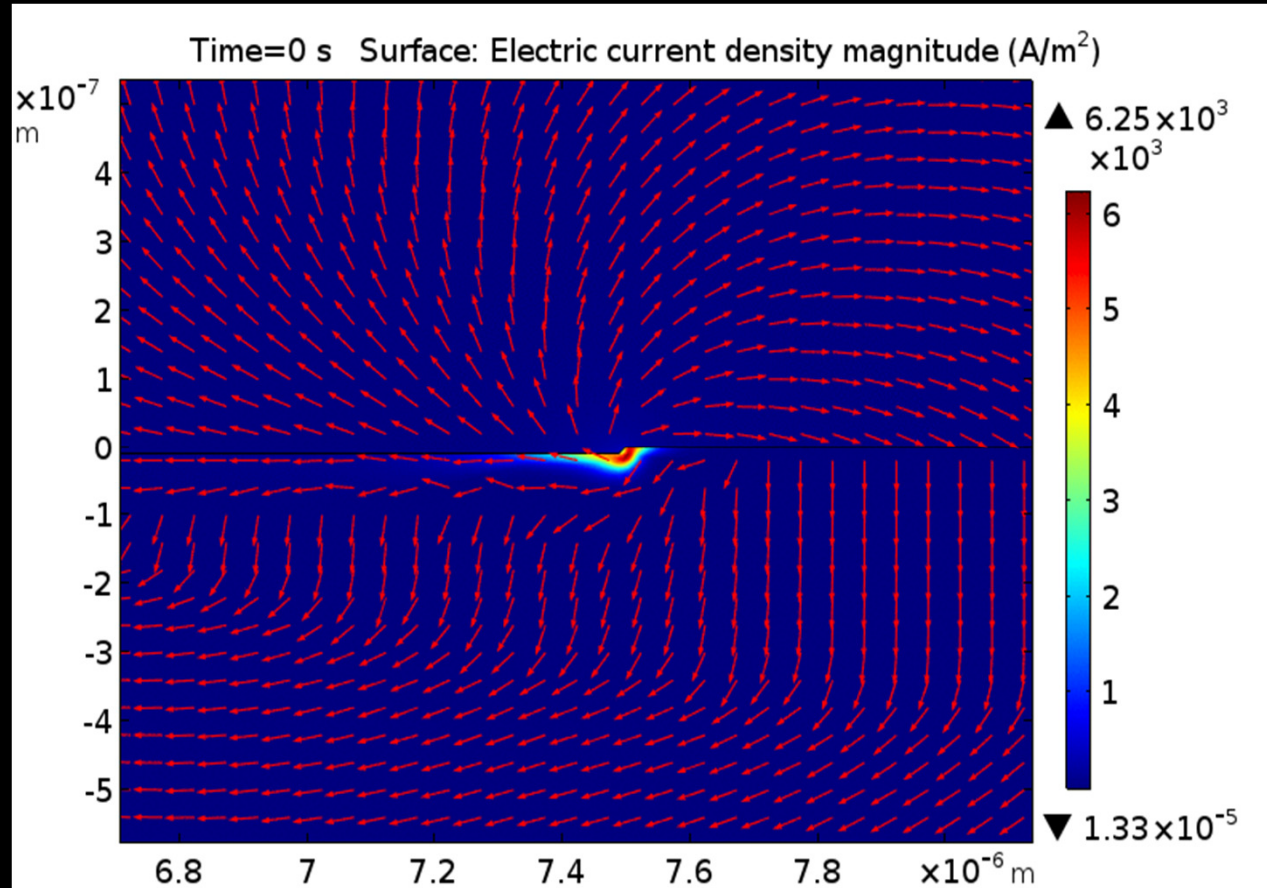


Region of interest

- Silicon: drift diffusion of carriers.
- Schottky barriers at Au/Si and Si/electrolyte interfaces.
- Butler-Volmer relationships for Au/electrolyte and Si/electrolyte.
- Electrolyte: ohmic conductor.

FIG. 4: 2D domain considered in calculation

- Etching rate is proportional to the electrical current between electrolyte and silicon.
- Gold is allowed to recede horizontally but keeps  $z$  value.



VIDEO. 1: Evolution of interfaces in MACE. Color scale shows electrical current density and arrows electrical current direction.

