Molecular dynamics simulation of bubble nucleation in Al nanoparticles embedded n-decane

Hongtao Zhang, Jun Xia
Dept. of Mech. & Aero. Engineering
Brunel University

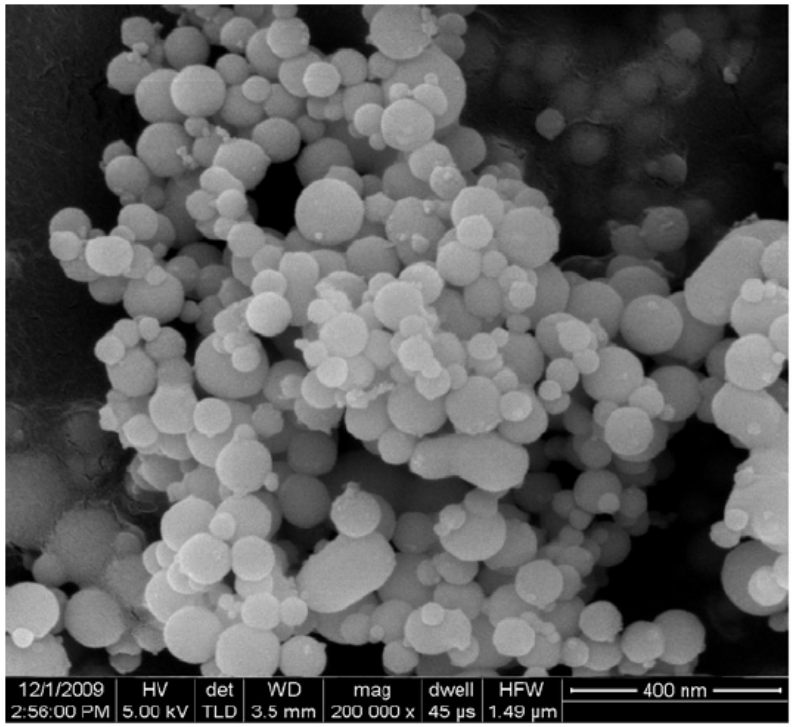
UKCTRF - Annual Meeting
16 September 2020

Introduction

- Background
- kerosene droplet combustion: Measurement
- MD simulation of nanoparticle effects on nucleation
- Conclusions

Background

Additive to enhance energy density:
nano-Aluminum particles



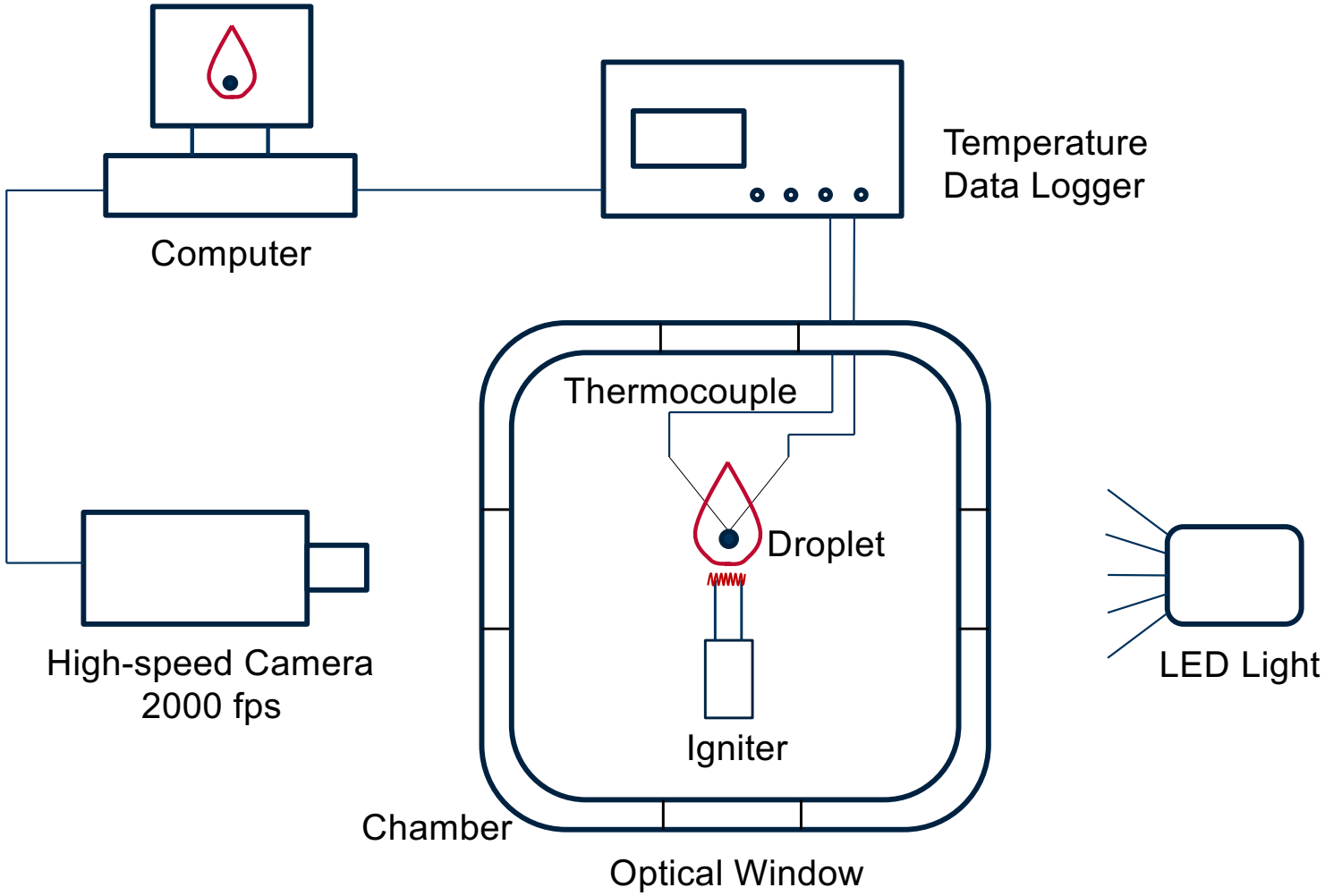
SEM photograph of 80nm nano-aluminium particles*

