

Supplementary information for "Indentation of graphene nano-bubbles"

Fahim Faraji,^{*,†,‡,¶} Mehdi Neek-Amal,^{*,§,‡} Erik C. Neyts,^{*,†,¶} and François M.
Peeters^{*,†,¶}

[†]*PLASMANT, Department of Chemistry, University of Antwerp, Universiteitsplein 1, 2610
Antwerp, Belgium*

[‡]*Condensed Matter Theory, Department of Physics, University of Antwerp,
Groenenborgerlaan 171, 2020 Antwerp, Belgium*

[¶]*Center of Excellence NANOlabor, University of Antwerp, Groenenborgerlaan 171, 2020
Antwerp, Belgium*

[§]*Department of Physics, Shahid Rajaei Teacher Training University, 16875-163 Tehran,
Iran*

E-mail: fahim.faraji@uantwerpen.be; mehdi.neekamal@gmail.com; erik.neyts@uantwerpen.be;
francois.peeters@uantwerpen.be

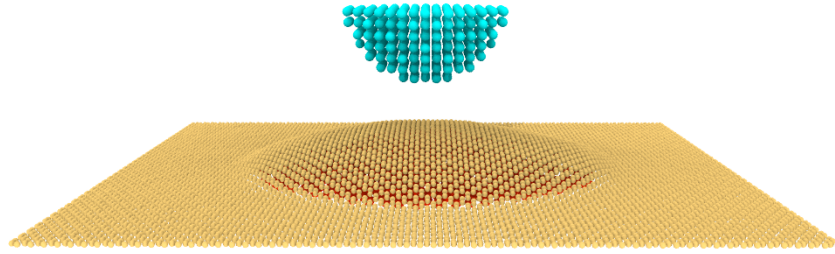


Figure S1: Schematic of the MD simulation system before the indentation for Ar bubble with $N_t = 1100$. A spheroidal surface tip with sphere radius of 2 nm made of silicon was placed above the graphene bubble.

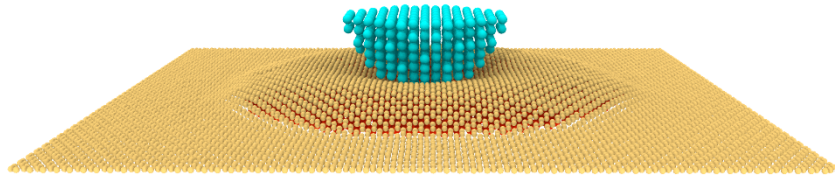


Figure S2: Schematic of the MD simulation system during the indentation for Ar bubble with $N_t = 1100$. The tip deforms the bubble until the point that the graphene sheet breaks.

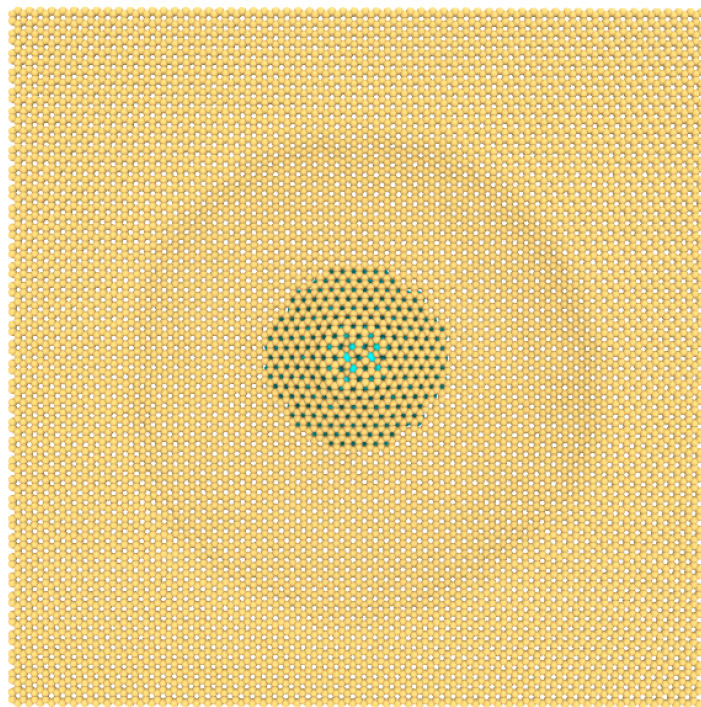


Figure S3: Schematic of the MD simulation system seen from the bottom for Ar bubble with $N_t = 1100$. The time frame is shown just before the graphene failure. The carbon bonds are under strong stretch. The substrate atoms are not shown here for a better illustration.

