Three-dimensional numerical study on hydrogen bubble growth at electrode

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Basilisk (Gerris) Users' Meeting 2025
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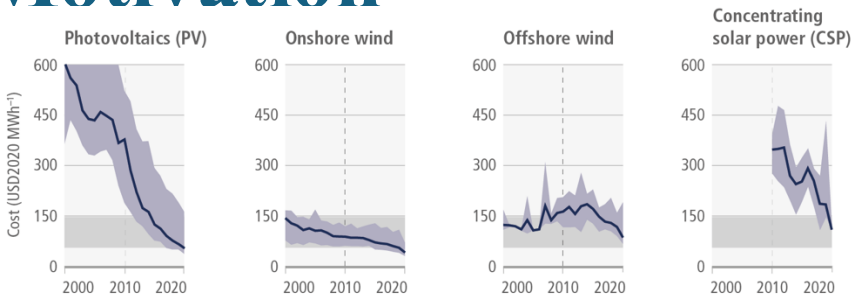
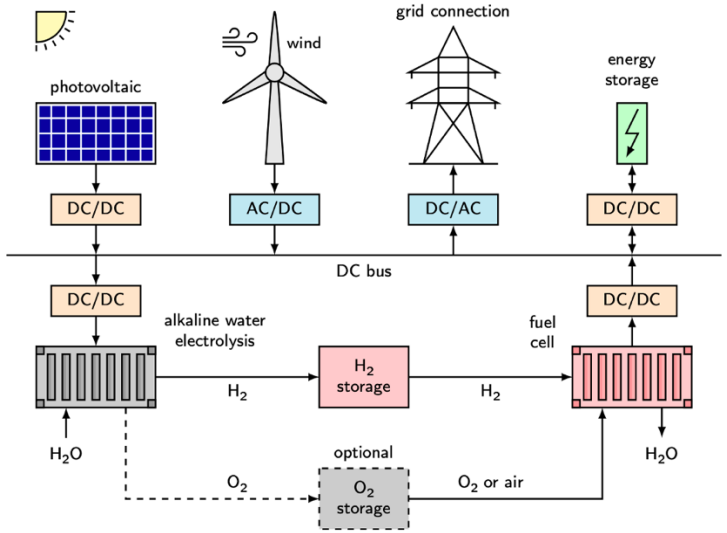
Outline

- Motivation
- Current work
- Conclusion & outlook

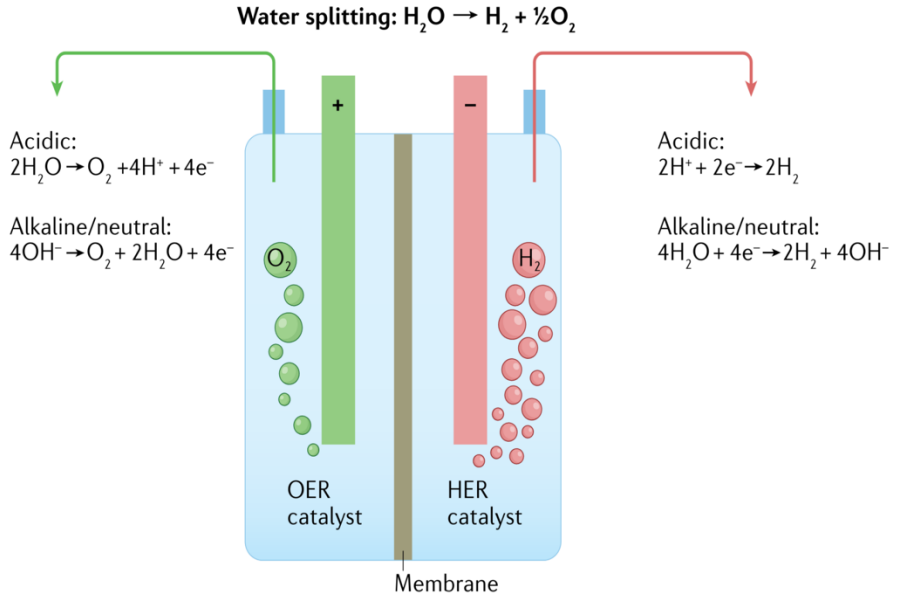
Motivation



Unit cost reductions for green energy production (IPCC 2022) [1].



A hydrogen/electric energy system (Nnabuife SG. 2024) [2].



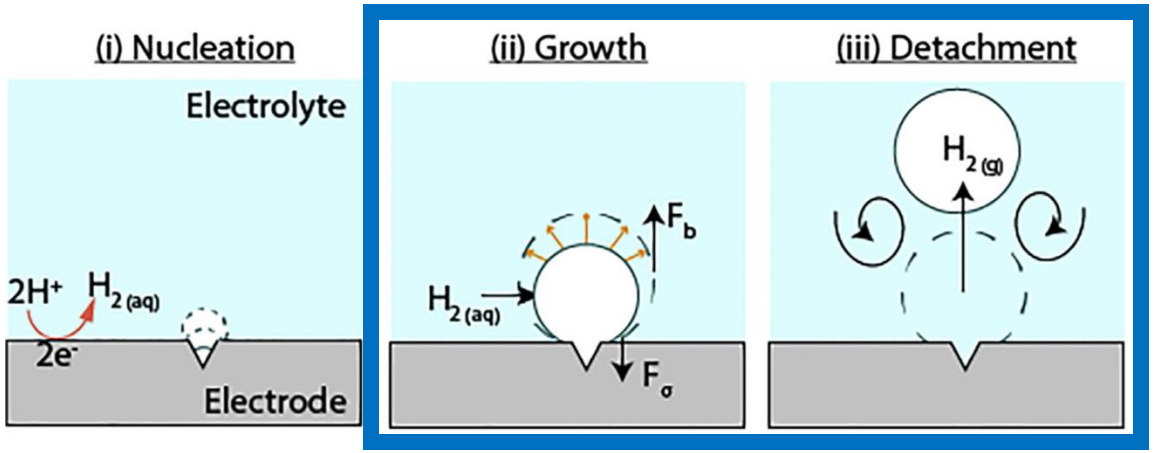
Schematic of a typical water electrolyzer. Oxygen is produced at the anode (+) and hydrogen at the cathode(–). HER, hydrogen evolution reaction; OER, oxygen evolution reaction (Shih 2022) [3].

[1] IPCC Sixth Assessment Report.

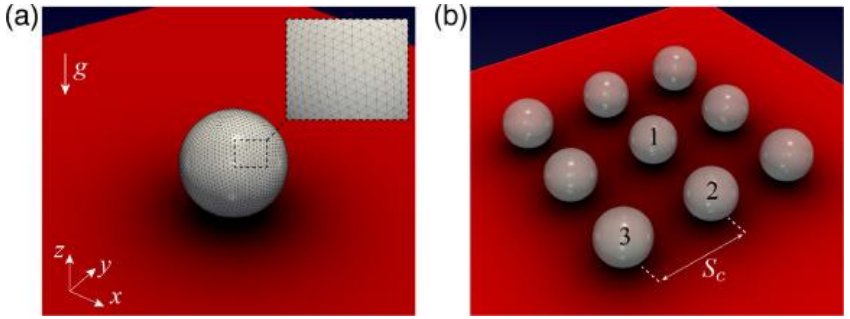
[2] Nnabuife SG, Hamzat AK, Whidborne J, Kuang B, Jenkins KW. Integration of renewable energy sources in tandem with electrolysis: a technology review for green hydrogen production. Int J Hydrogen Energy 2024

[3] J.Shih et al. Water electrolysis. Nature Reviews Methods Primers, 2(1):84, October2022.

Objective



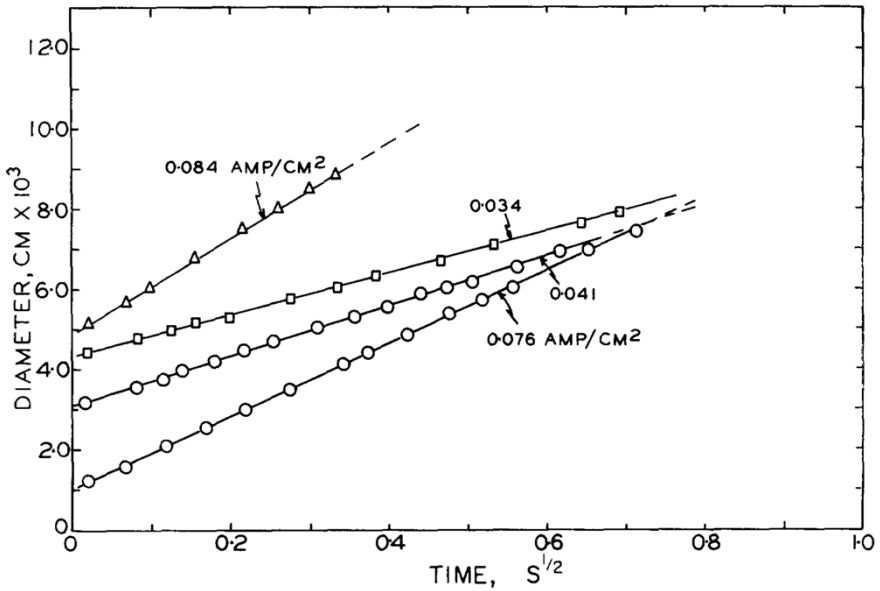
Various stages of bubble evolution on electrodes. (i) bubble nucleation, (ii) bubble growth , (iii) detachment of bubbles (Angulo 2020) [4].



(a) the basic simulation setup with a single bubble in the center of the domain and (b) a 3 × 3 bubble cluster with spacing (Sepahi 2024) [6].