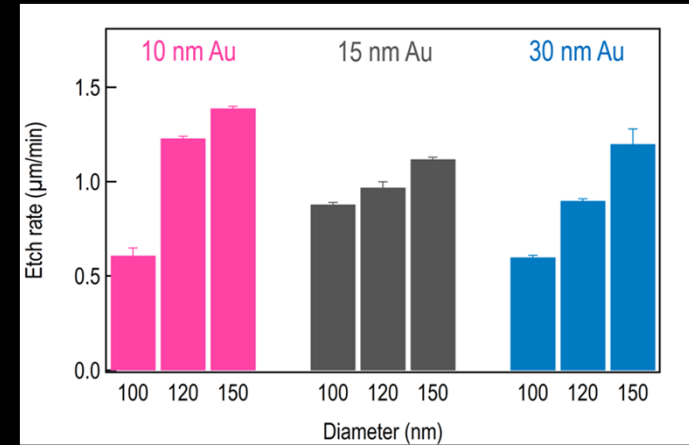
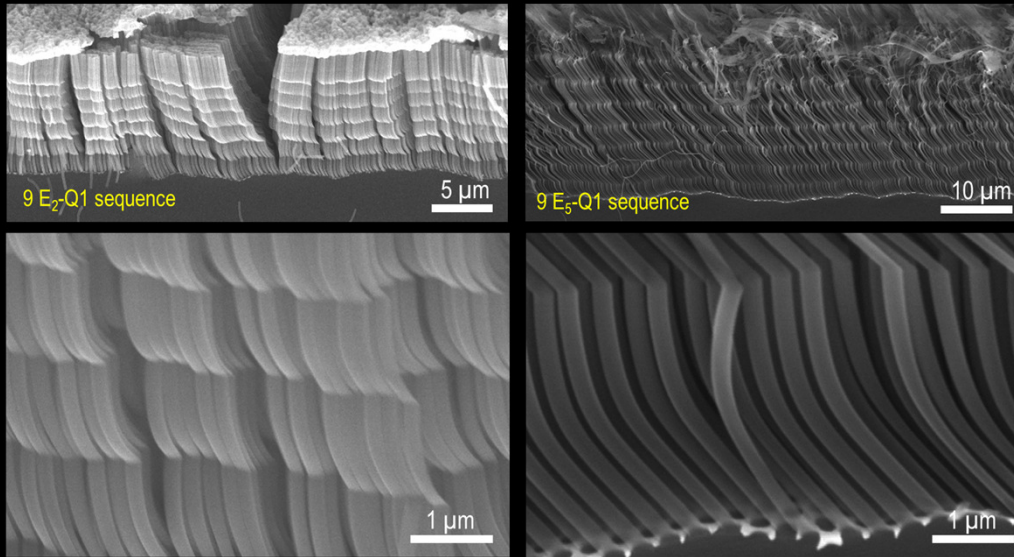
# Features of the 2D model

- Etching more pronounced near gold pattern
- Fast etching due to tight contact between gold and silicon
- Previous qualitative models put forward are consistent with the numerical calculation

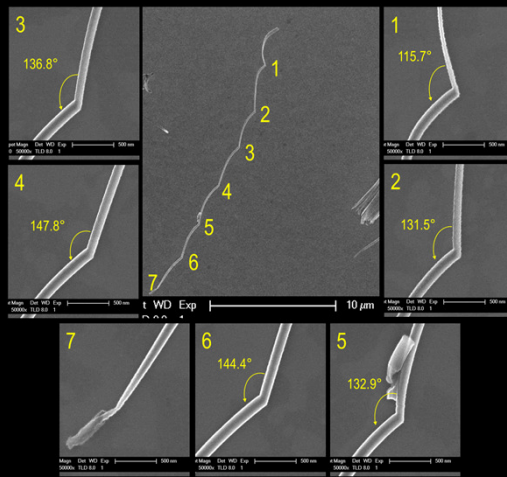
# Kink formation model

- Kink formation requires placing the sample in a reaction quencher, such as methanol, and putting back the sample in reactant.
- The process is complex, involving fluid dynamics, chemical reactions and diffusion of species.
- Experimentally, a myriad of configurations can be obtained.