- Higher energy density
- Less CO_2 & NO_x
- Shortened ignition delay time
- Enhanced fuel oxidation by catalytic effect

*Y. Gan, L. Qiao / Combustion and Flame 158 (2011) 354–368

Kerosene droplet combustion: Measurement

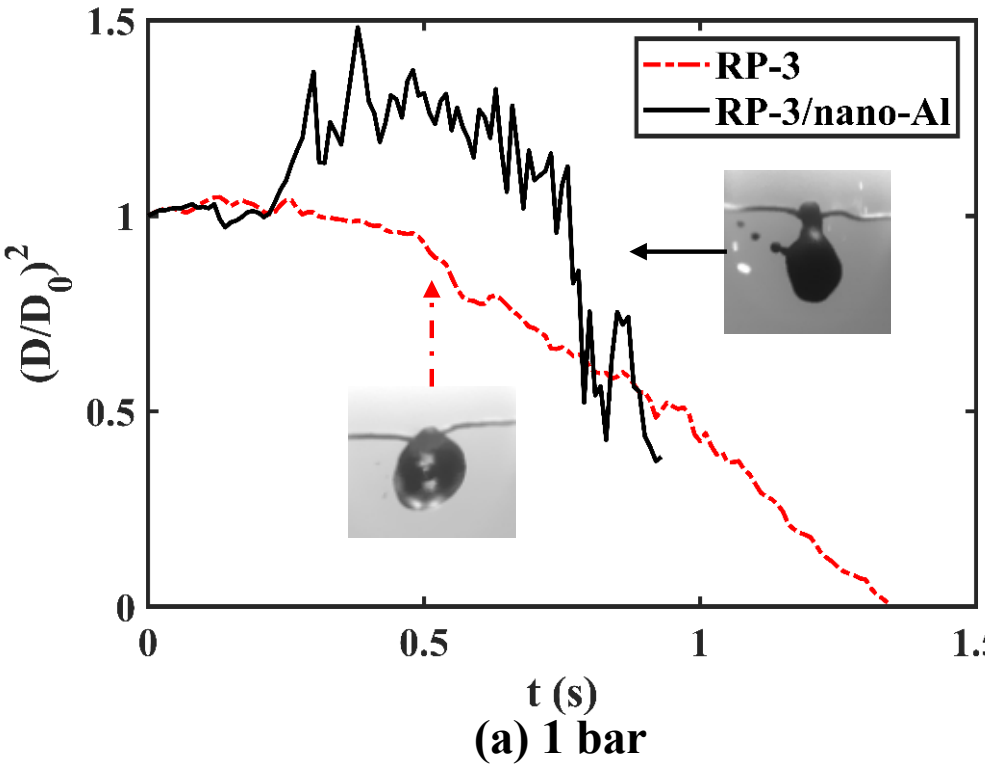
Experimental Setup @ Zhejiang University, China