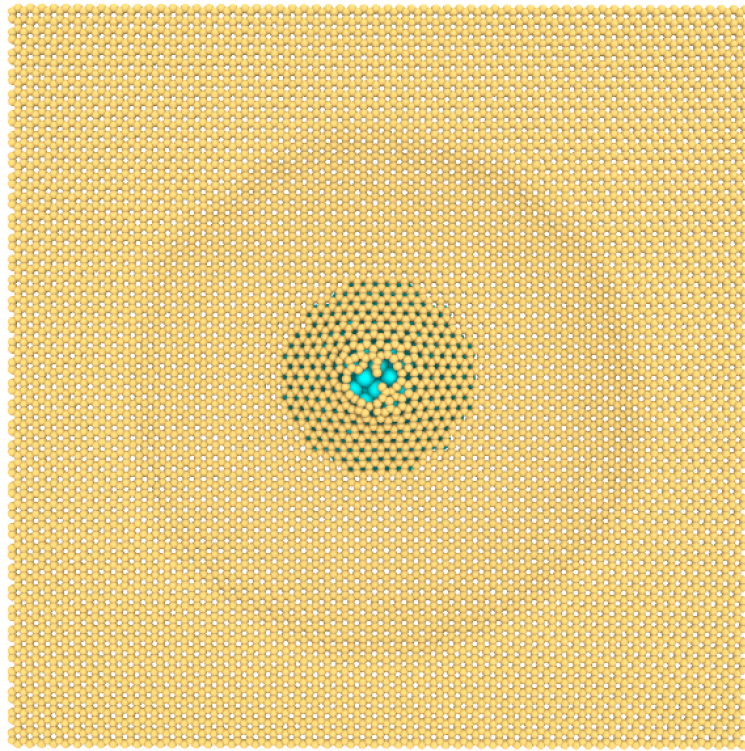


Figure S4: Schematic of the MD simulation system seen from the bottom after the graphene failure for Ar bubble with $N_t = 1100$. The substrate atoms are not shown here for a better illustration.

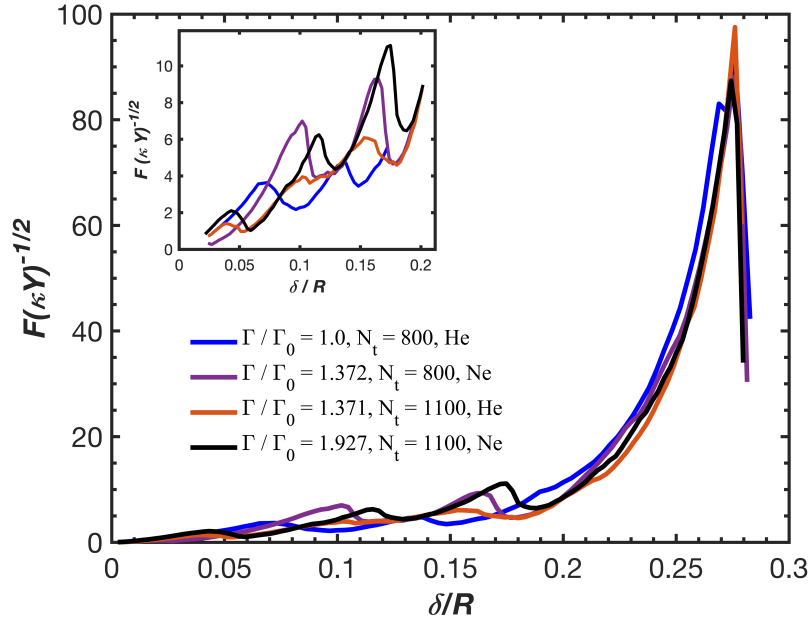


Figure S5: The force applied on the tip versus the bubbles deformation at $T = 5K$. The inset magnifies the region of the partial drops associated with the buckling transitions.