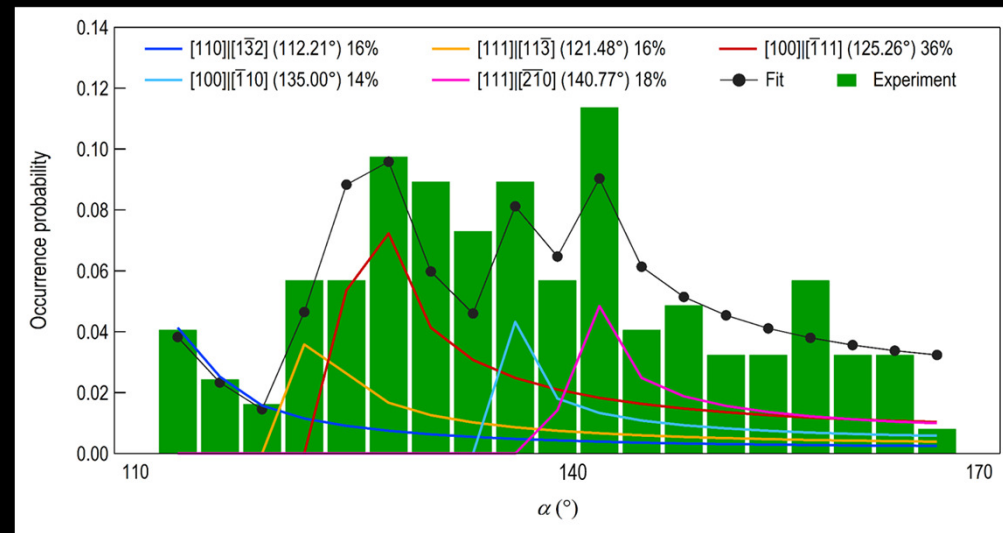




a



c



d

FIG. 5: a) Multiple kinks in nanowires, with segments length controlled by etching rate and time depending on gold mask thickness as characterized in b); c) kinked nanowire with different angles; d) populations of kink angles.

# Which will be the preferential location for methanol nanodroplets near a tilted nanowire?

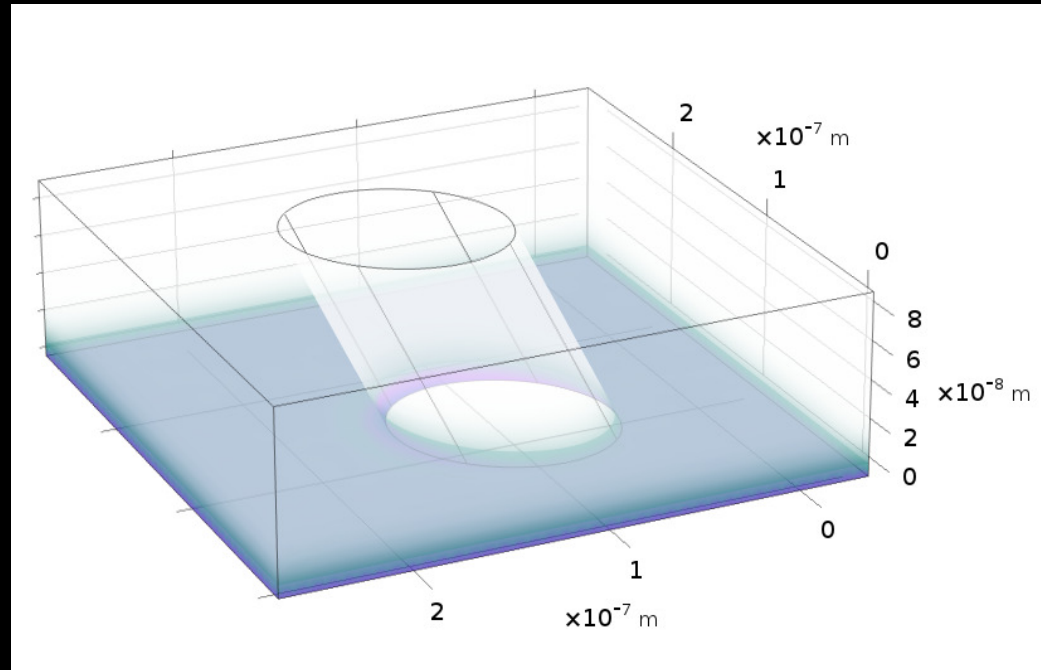
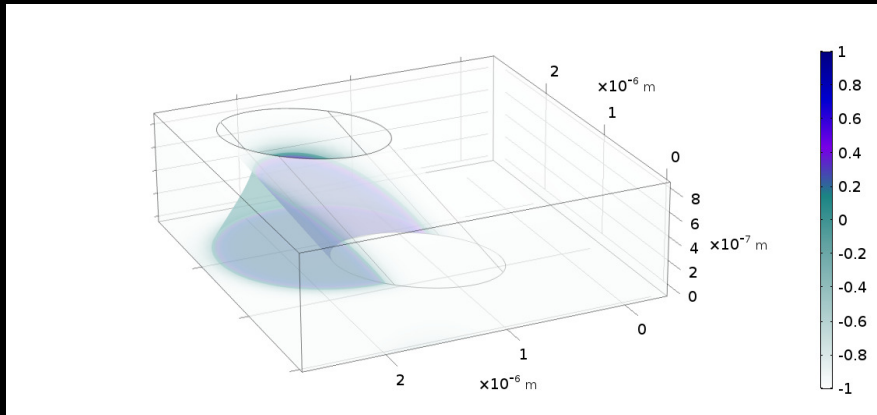