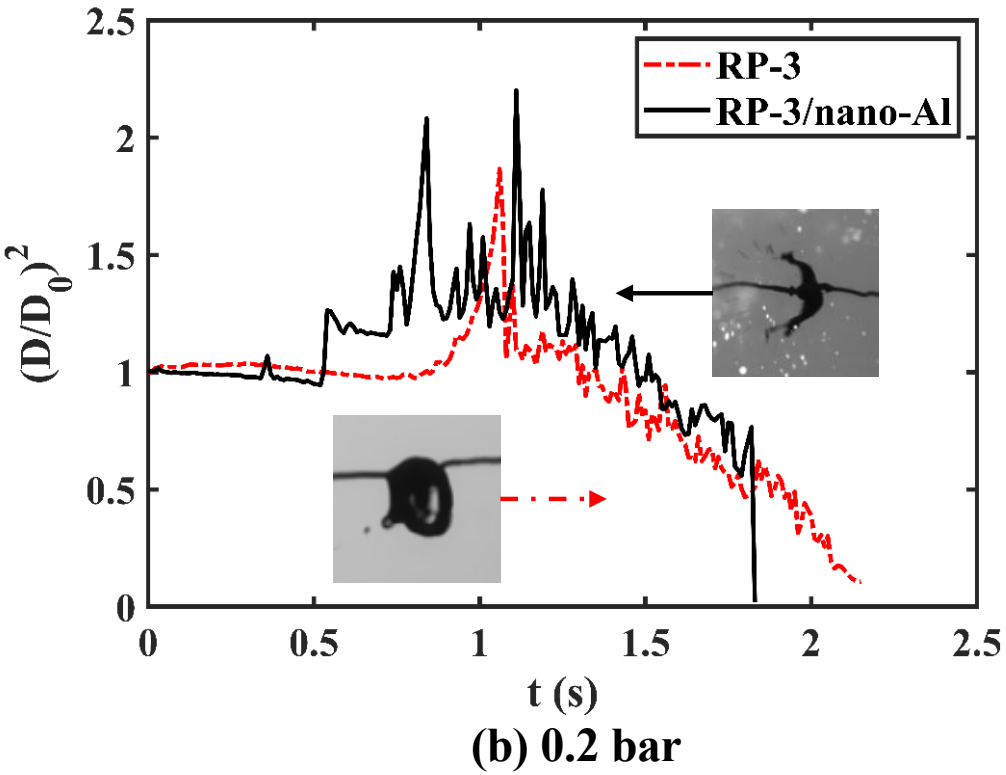
Kerosene droplet combustion

Major components of Chinese RP-3 kerosene (mass fraction)

Saturated hydrocarbons				Aromatic hydrocarbons			
Alkanes	Naphthenes			Alkyl Benzenes	Indan & Tetralin	Naphthalene	Naphthalene derivatives
	Monocyclic	Bicyclic	Tricyclic				
52.2	33.8	6.0	0.1	5.1	1.3	0.6	0.9