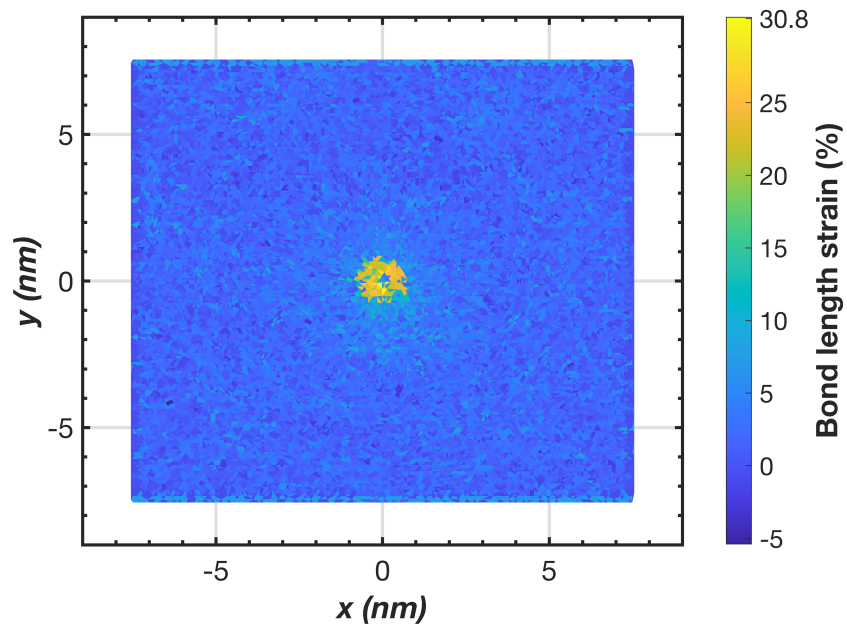


Figure S6: Strain rates of bond length across the graphene sheet for Ne bubble with $N_t = 800$ at room temperature.

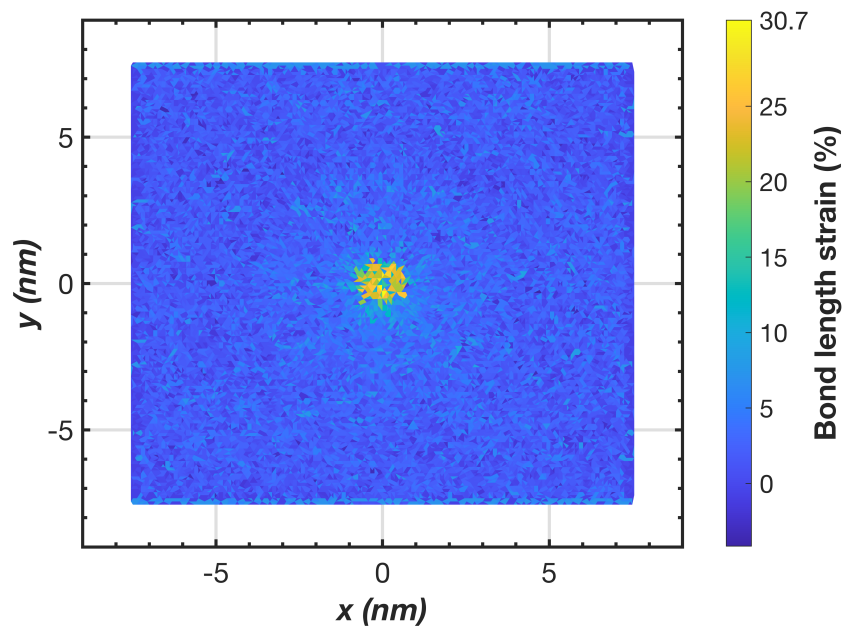


Figure S7: Strain rates of bond length across the graphene sheet for Ne bubble with $N_t = 1100$ at room temperature.

