Liquid Metal Bubble Synthesis and Simulation of Thin 2D Nitride Materials

Jacob Ahmed[1], Jiayun Liang[2], Sara C. Susanto[2], Zakaria Y. Al Balushi[2]
[1]College of Alameda, Alameda CA
[2]Department of Materials Science and Engineering, University of California, Berkeley CA
Contact: jacobahmedd@berkeley.edu (510-372-4770)

Berkeley UNIVERSITY OF CALIFORNIA — TRANSFER-TO-EXCELLENCE PROGRAM

E3S — COLLEGE OF ALAMEDA

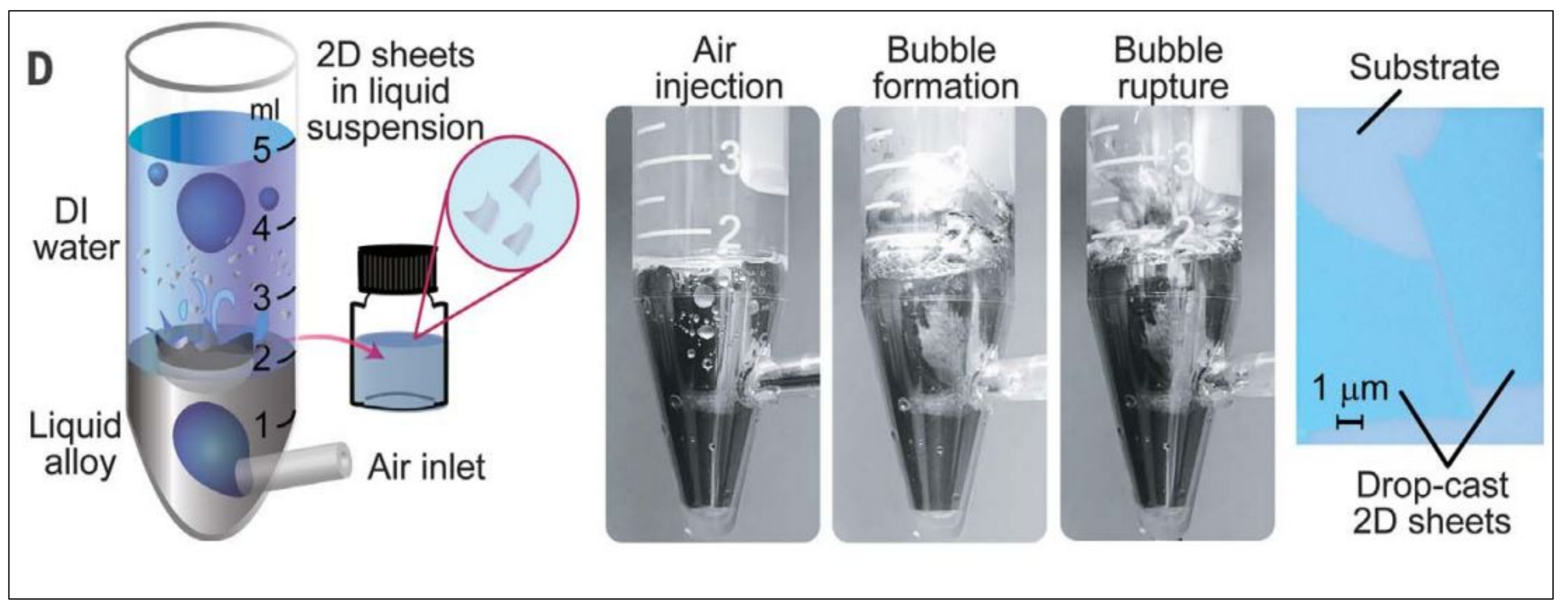
2021 Transfer-to-Excellence Research Experiences for Undergraduates Program (TTE REU Program)

ABSTRACT - Two-dimensional (2D) materials, group-III nitrides are versatile, however, their synthesis using current approaches is difficult. In this project, we approach their novel synthesis via a three-phase bubbling process through liquid metal as the synthesis medium. Using a finite element simulation program, COMSOL Multiphysics, we developed and understood the physics and Cahn-Hilliard/Navier-Stokes equations behind three-phase flow models. This can be used to analyze and provide theoretical guidance to how radius, temperature, and velocity can affect bubble shape and time for burst. Our final goal is to harvest 2D Gallium Nitride (GaN) and apply them onto various energy harvesting applications.