Scriven's scaling: $R \propto t^{\frac{1}{2}}$

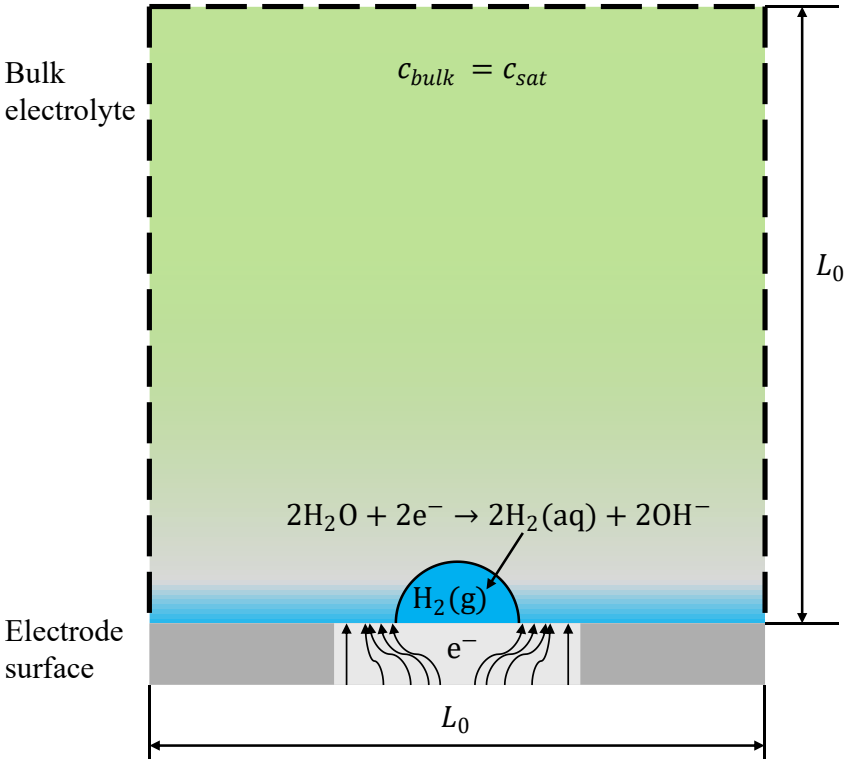
Growth controlled by diffusion



Result from Glas experiment measurement (Glas 1964) [5].

[4[Andrea Angulo et al. Influence of Bubbles on the Energy Conversion Efficiency of Electro-chemical Reactors. Joule, 4(3):555–579, March 2020.
[5] J. P. Glas and J. W. Westwater. Measurements of the growth of electrolytic bubbles. International Journal of Heat and Mass Transfer, 7(12):1427–1443, December 1964.
[6] Farzan Sepahi,et al. The effect of buoyancy driven convection on the growth and dissolution of bubbles on electrodes, Electrochimica Acta, 2022.

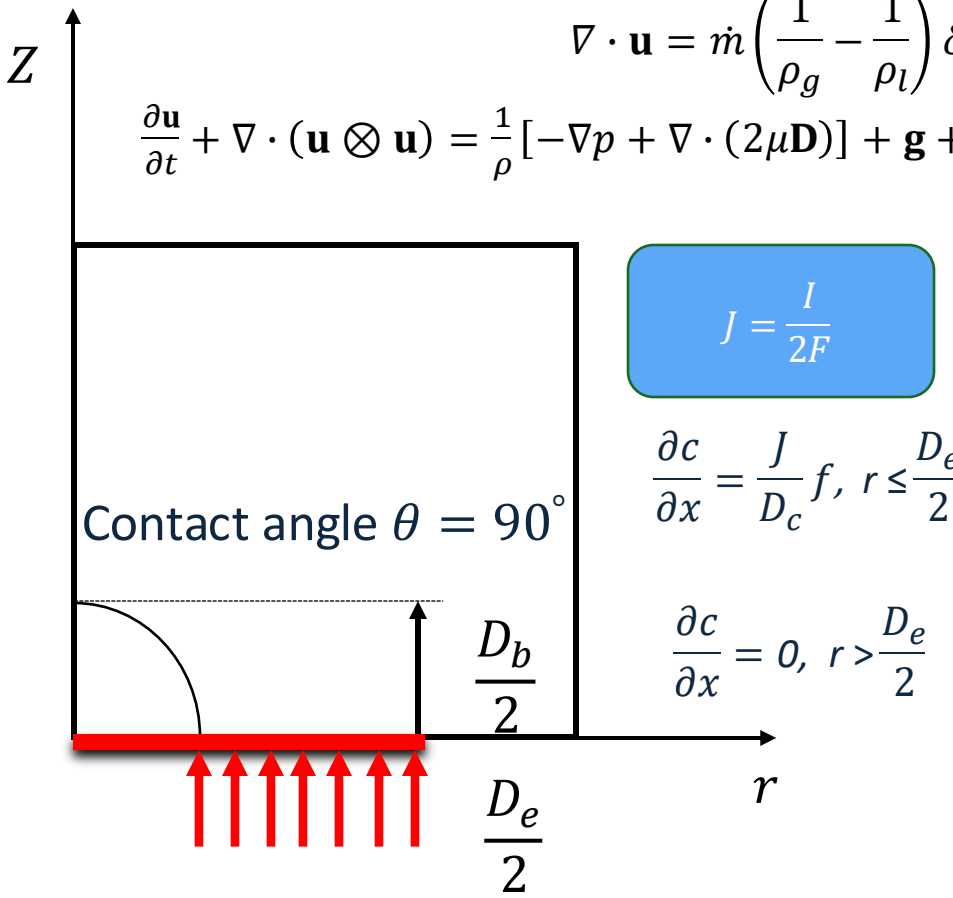
Configuration



Schematic representation of the two-phase electrochemical system with relevant chemical reactions and boundary conditions at the cathode.

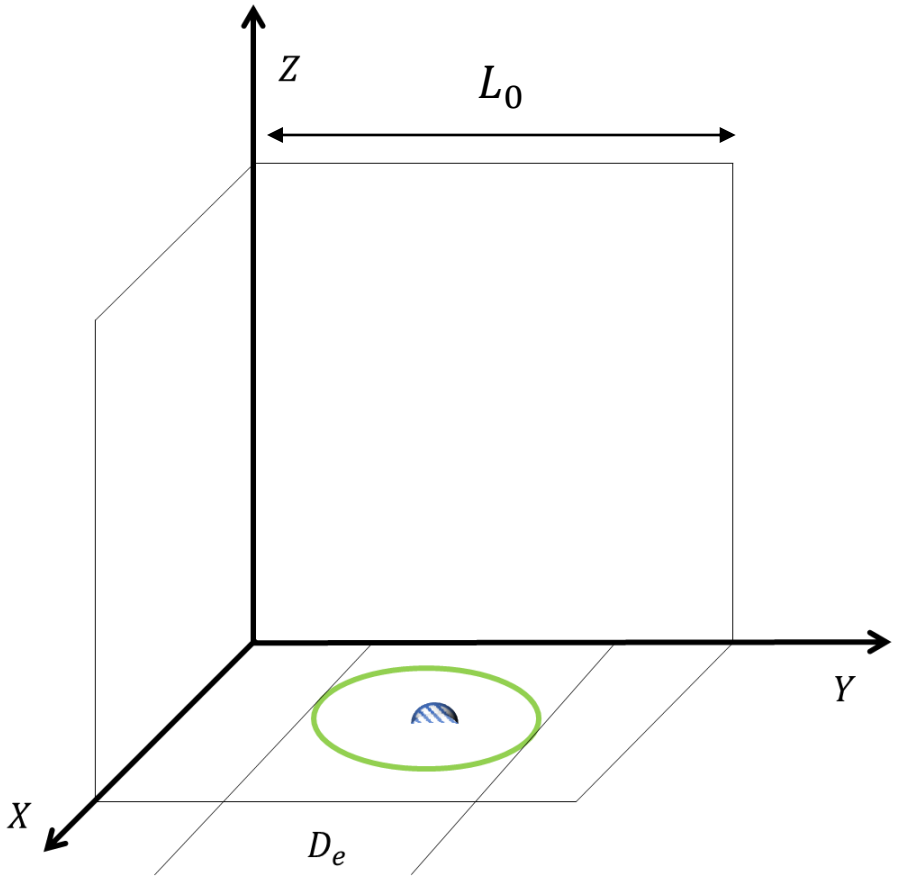
$$\nabla \cdot \mathbf{u} = \dot{m}\left(\frac{1}{\rho_g} - \frac{1}{\rho_l}\right)\delta_\Sigma$$

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) = \frac{1}{\rho}[-\nabla p + \nabla \cdot (2\mu \mathbf{D})] + \mathbf{g} + \frac{\sigma k \mathbf{n}_\Sigma}{\rho}\delta_\Sigma$$