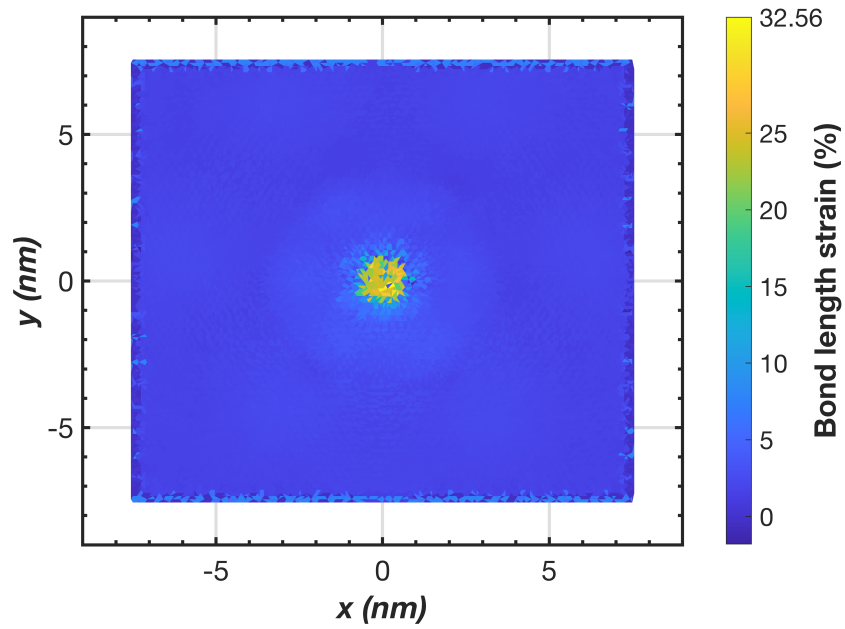


Figure S8: Strain rates of bond length across the graphene sheet for Ne bubble with $N_t = 800$ at $T = 5\text{K}$.

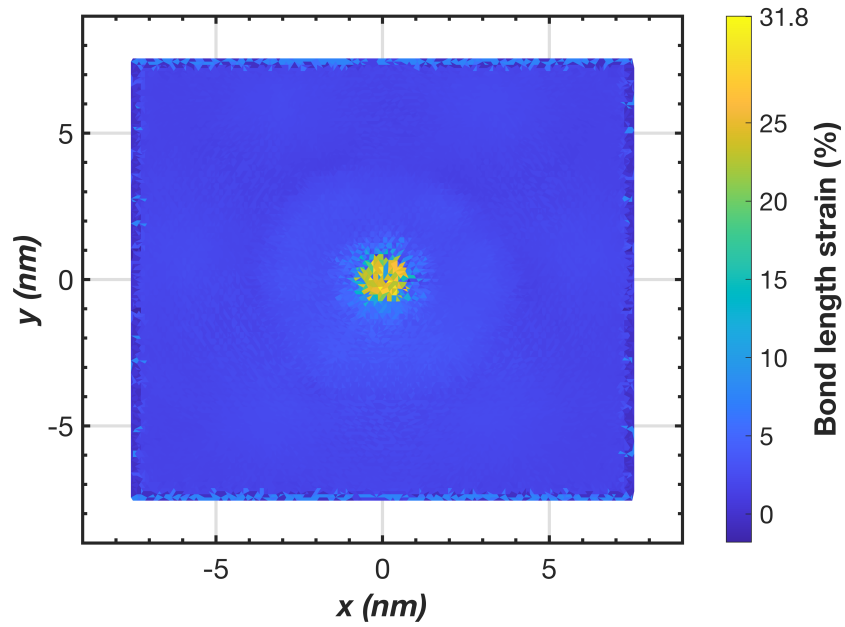


Figure S9: Strain rates of bond length across the graphene sheet for Ne bubble with $N_t = 1100$ at $T = 5\text{K}$.

