Electronic Supplementary Material (ESI) for Soft Matter.

Solutal Marangoni force controls lateral motion of electrolytic gas bubbles

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Supporting information

S.1. The introduction of initial bubbles for MD

In our MD simulation, the initial condition is a cell filled with only liquid atoms. As the reaction progresses, the gas supersaturation (concentration) near the electrode gradually increases. When the nucleation condition is fulfilled, bubbles will spontaneously form, as shown in the following figure. During the nucleation stage, bubbles gradually grow and finally cover the electrode completely. Then, the surrounding undersaturated liquid will cause gas diffusion loss from the top of the bubble and promote contraction of the nanobubble, causing partial electrode exposure. Finally, the bubbles reach a dynamic equilibrium accompanied by lateral oscillations.

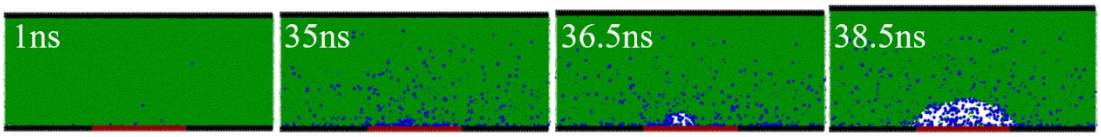

Figure S1: A typical representation of the bubble formation.

S.2. Concentration boundary condition from MD

Take $0.15/ns$ as an example to illustrate that the concentration distribution extracted from MD is used for CFD calculation. To eliminate the interface gas enrichment effect, we select the gas concentration distribution $10 \sim 20\sigma$ away from the bubble interface as the boundary condition for CFD calculation. The following figure shows the gas concentration distribution along the gas-liquid interface at different positions from the interface. $L_{XZ} = 0$ represents the electrode surface.

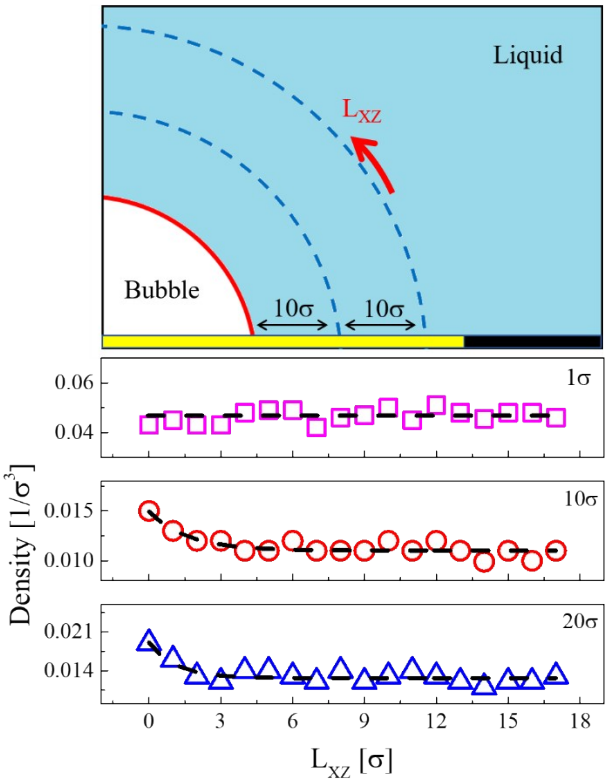

Figure S2: Concentration distribution along gas-liquid interface.

S.3. Marangoni force in vertical direction

In addition to the horizontal gas concentration gradient, the dissolved gas is also not uniformly distributed in the vertical direction, with a gradient pointing from the bottom electrode towards the bulk electrolyte. This results in a vertical component of the solutal-Marangoni force, similar to that observed in Lubetkin.[14]

The following table compares the magnitudes of the Marangoni force in horizontal (f_x) and vertical (f_y) directions obtained from CFD simulations using Approach A. As can be seen, f_y points downwards from bulk electrolyte towards the electrode with enriched gas, and is weaker in value compared to the horizontal component f_x.

Table S1: Comparison of the magnitudes of Marangoni force in horizontal (f_x) and vertical (f_y) directions

Reaction rate v $[1/ns]$	f_x $[nN]$	f_y $[nN]$
0.1	0.01848	− 0.01368
0.11	0.01689	− 0.01373
0.12	0.01709	− 0.01525
0.13	0.01767	− 0.01557
0.14	0.01861	− 0.01471
0.15	0.01865	− 0.01415