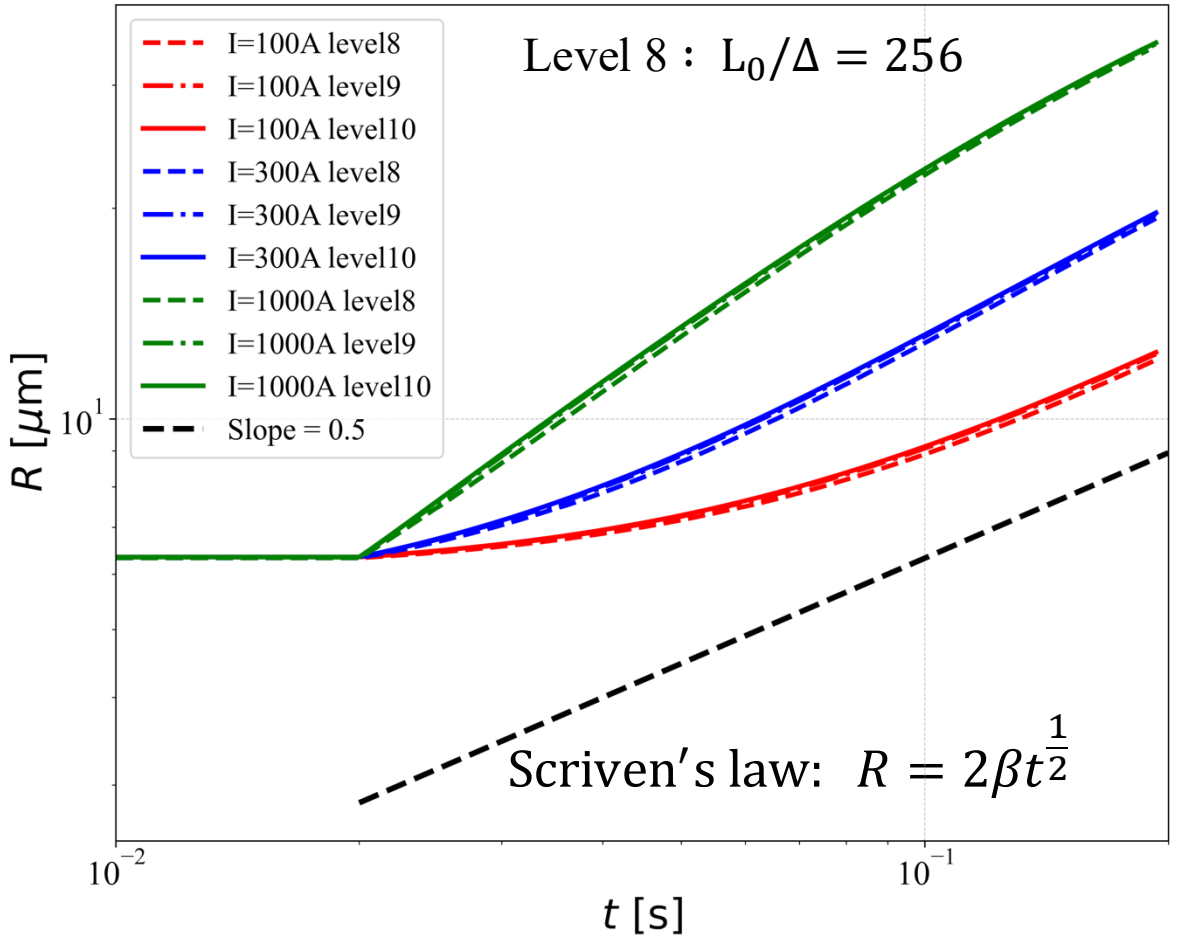


Sketch of the axisymmetric simulation setup.

Mesh independence analysis

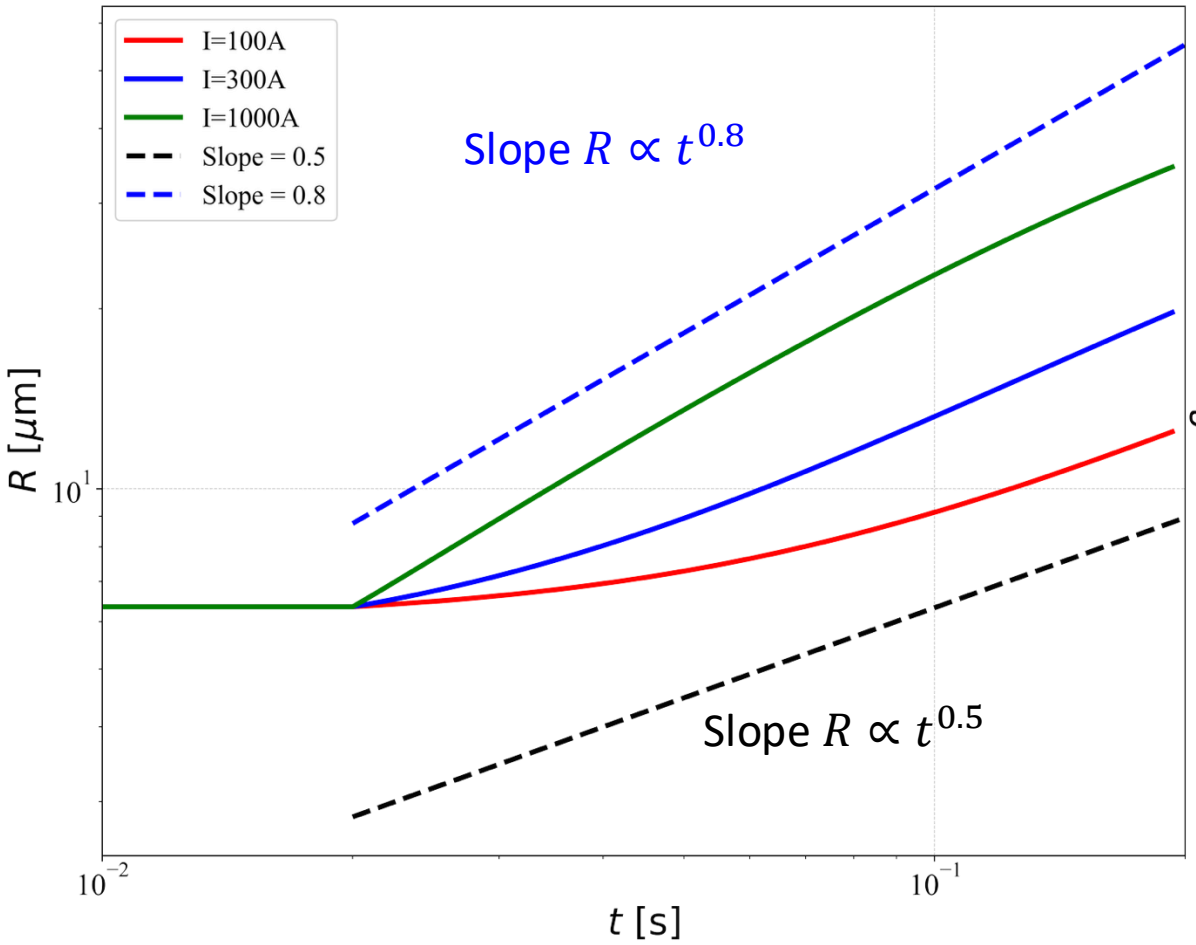


Sketch of the 3D simulation setup.



Bubble radius growth for varying current density.

Influence of current density on bubble growth



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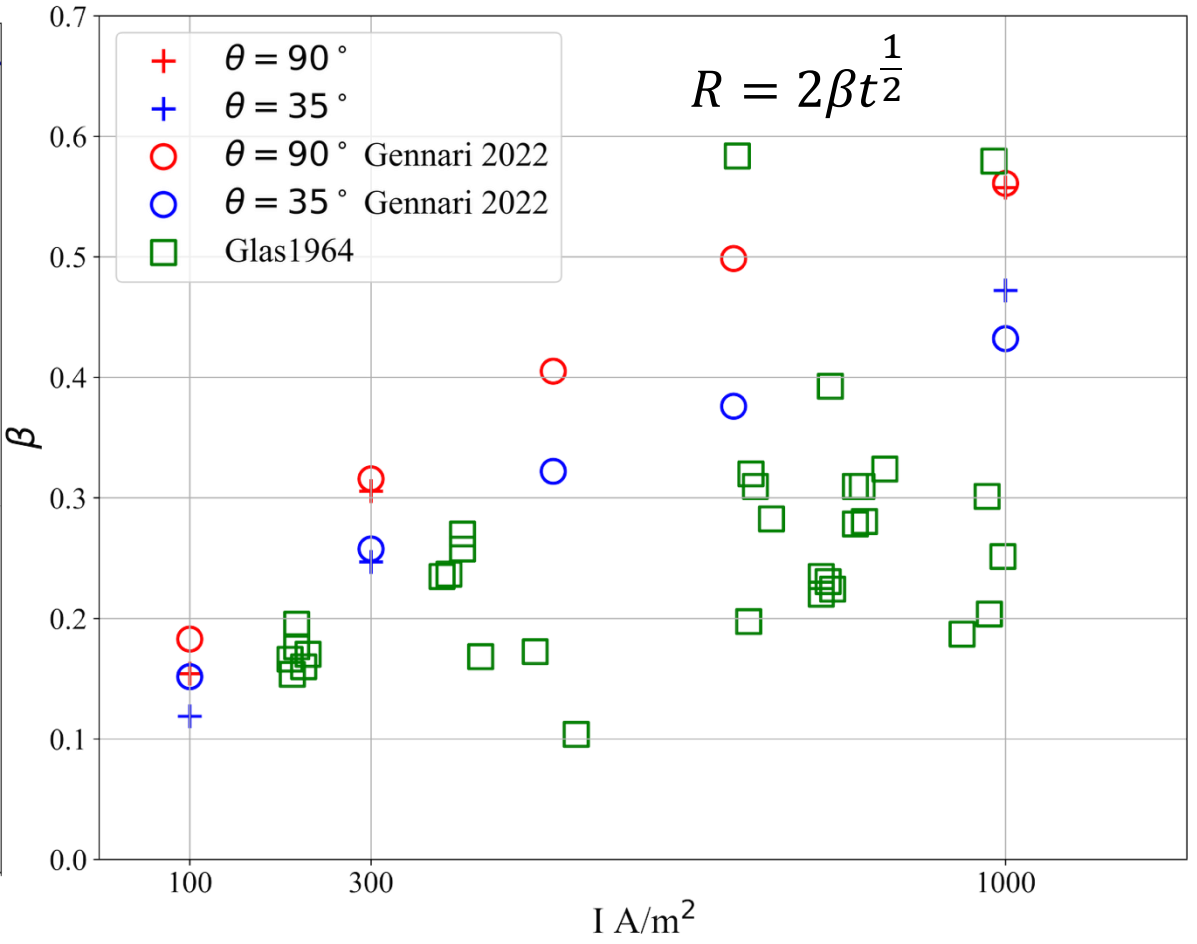
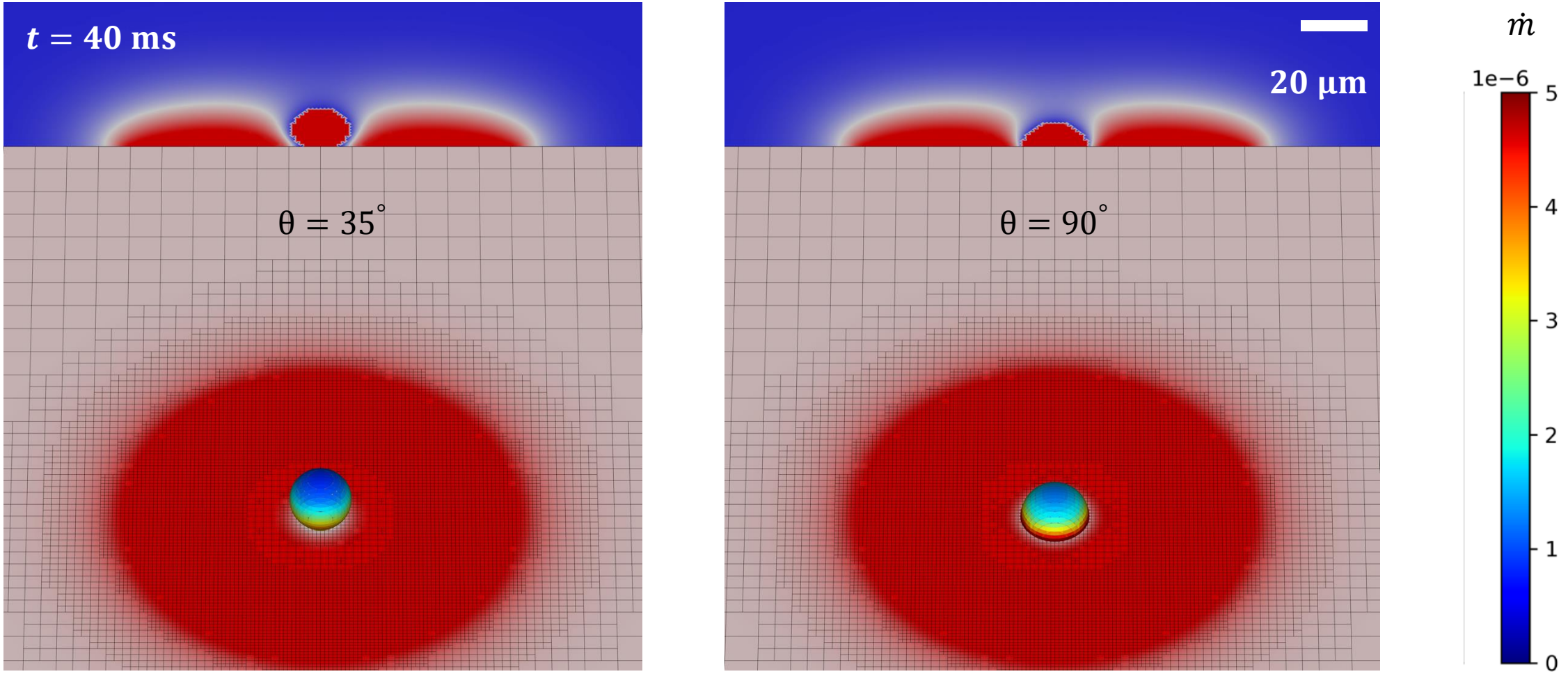