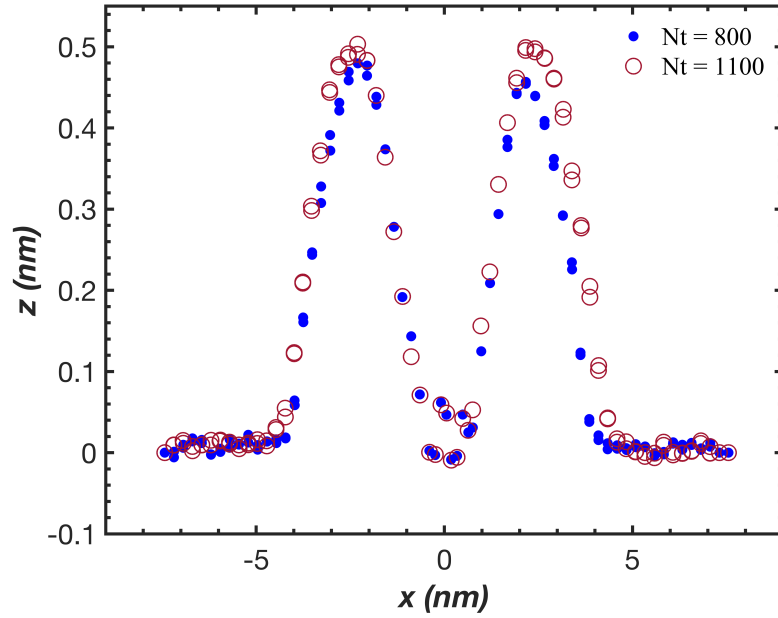


Figure S10: Cross section of the Ne bubble profile at the time frame before the graphene failure for $N_t = 800$ and $N_t = 1100$ at room temperature.

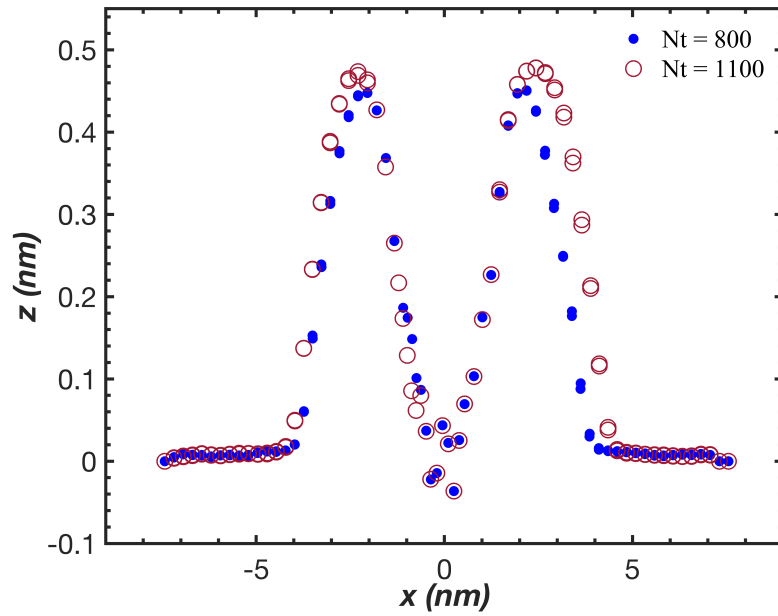


Figure S11: Cross section of the Ne bubble profile at the time frame before the graphene failure for $N_t = 800$ and $N_t = 1100$ at $T = 5\text{K}$.