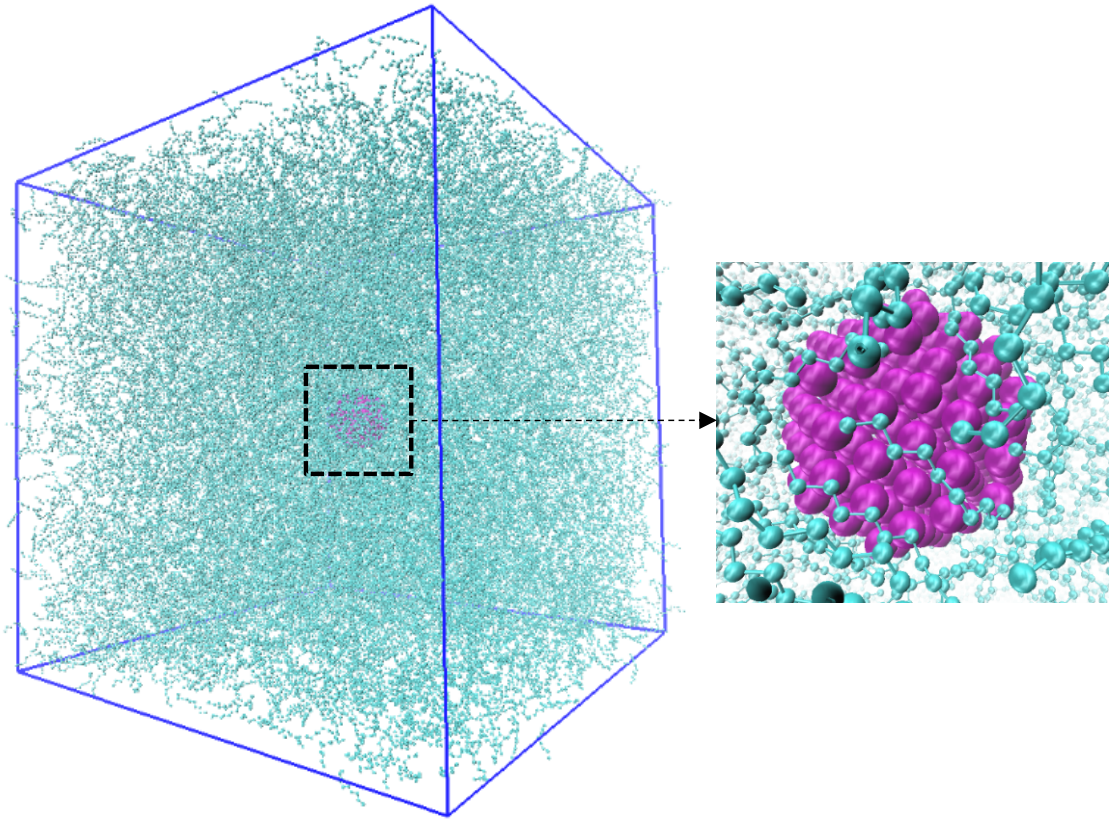
(a) 1 bar



(b) 0.2 bar

MD simulation of nanoparticle effects on nucleation

Numerical setup



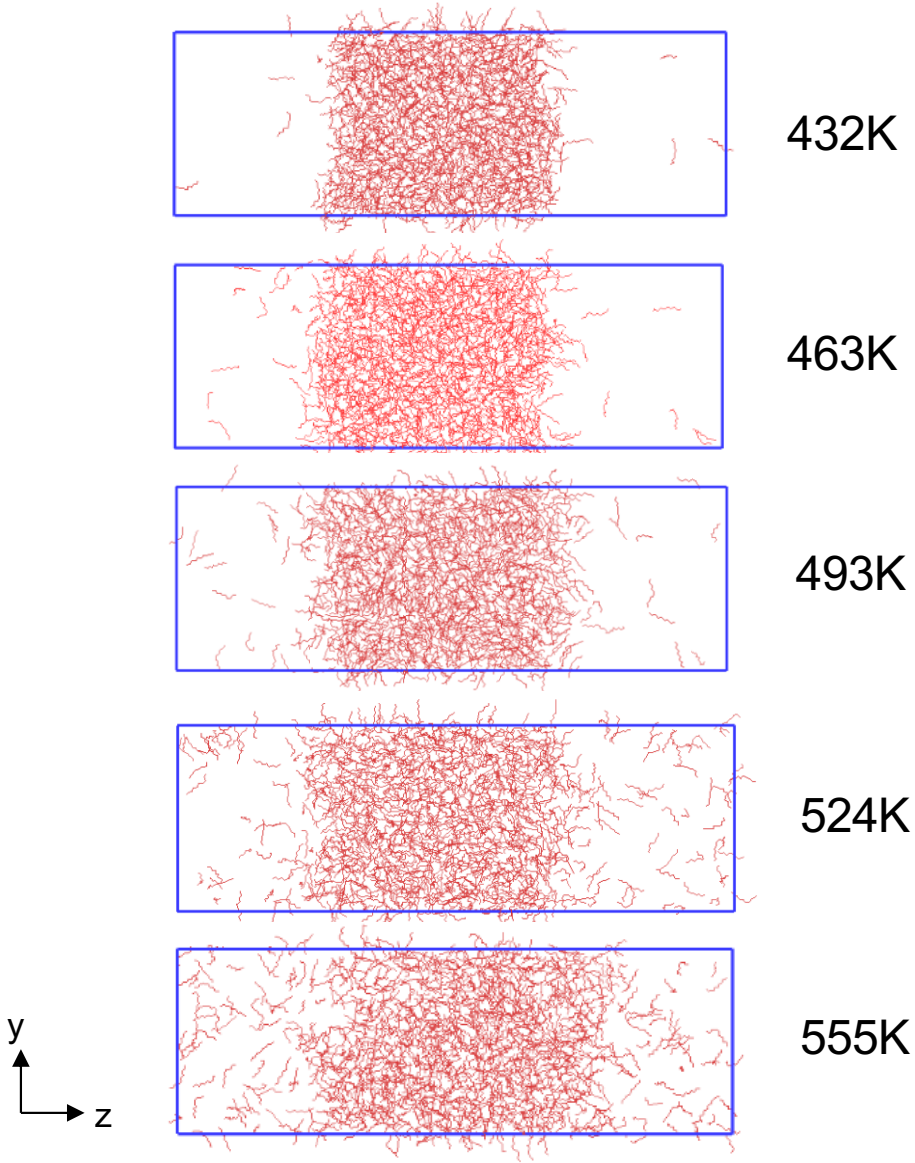
- Software: LAMMPS
- Force field: TraPPE-UA

- Using single interaction sites to represent a carbon atom together with all of its bonded hydrogen atoms.

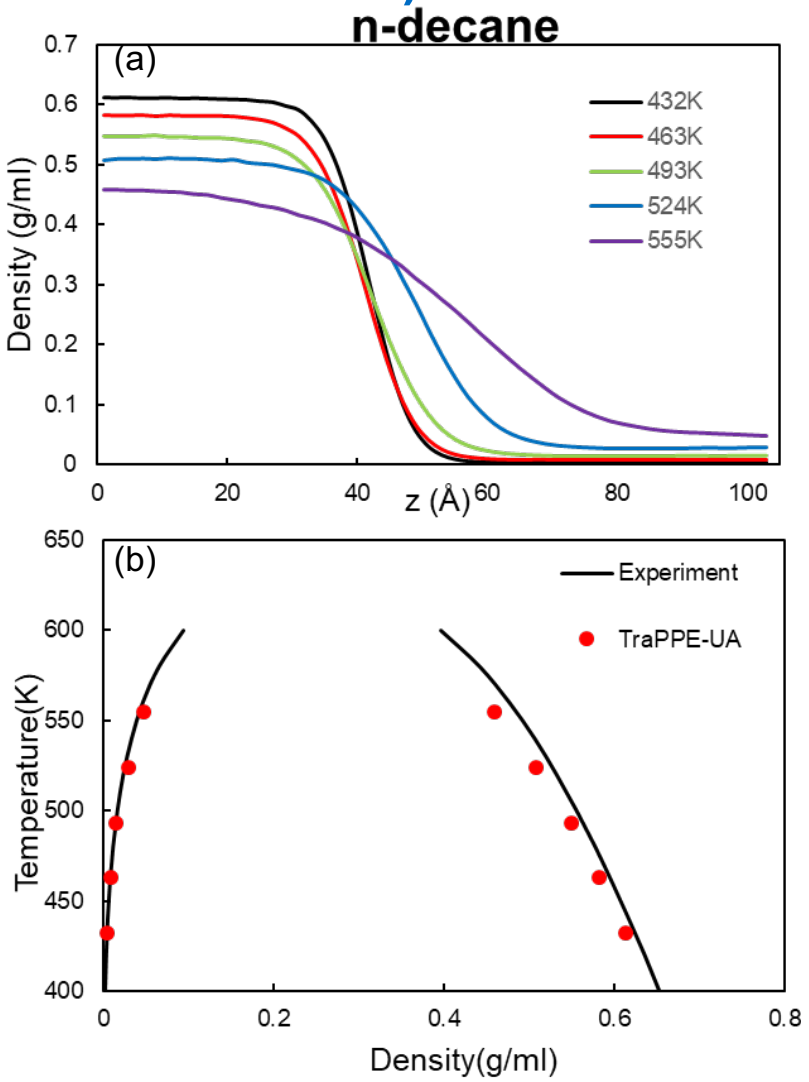
- Ensemble: NVT
- Molecule number: 30000
- Nanoparticle radius: 10 / 20 Å
- Nanaparitcle number: 1 / 8
- Sample T: 524 K(85% $T_{c\text{-}decane}$)