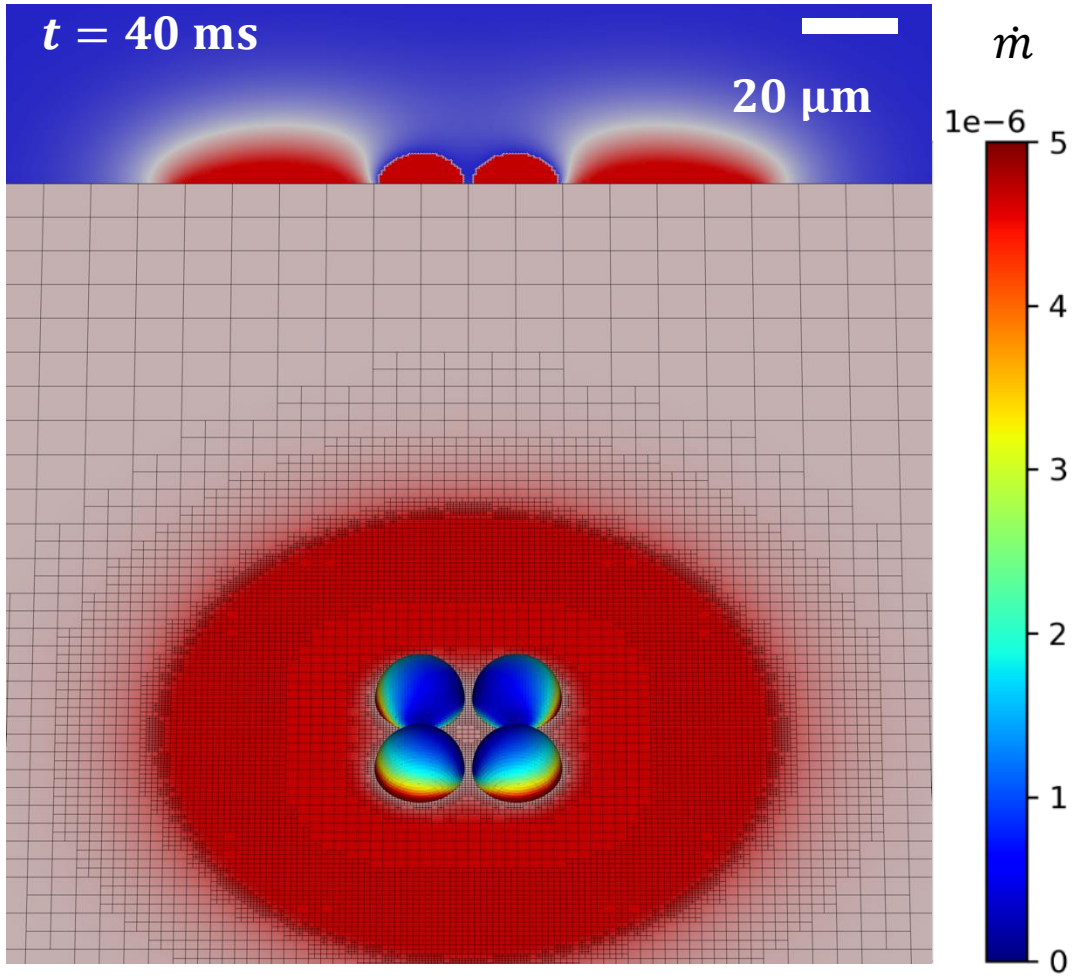
Influence of current density and contact angle on the growth coefficient.

Influence of contact angle on bubble growth

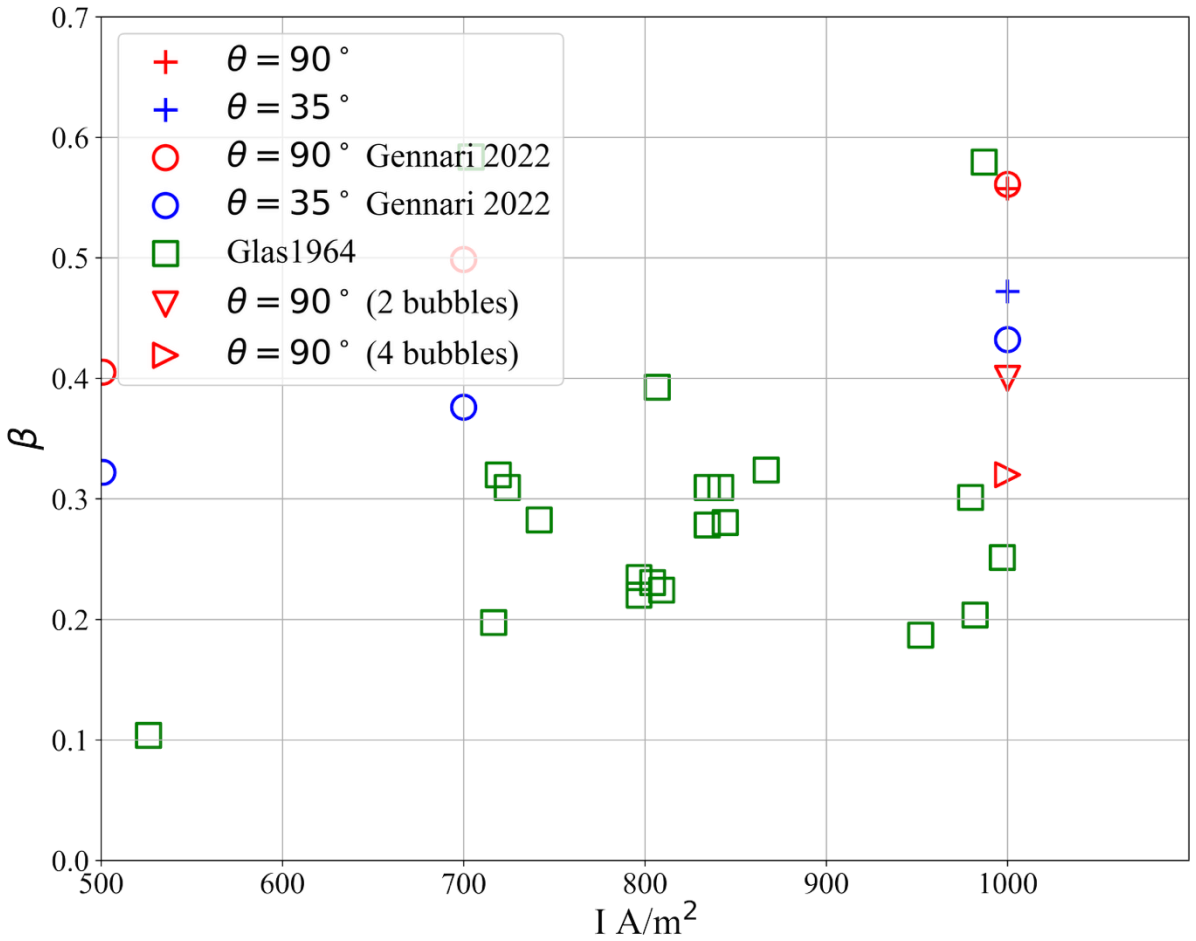


Snapshots of hydrogen bubble evolution for different contact angle. The current density is $1000\ \mathrm{A/m^2}$.