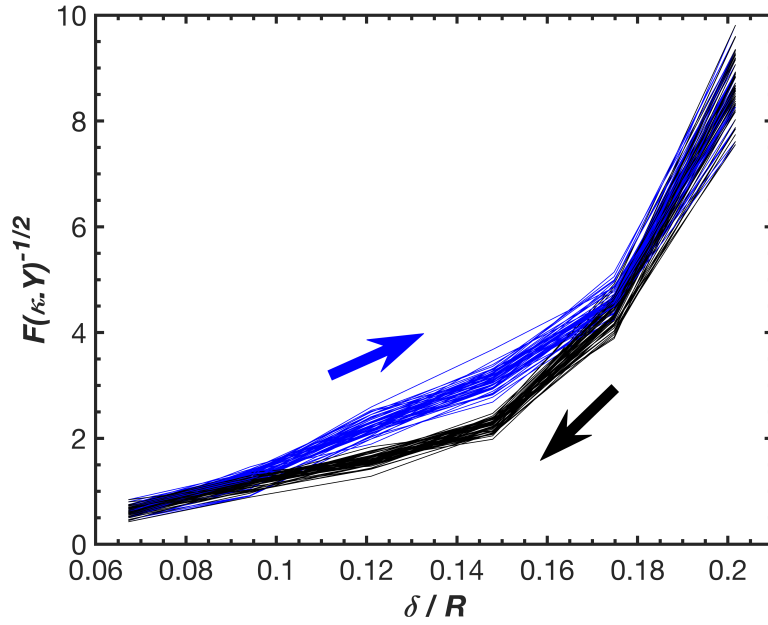


Figure S12: The force-displacement curve for periodic indentation after 50 cycles for Ne bubble with $N_t = 800$ at $T=5\text{K}$.

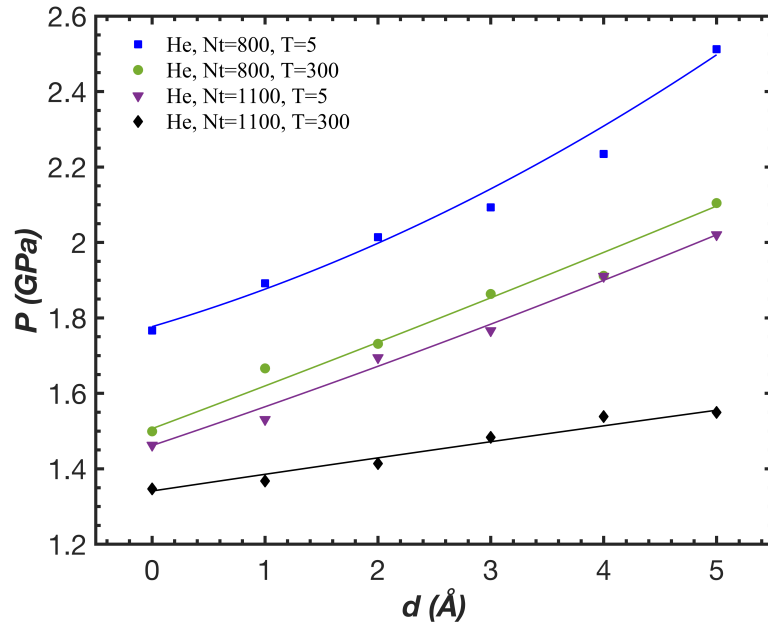


Figure S13: Trapped materials hydrostatic pressure for He bubbles as function of tip displacement for different N_t and temperatures. The curves are guide to the eye.