FIG. 7: 100 nm tilted Si nanowire with methanol pool

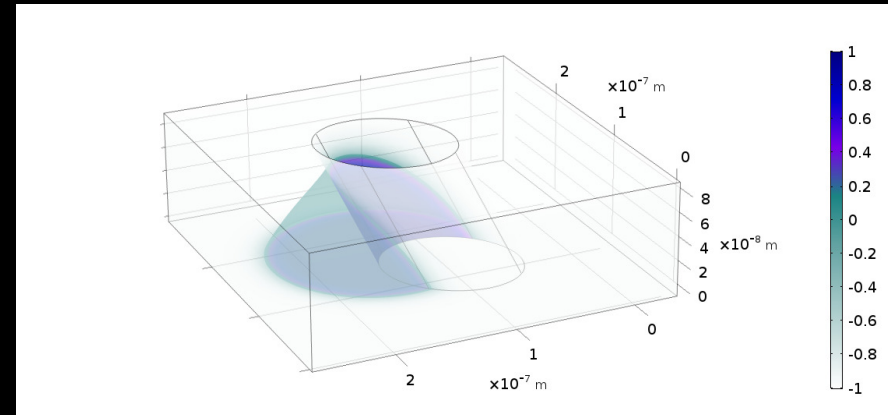
## Phase field method

- Allows study of fluid interfaces considering surface tensions and contact angles in 3D
- Fluid flow neglected and periodic boundary conditions

a



b



c

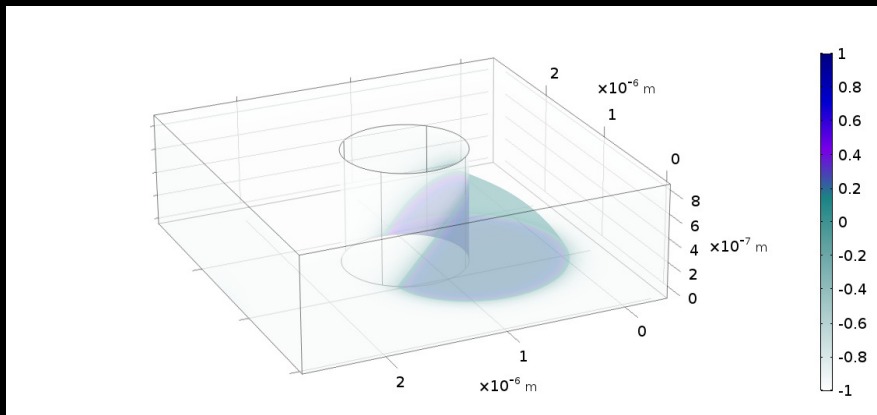


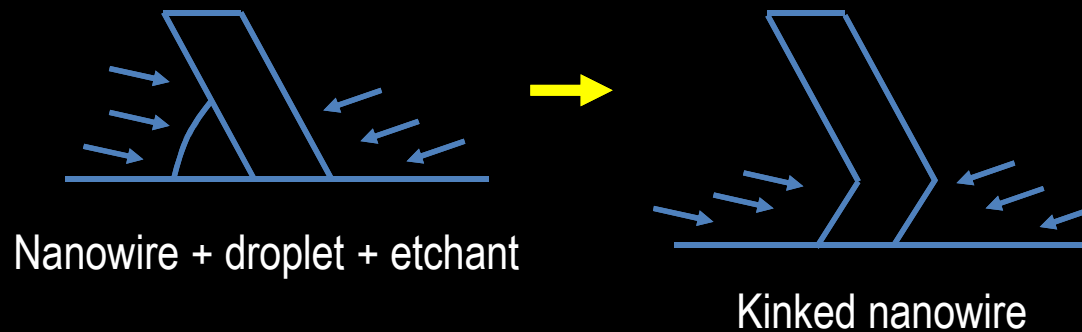
FIG. 8: 60° contact angle, 22.7 mN/m surface tension. a) 45° tilted nanowire, b) 60°, c) 90°. Color bars indicate phase field value.

# Features of the kink formation model

- Droplet accumulates always in the inner part of the nanowire/base architecture.
- Vertical nanowires produce random results due to symmetry.
- Similar results for  $35^\circ$ ,  $60^\circ$ , and  $90^\circ$  contact angles.

# Kink formation in MACE

- Droplets of quencher will preferentially accumulate in the inner parts of the Si nanowire – substrate system.
- Upon continuation of MACE, there will be a change of direction, due to reduced concentration of the etchant in the region of accumulated quencher.



# Conclusions

- A physical model including most relevant properties was developed for MACE of Au/Si, showing expected features.
- Droplet formation is studied for tilted Si nanowires, showing preferential sites.
- Droplet model is used to explain formation of kinked Si nanowires.