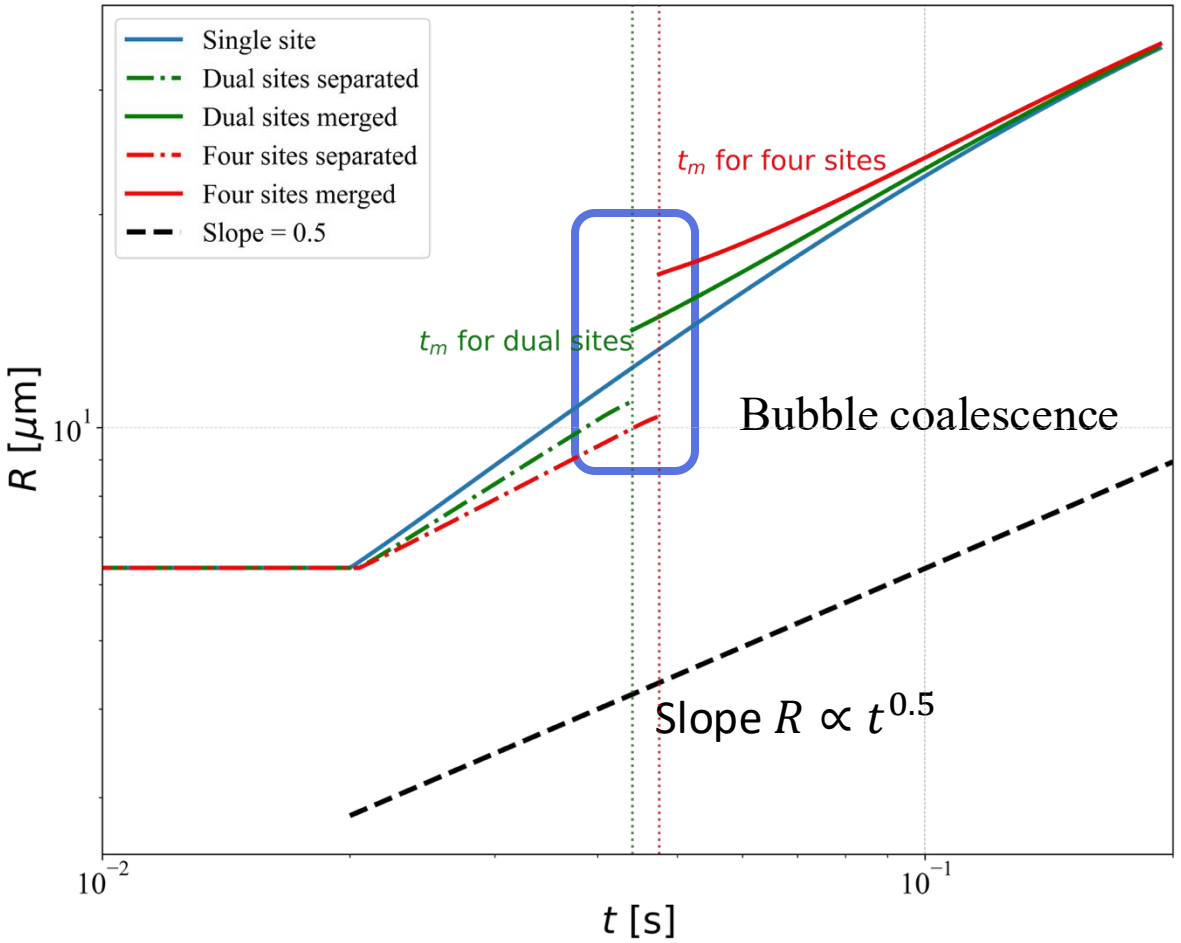
Influence of nucleation sites on bubble growth



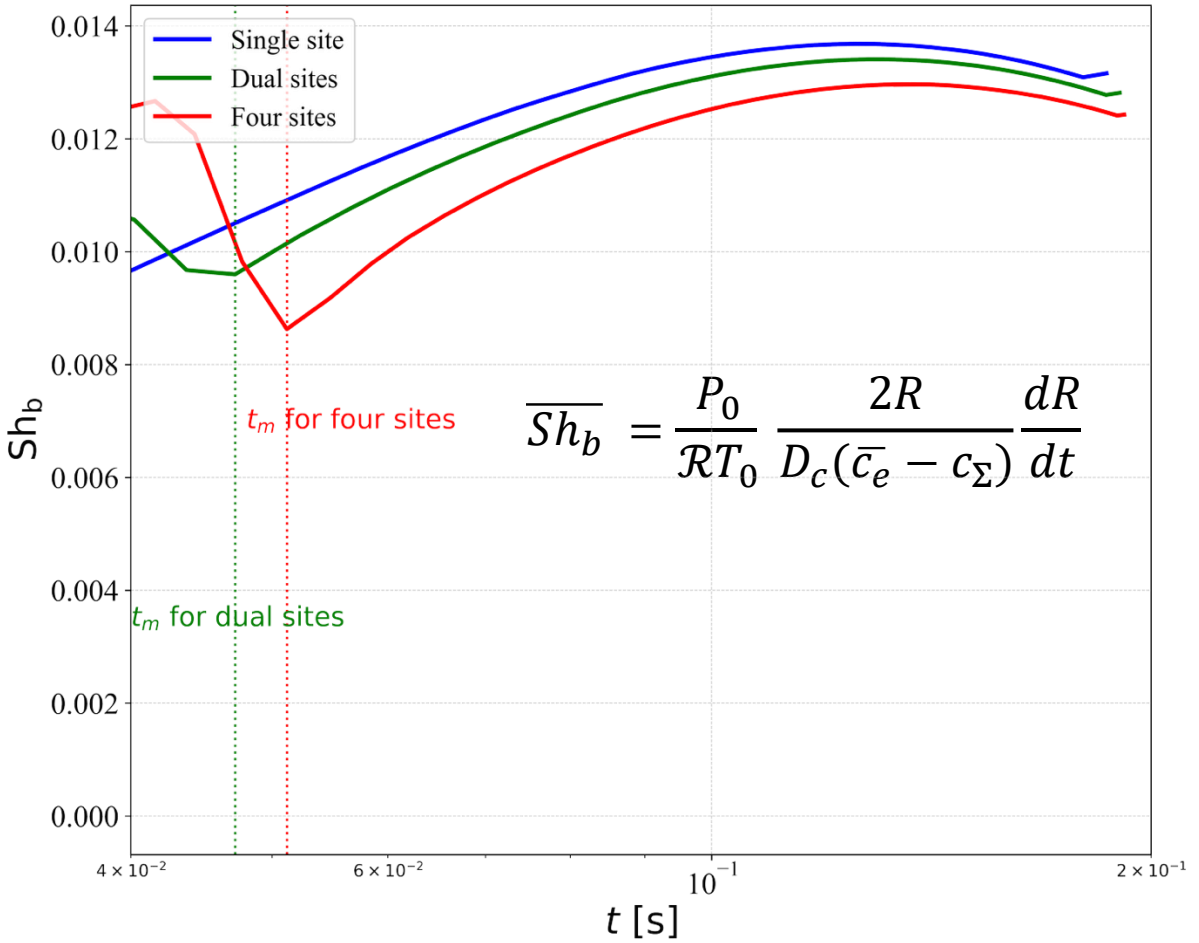
Snapshots of bubble growth for 4 nucleation sites.
The current density is 1000 A/m^2



Influence of current density and contact angle on the growth rate.

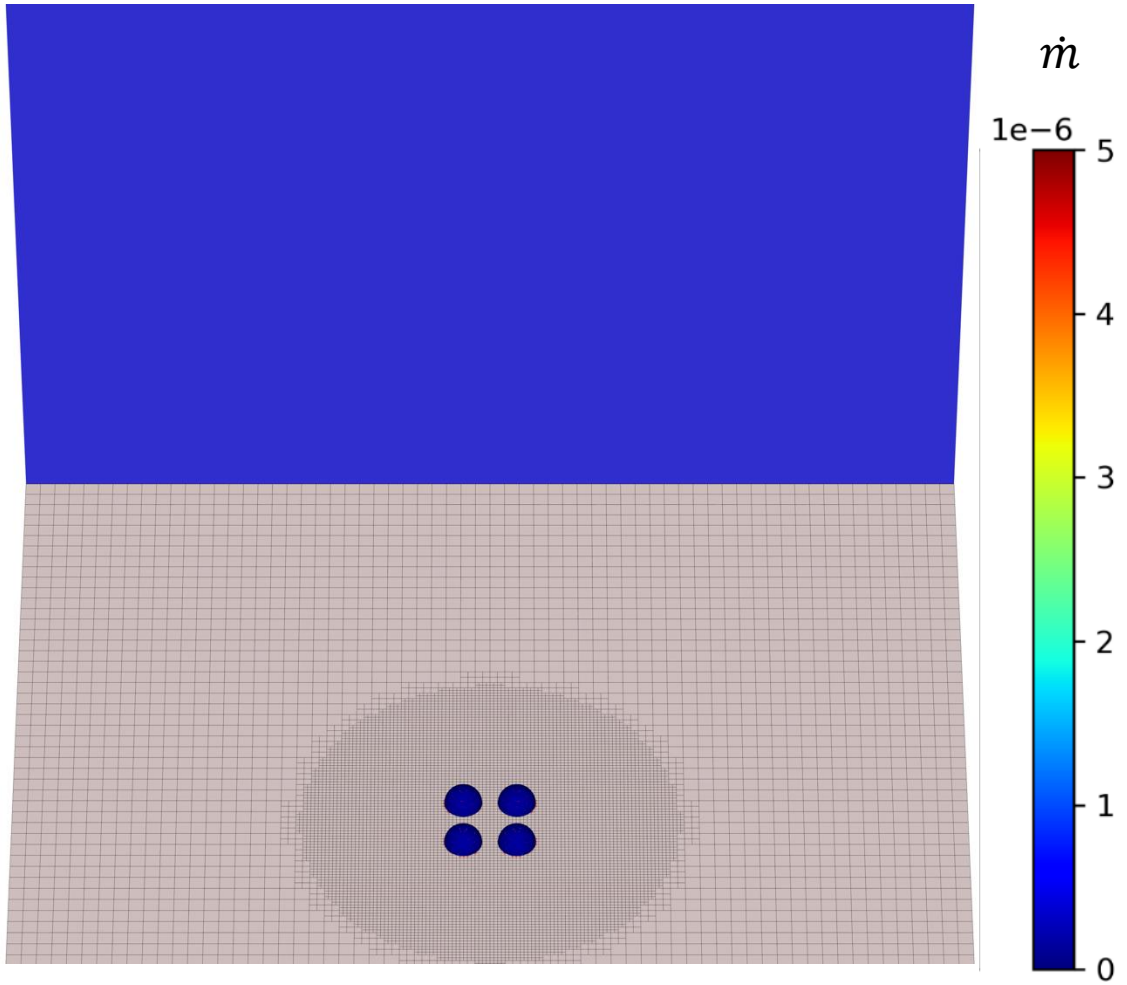


Bubble radius growth for multiple nucleation sites.