MD simulation of nanoparticle effects on nucleation

Validation for TraPPE-UA force field(VLE simulations)



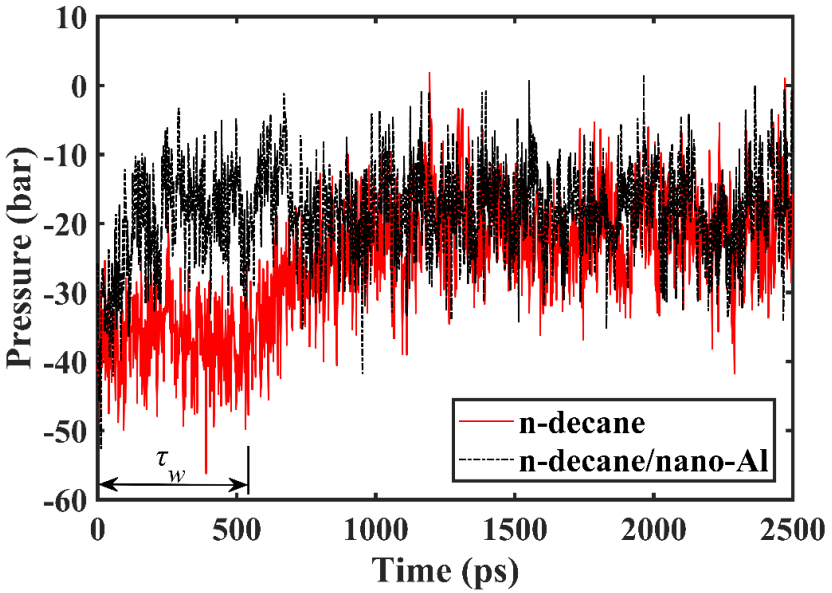
Evaporation of n-decane at different temperatures



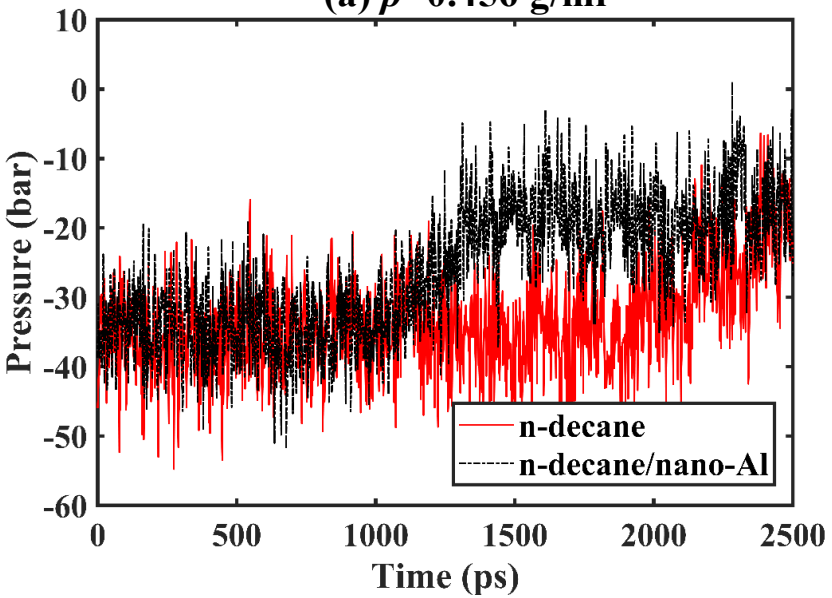
(a) Density as a function of distance from the liquid-slab center of mass

