Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Electrocatalytic generation and tuning of ultra-stable and ultra-dense nanometre bubbles: An *in situ* molecular dynamics study

Wenjing Xi[1], Hao Feng,[1] Dong Liu,* Longfei Chen, Ying Zhang, Qiang Li*

MIIT Key Laboratory of Thermal Control of Electronic Equipment, School of Energy and Power Engineering, Nanjing University of Science and Technology, Nanjing 210094, China

[1]These authors contributed equally.

*Corresponding Authors: liudong15@njust.edu.cn; liqiang@njust.edu.cn.

Contents

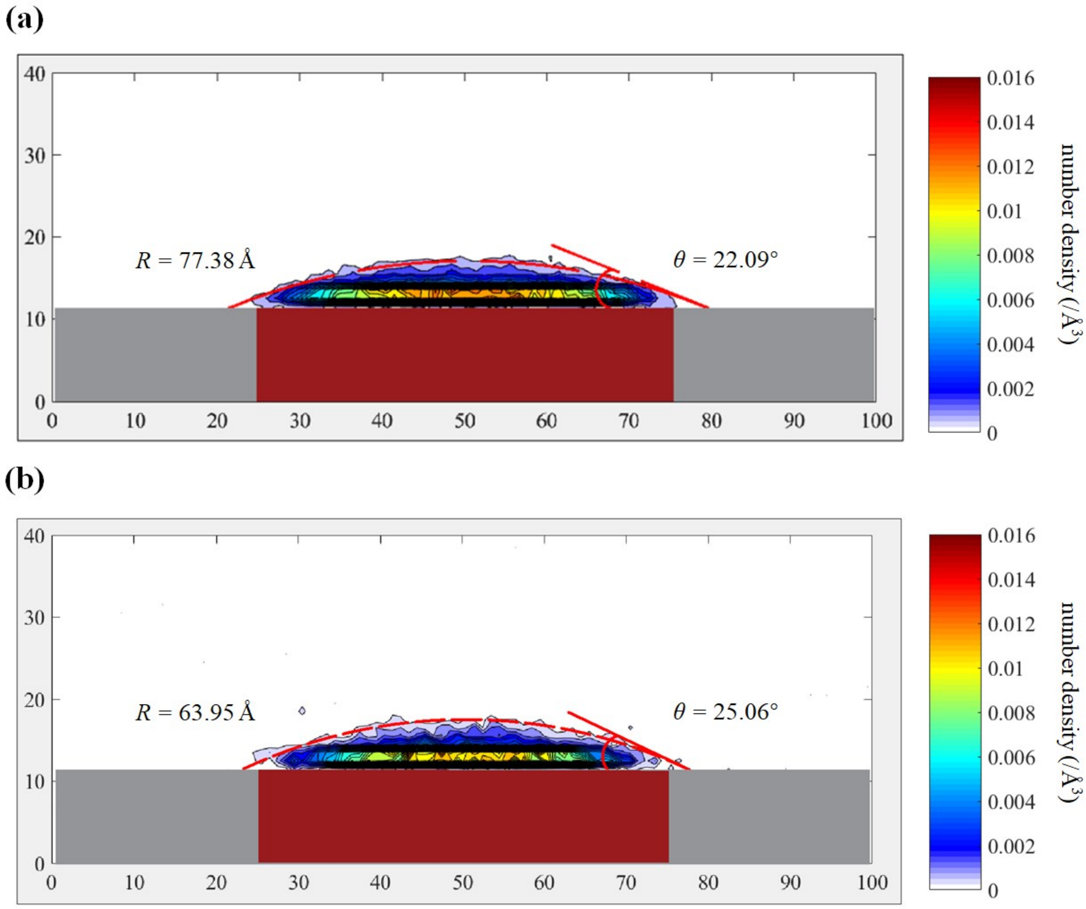

Figure S1. Properties of stationary nanobubbles for (a) ε_{WE}=0.35 and (b) ε_{WE}=0.40.

Figures 3 and S1 tell that the contact angles of stationary nanobubbles also increase with increasing ε_{WE} and decreasing hydrophobicity.

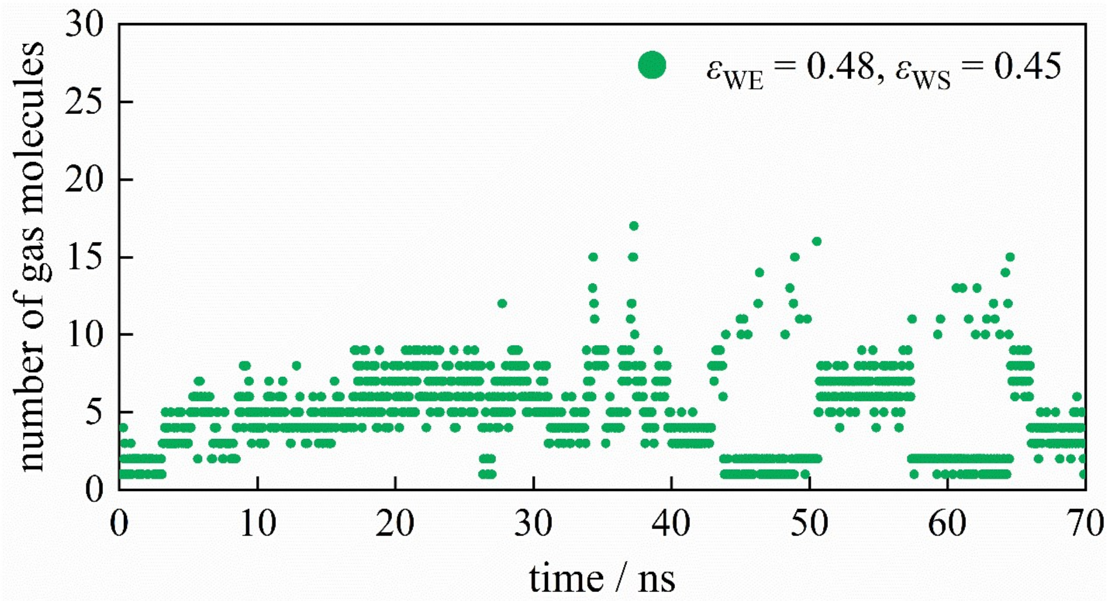

Figure S2. Variations of the number of gas molecules inside the largest gas cluster with time for ε_{WE}=0.48 and ε_{WS}=0.45. Nanobubble neither forms on the nanoelectrode nor on the silica surface with higher hydrophobicity, which means that the formation of nanobubbles is mainly affected by the hydrophobicity of the nanoelectrode.

Table S1. The critical time for nanobubble nucleation[a] and the contact angles of critical gas nuclei for various ε_{WE}

ε_{WE}	critical time for nanobubble nucleation (ns)	contact angle of critical gas nucleus (°)
0.35	3.5	13.8
0.40	10.5	16.4
0.45	13.3	18.9

[a]The nucleation point features abrupt increase of the slope of the *N*-*t* curve and is captured in the insets of Figure 6