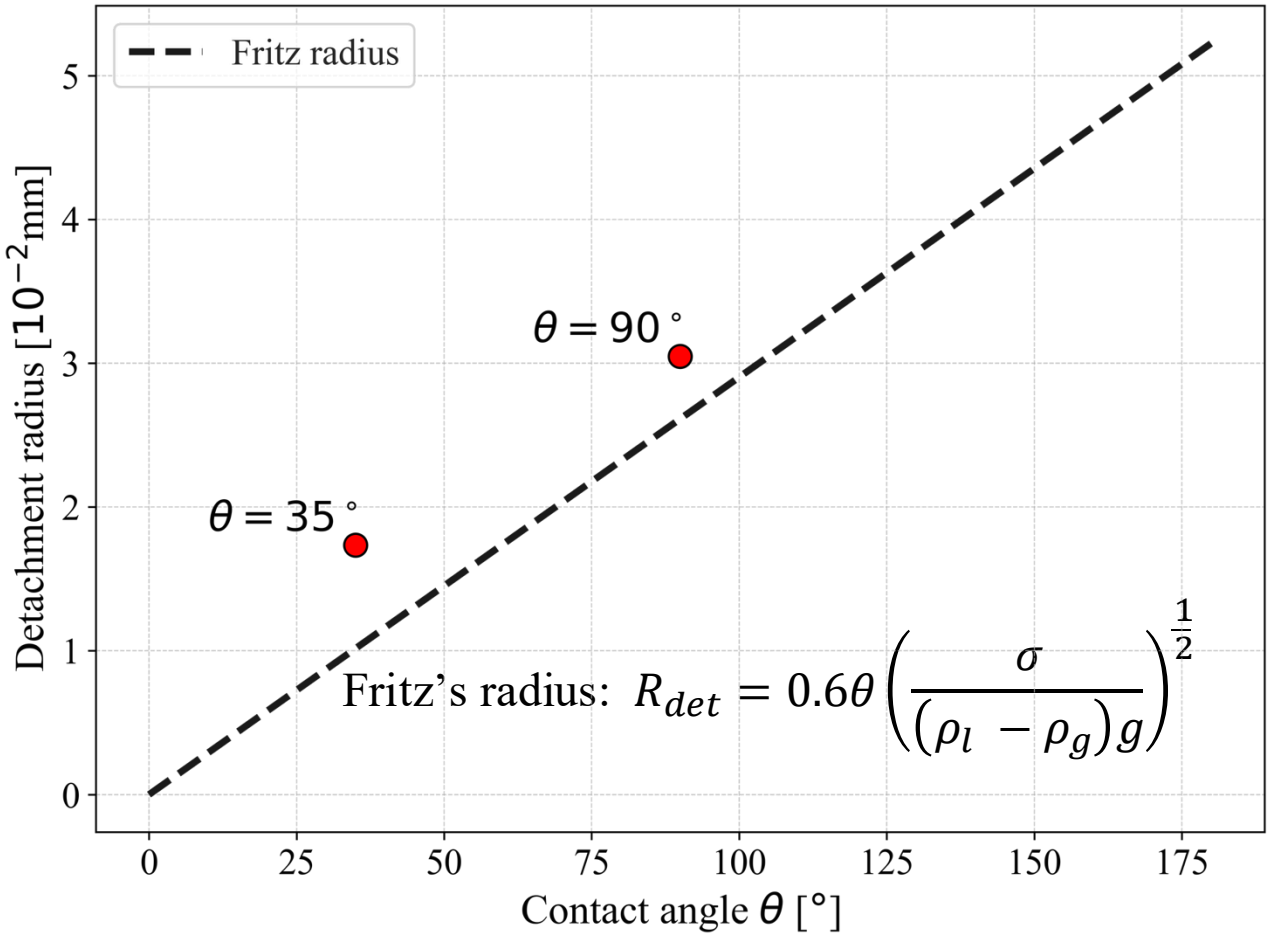


Bubble Sherwood number for multiple nucleation sites.

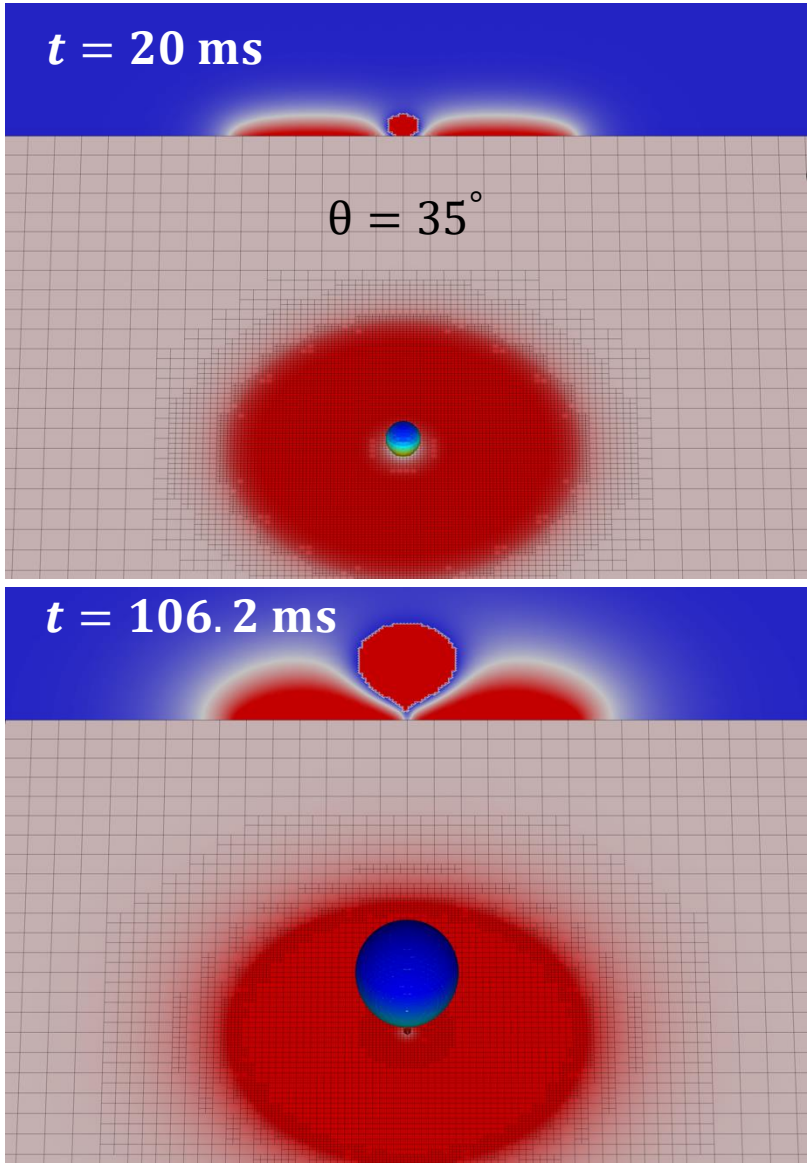
Factors influencing bubble detachment

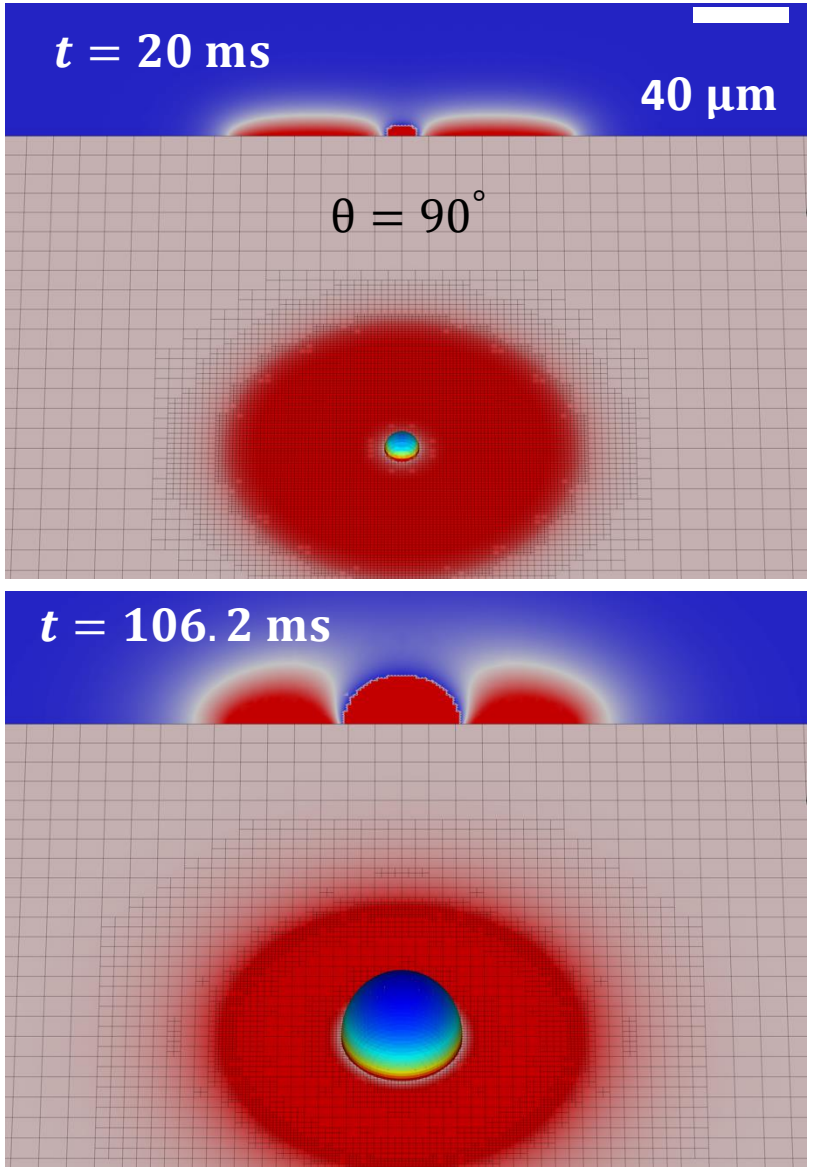


Bubble growth for 4 nucleation sites.