(b) Vapor-lquid coexistence curve

MD simulation of nanoparticle effects on nucleation

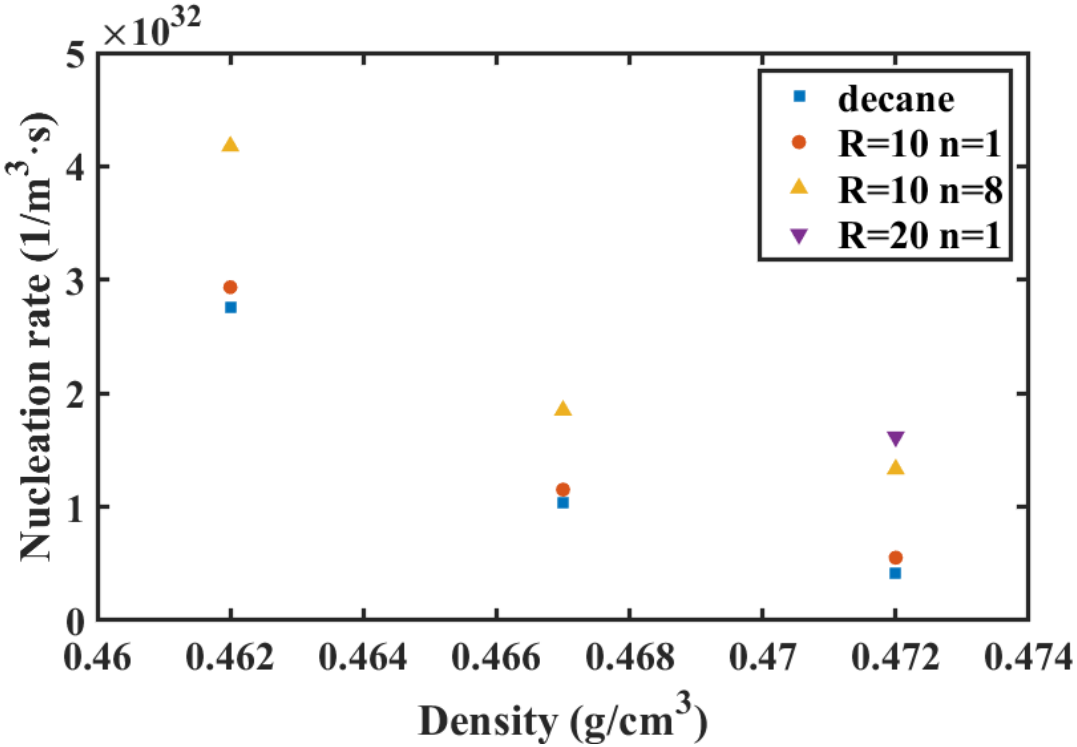


(a) ρ=0.456 g/ml

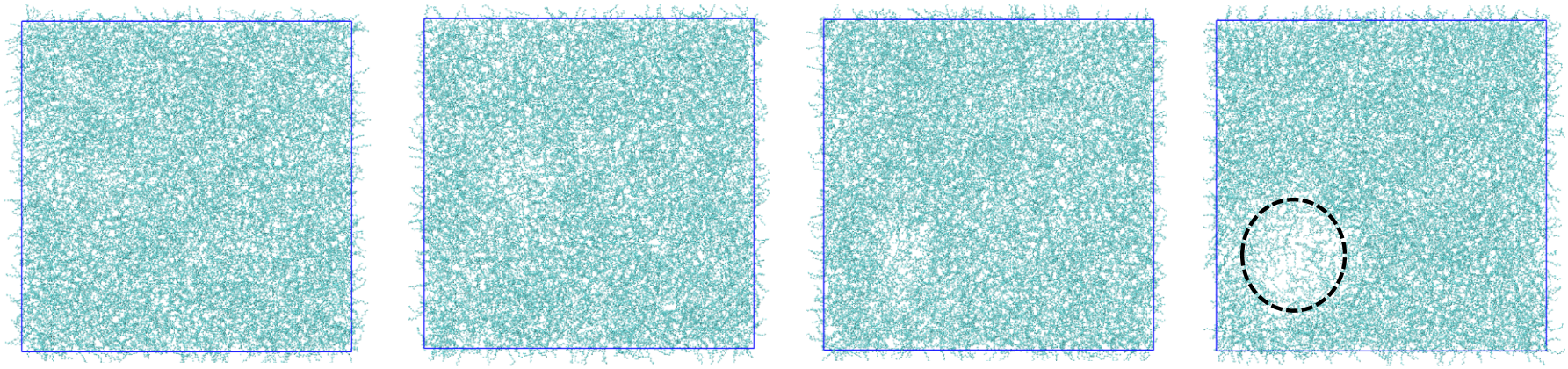


(b) ρ=0.462 g/ml

$$J_{sim} = 1/(\tau_w V)$$

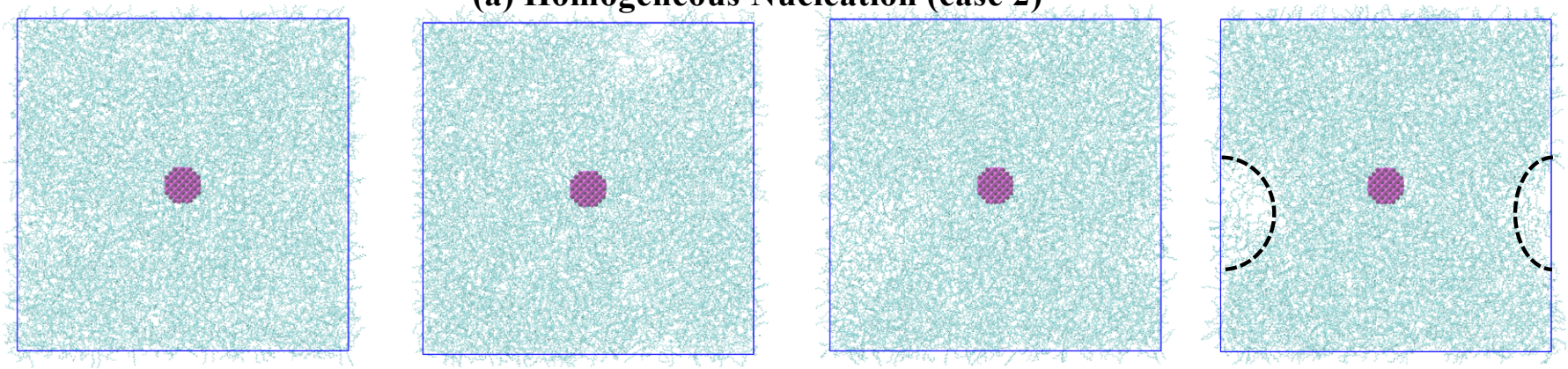


MD simulation of nanoparticle effects on nucleation



t=1632ps t=1800ps t=2016ps t=2294ps

(a) Homogeneous Nucleation (case 2)

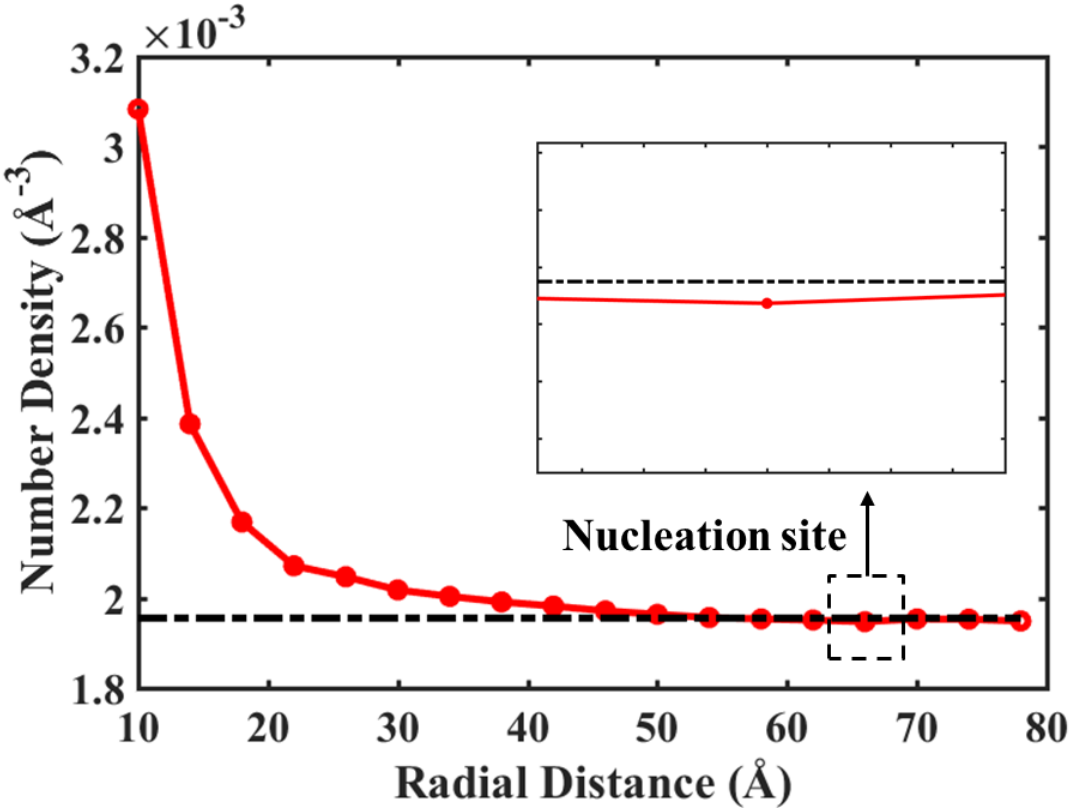


t=400ps t=900ps t=1304ps t=1490ps

(b) Heterogeneous Nucleation (case 4)

Snapshots of bubble formation and growth when ρ = 0.462 g/ml，R = 10 Å, n=1

MD simulation of nanoparticle effects on nucleation



Number density of the n-decane molecules surrounding the nanoparticle for the heterogeneous nucleation case (ρ = 0.462 g/ml) averaged over the initial 200 ps. Dash line: average number density of n-decane for the homogeneous nucleation case.

