Surface tension of lipid monolayer under rapid deformation, and calculation of local surface tension

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1. Project Purpose

The use of oscillation of bubbles under ultrasound has recently gained attention in medical applications. In this application, microbubbles are coated by lipid monolayer. The surface tension of the coating monolayer is known to be varying nonlinearly with strain, therefore affects ultrasound-induced oscillation of bubbles and ultrasound propagation in medium with bubbles.

Conventional surface tension models are based on experiments. However, experiments can only probe low frequency range (10^{-1}~10^{1} Hz) while behavior and mechanical properties in the high frequency regime (10^{5}~10^{6} Hz), corresponding to ultrasound-induced bubble oscillations, remain unclear. Therefore, to properly describe bubble oscillations, it is necessary to develop a new surface tension model for lipid monolayers.

By using Molecular Dynamics simulation (MD), this study explores the behavior and the surface tension of lipid monolayers under high deformation rate (high frequency). The trends and the tendency of the surface tension from molecular simulation is then used to construct the continuum surface tension model. Furthermore, the local surface tension is probed to understand how local tension is related to local deformation.

2. Results

The simulation is as follows: a system of two monolayers (each with 64 molecules of DPPC lipid) sandwiching a water layer is prepared, with area per lipid (APL) at 0.63nm^2. After equilibration, system is subjected to NVT simulation for 8ns to record surface tension. Then, system is deformed by changing box size bilaterally for 8ns. After that, the system is kept at deformed state for 8ns with unchanged box size. The deformation is conducted with two types: (a) compression or (b) expansion, both at constant deformation rate. During the compression, the trajectories are recorded, and the local surface tension field is averaged every 250 steps during 100.000 steps, using Nakamura patch for LAMMPS (Comput. Phys. Commun., 2015), with Python code for extracting surface, normal vector, aligning stress tensor with normal vector. Figure 1 shows the surface tension of whole system. With constant-rate expansion (red), the surface tension increases linearly while with constant-rate compression (blue), the surface tension drops nonlinearly and is much more pronounced. Moreover, right after deformation, the surface tension in expansion case oscillated mildly, while in compression case, a recovery of surface tension appeared. Figure 1 also shows that, the deformation, even in compression case, the surface tension and APL have a linear relation, until surface tension near zero.

Figure 2 shows the local surface tension field during the compressing process. As the lipid monolayer becomes more deformed, the local surface tension field reaches higher amplitude, with negative values are more dominant. It should be noted that the current results are not converged yet, as evidenced by the high values of surface tension, and by the dependence on grid size.

3. Roles of the MCRP and its significance

The MCRP has provided necessary computational resources for the preparation and the simulation of lipid monolayer under deformation. Moreover, MCRP has supported significant storage, necessary for the calculation of local surface tension. In overall, MCRP has enabled the research of lipid monolayer under high deformation rate and local surface tension rate, which accelerate the knowledge on understanding and designing lipid monolayer for medical applications.

4. Future plan

In the future, we will compare the simulation results with the prediction from continuum theory. Then by using both simulation and theoretical results, we aim to propose a new model for surface tension. The replicated simulations will also be conducted, and the periodic boundary conditions effects, the convergence of local surface tension field, will also be examined.

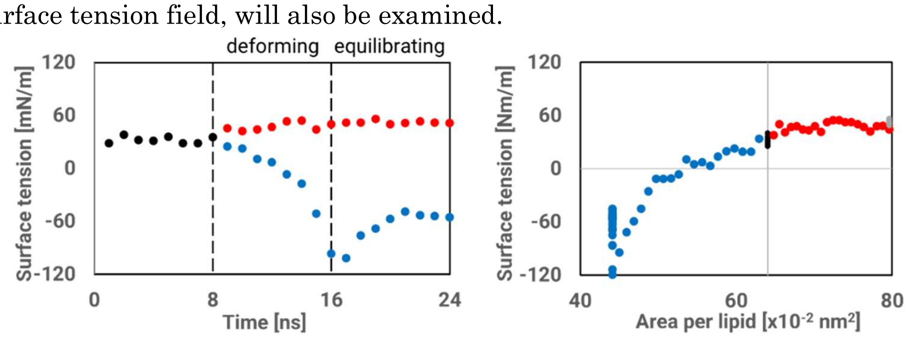

Figure 1: Surface tension versus time (left), and surface tension versus area per lipid (right) of lipid monolayer.

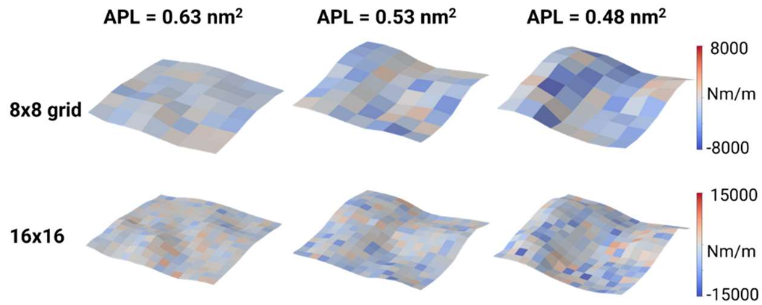

Figure 2: Local surface tension of lipid monolayer of different area per lipid during compressing process.

５． Publications and conference presentations

(1) Journal papers

(2) Presentations

[1] Nguyen, Mabuchi & Kanagawa: Calculation of Surface Tension Field of Lipid Monolayer under High Strain Rate, 22nd International Conference on Flow Dynamics ICFD2025, Sendai, (2025), CRF-71.

[2] Nguyen, Mabuchi & Kanagawa: Molecular Dynamics study on surface tension model for phospholipid coated (micro)bubble ultrasound contrast agents, 第 12 回混相流国際会議 ICMF2025, Toulouse, (2025), ID: 340.

[3] Nguyen, Mabuchi, Takeishi & Kanagawa: 医療用気泡を覆う脂質単分子膜の力学挙動の考察：変分法に基づく膜の数理モデルと分子動力学計算, 混相流シンポジウム 2025, 神戸, (2025), SS0505.

[4] Nguyen, Takeishi, Mabuchi & Kanagawa: MHz 帯で振動する脂質単分子膜の理論解析と分子動力学計算, 第 36 回バイオフロンティア講演会, 弘前, (2025), 2A03.

[5] Nguyen, Takeishi, Kanagawa: Dynamics of lipid monolayer coating microbubbles for ultrasound medicine, 超音波研究会（US）, 仙台, (2025).

(3) Others

Supercomputer	Use	Allocated resources*		
		Initial resources	Transferred resources**	Purchased resources
Pegasus	Yes	14400		
Miyabi-G	Yes	32400		
Miyabi-C	No			
	*in units of node-hour product ** If the budget transfer was performed, fill in here, such as "+2000" and "−1000".			