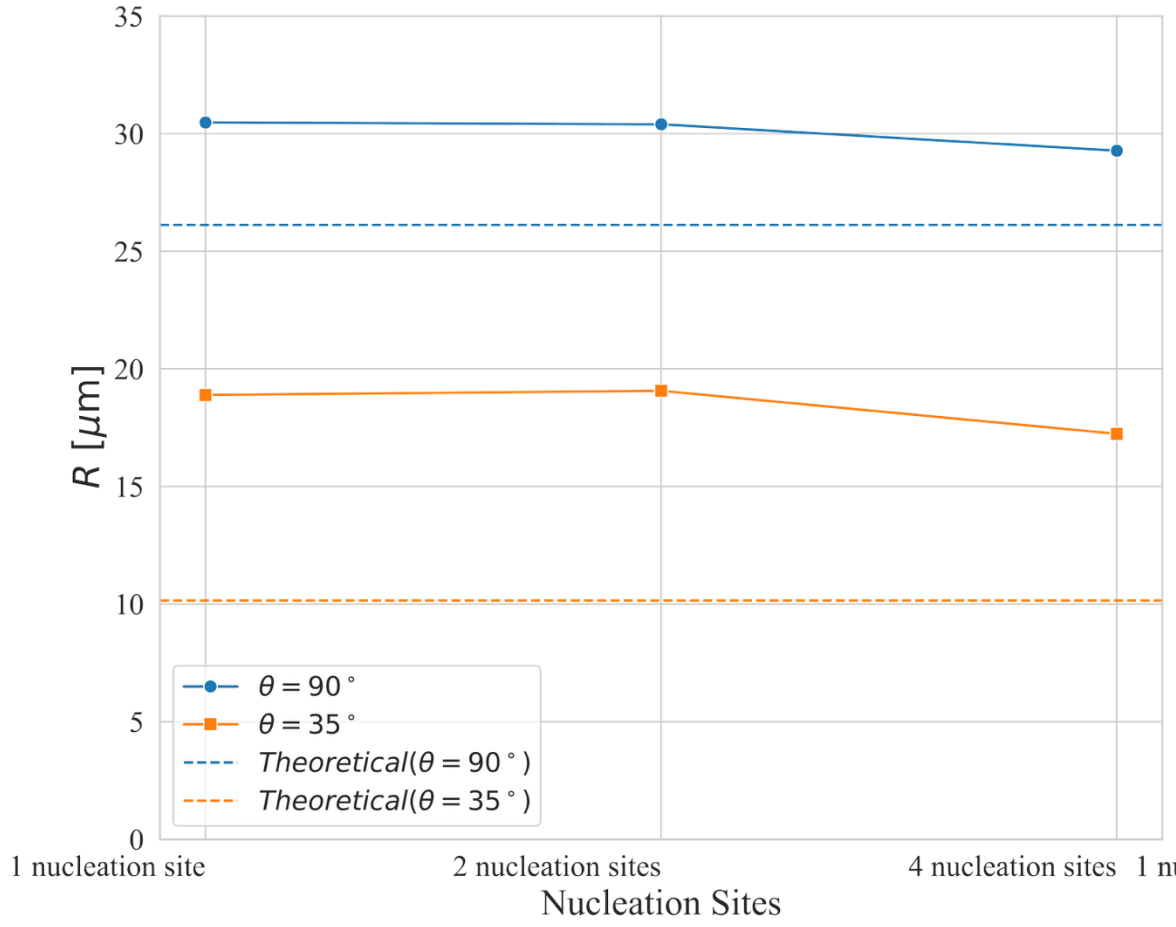


Theoretical Fritz radius for varying contact angle.

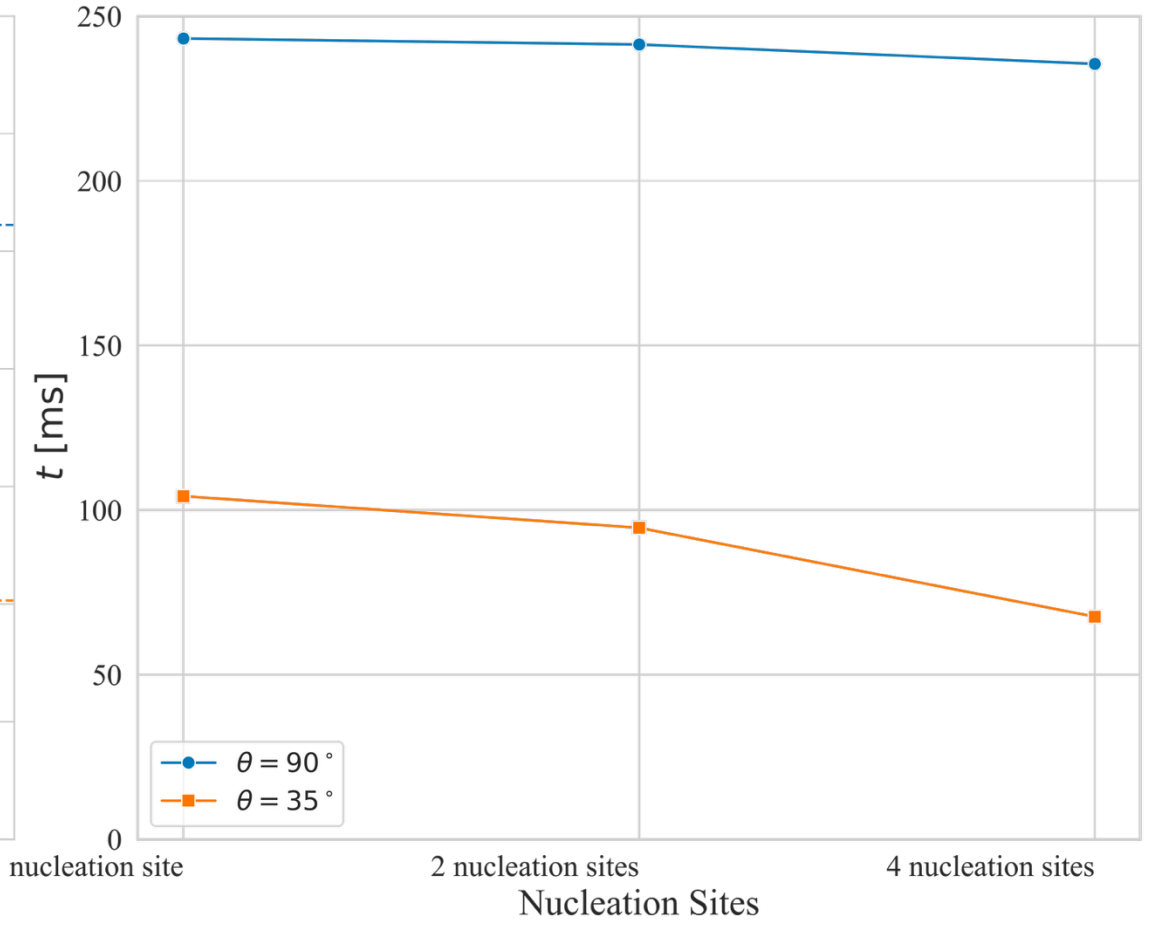




Snapshots show the detachment evolution for varying contact angle. The current density is 1000 A/m^2.