12-6 Lennard-Jones potential

$$E_{ij} = \begin{cases} 4\varepsilon_{ij}\left(\left(\frac{\sigma_{ij}}{R_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{R_{ij}}\right)^{6}\right) & R_{ij} \le r_C, \\ 0 & R_{ij} > r_C, \end{cases}$$

$$\left(\sigma_{ij} = \frac{1}{2}(\sigma_i + \sigma_j)\right) \quad \text{and} \quad \left(\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}\right)$$

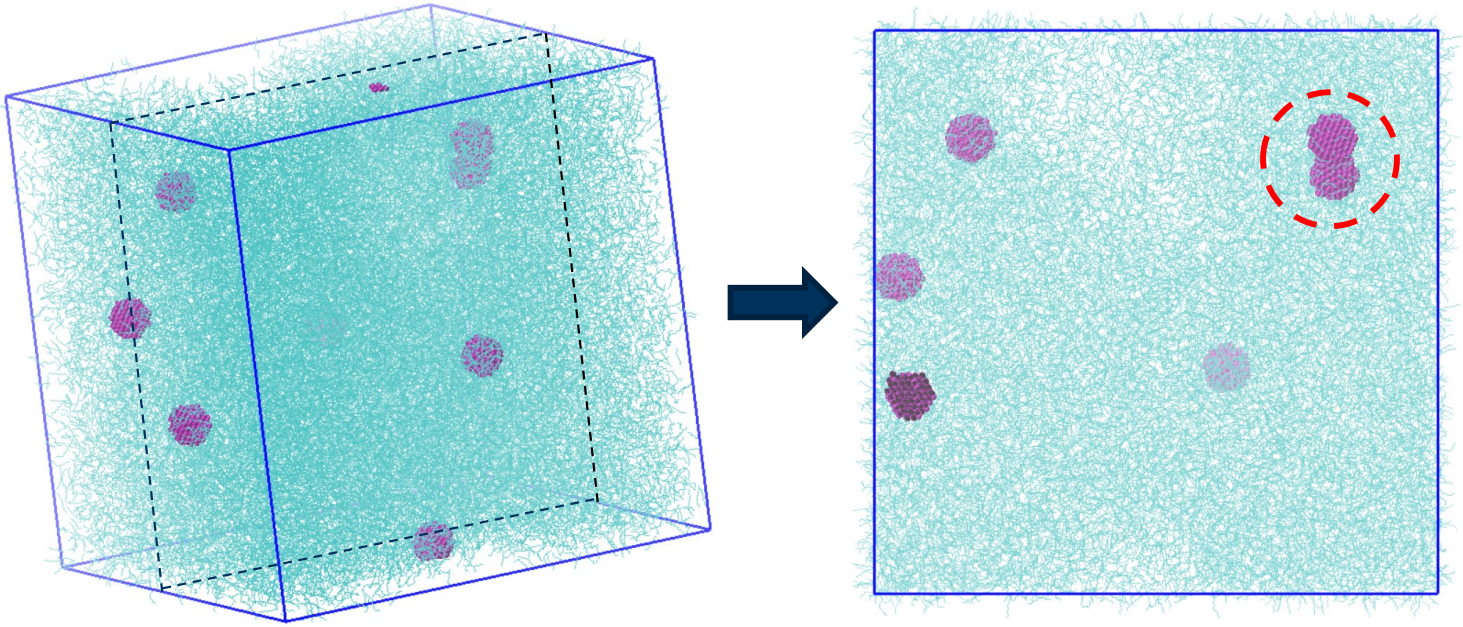
$\varepsilon_{CH3} = 0.815$ kJ/mol

$\varepsilon_{CH2} = 0.407$ kJ/mol

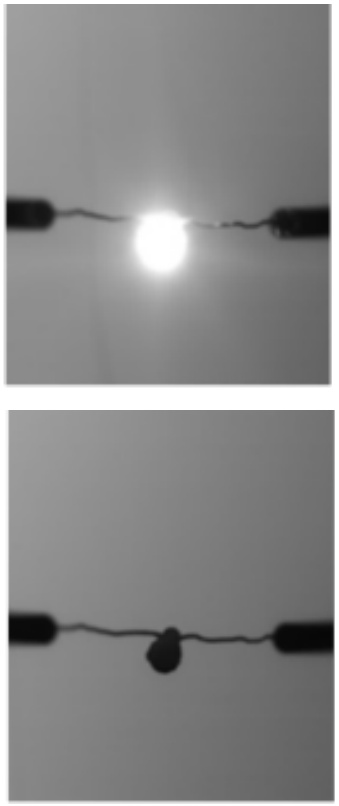
$\varepsilon_{Al} = 37.839$ kJ/mol

MD simulation of nanoparticle effects on nucleation

Al nanoparticles aggregation



Snapshot of nano particles distribution when ρ = 0.472 g/ml，R = 10, n = 8, t = 2500 ps



Al-aggregation combustion and residue

Conclusions

- The TraPPE-UA force field was first demonstrated to be able to properly predict phase transition via vapor-liquid equilibrium simulations.
- For ρ = 0.456 g/ml, the metastable system became unstable with addition of the nanoparticle. For ρ = 0.462-0.472 g/ml, the nanoparticle was found to enhance the nucleation rate. With the increase of the particle size and number, the nucleation rate was enhanced.
- A density gradient was observed near the surface of the nanoparticle because of a larger van der Waals force between Al atoms and n-decane molecules, leading to easier formation of bubbles and thus an increase of the nucleation rate further than 65 Å away from the nanoparticle surface.
- And a larger van der Waals force between Al atoms leads to the aggregation of Al nanoparticles, which agreed with the founding in experiments.

Acknowledgements

- Financial support by the China Scholarship Council (CSC) for a research visit of Hongtao Zhang to Brunel University London is gratefully acknowledged.
- Code: **LAMMPS**; ARCHER resources: **8,500 kAUs**.