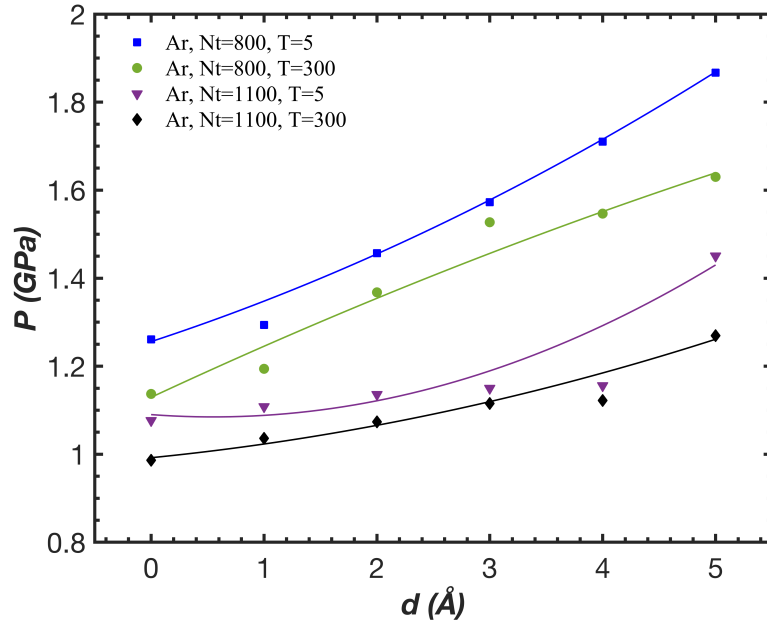


Figure S14: Trapped materials hydrostatic pressure for Ar bubbles as function of tip displacement for different N_t and temperatures. The curves are guide to the eye.

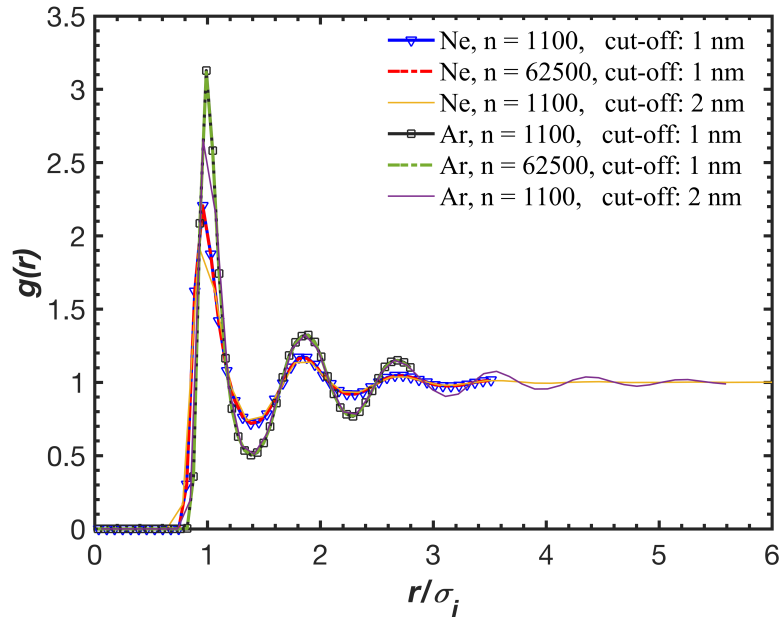


Figure S15: Radial distribution functions for Ne and Ar gases simulated with Lennard-Jones (LJ) potential in an isothermal-isobaric (NPT) ensemble (at room temperature and corresponding bubble pressure) for different system size and MD cut-off radius.

Supplementary movies

Supplementary movie 1:

The video shows the graphene sheet for Ar bubble with $N_t = 1100$ during the indentation until graphene fails.

Supplementary movie 2:

This video shows He atoms ($N_t = 800$) inside the bubble seen from the bottom during the indentation up to the graphene failure point. It appears that He atoms are in the liquid state inside the bubble at room temperature.

Supplementary movie 3:

This video shows Ne atoms ($N_t = 800$) inside the bubble seen from the bottom during the indentation up to the graphene failure point. It appears that Ne atoms are in the solid state inside the bubble at room temperature.

Supplementary movie 4:

This video shows Ar atoms ($N_t = 800$) inside the bubble seen from the bottom during the indentation up to the graphene failure point. It appears that Ar atoms are in the solid state inside the bubble at room temperature.

Supplementary movie 5:

In this video, atoms of Ne are shown within a periodic box resembling a bulk condition. MD simulation is performed in an isothermal-isobaric (NPT) ensemble at room temperature and the corresponding bubble pressure. Ne atoms appear to be in the liquid state at this particular temperature and pressure.

Supplementary movie 6:

In this video, atoms of Ar are shown within a periodic box resembling a bulk condition. MD simulation is performed in an isothermal-isobaric (NPT) ensemble at room temperature and the corresponding bubble pressure. Ar atoms appear to be in the liquid state at this particular temperature and pressure.