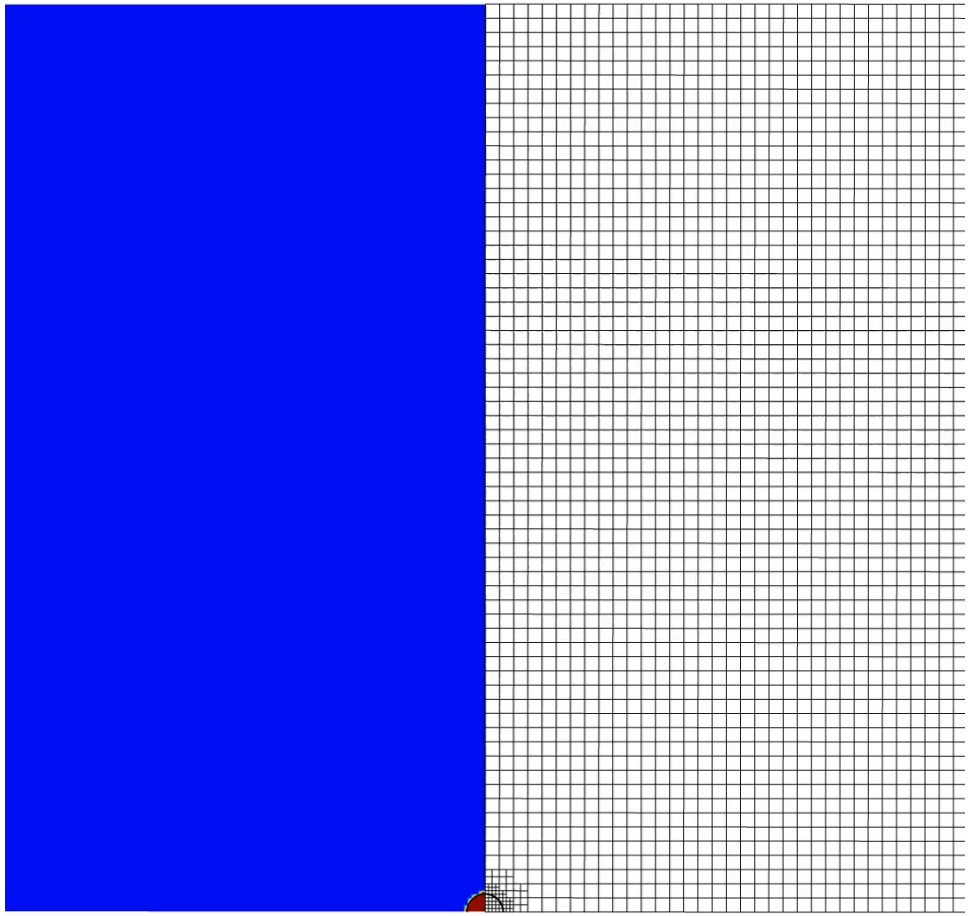


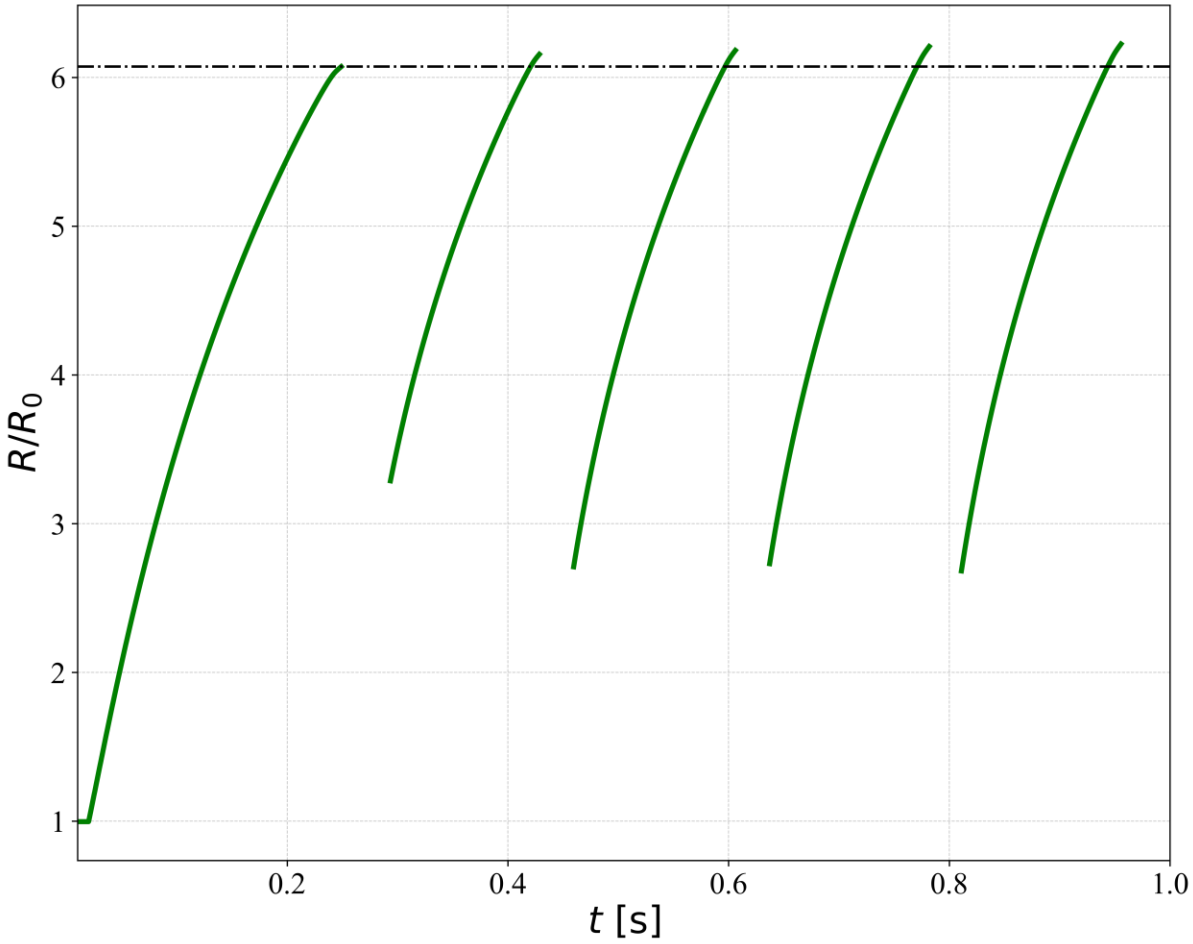
Bubble detachment radius for varying nucleation sites.



Bubble detachment times for varying nucleation sites.

Successive bubbles detachment





Radius of the successively growing bubbles as function of time.

Conclusion & outlook

Bubble growth study	Contact angle influences the growth significantly.
	Multiple bubbles can suppress mass transport mutually.
Detachment study	Smaller contact angle leads the earlier bubble detachment.
	Bubble coalescence accelerates detachment.
Outlook	Successive processes of bubble growth and rise

Thank you!

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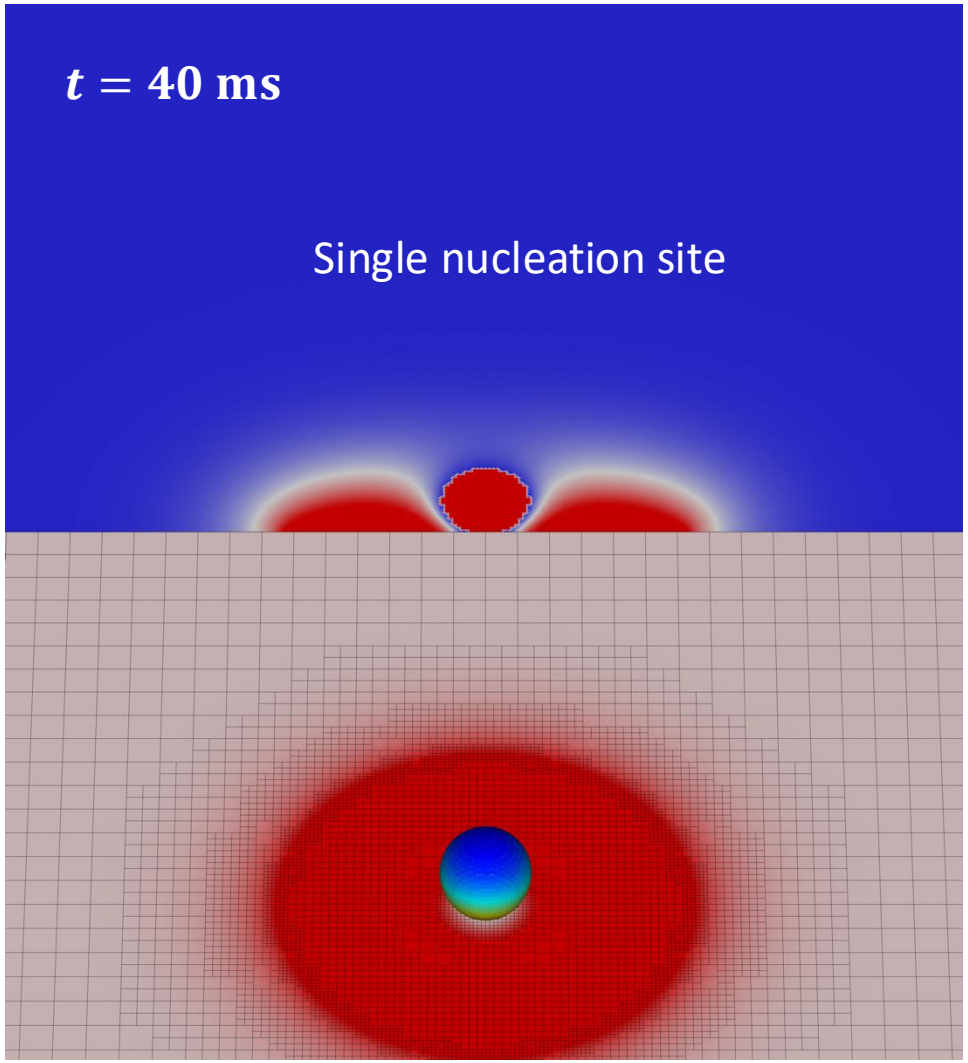

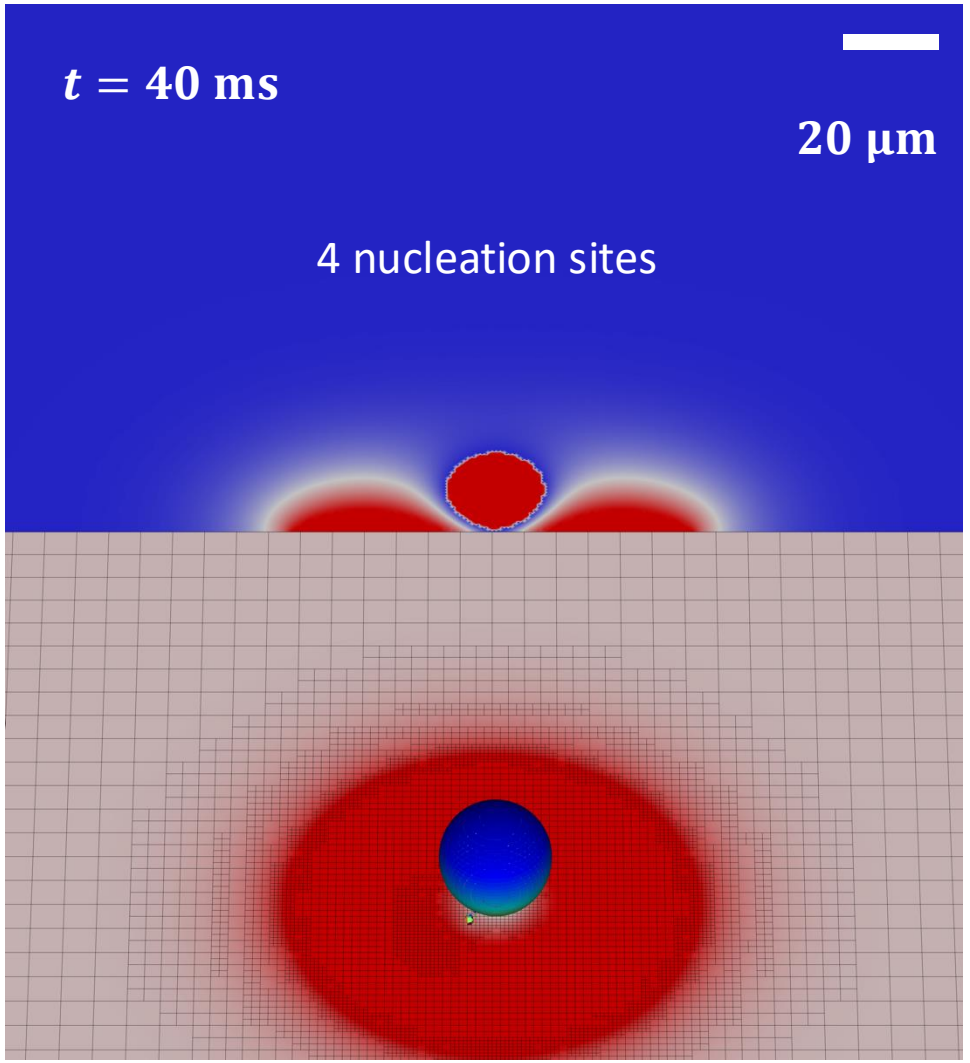

Snapshots of hydrogen bubble detachment evolution. The current density is $1000\ \mathrm{A/m^2}$.