Background

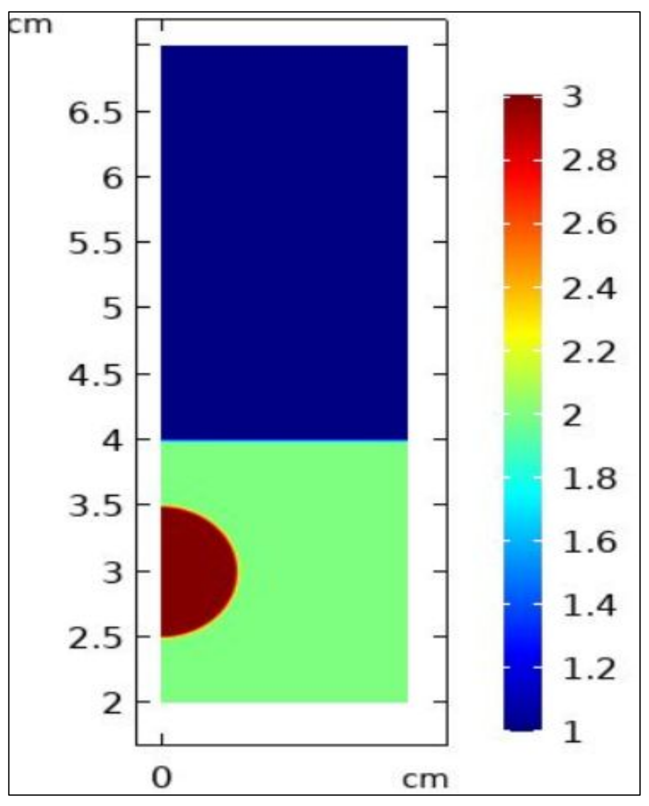
Experimental - Inject nitrogen gas into liquid gallium. Bubbles react with the liquid Ga to create GaN film inside the bubble. Bubble pops in the suspension fluid above (water)

Fig. 1. The inspiration behind our project provided by [1]



Simulation - Replicated the physical experimental apparatus and implemented initial values. By changing the parameters and initial values, such as velocity, radius, temperature, of the simulation, we can then study the experiment.

Fig. 2. To the right is the geometric setup before simulation begins.
- Phase 3 - Nitrogen gas
- Phase 2 - Liquid Gallium
- Phase 1 - Water



Methods

Physical Experiment -
- Beaker with water, along with aluminum disks, placed on hot plate (30-50ºC).
- Bubbler filled with liquid Ga to 3-6cm above gas inlet
- Solution is placed 5-8cm above liquid Ga
- Mass flow rate of nitrogen gas is 5-10sccm
- Microwave generator used to flow nitrogen gas into liquid Ga for 5 min
- Samples are deposited on silicon substrates, allowed to evaporate

COMSOL Finite Element Modeling -
- Set up model correctly, mirroring physical apparatus
- Introduce varying parameters and variables such as velocity, radius, pressure, and temperature
- Run models

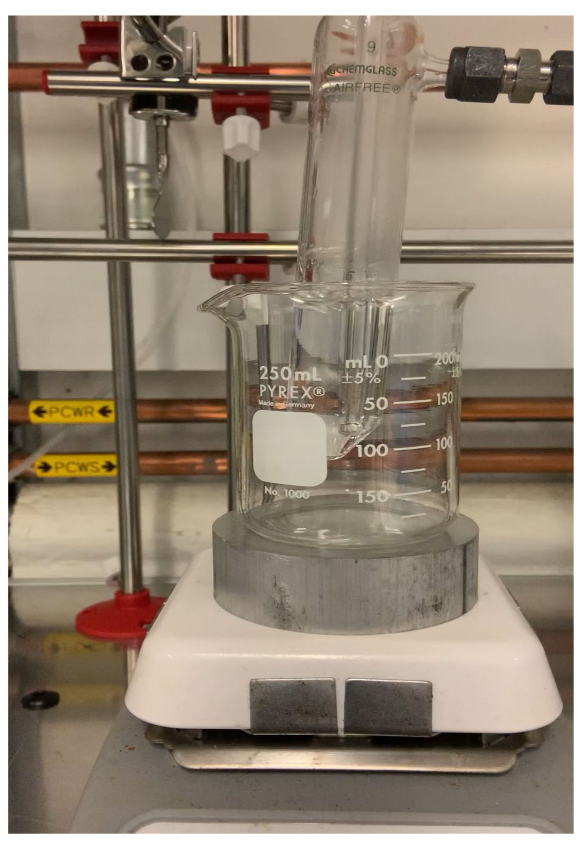


Fig. 3. The physical experiment apparatus. The photo was provided by my Senior Colleague Sara Susanto.

Results and Final Discussions

Reynolds and Eötvös Numbers
- The Reynolds number (Re) is the ratio of interior forces to viscous forces within a fluid
- The Eötvös number (Eo) is the ratio of gravitational forces to surface tension forces.

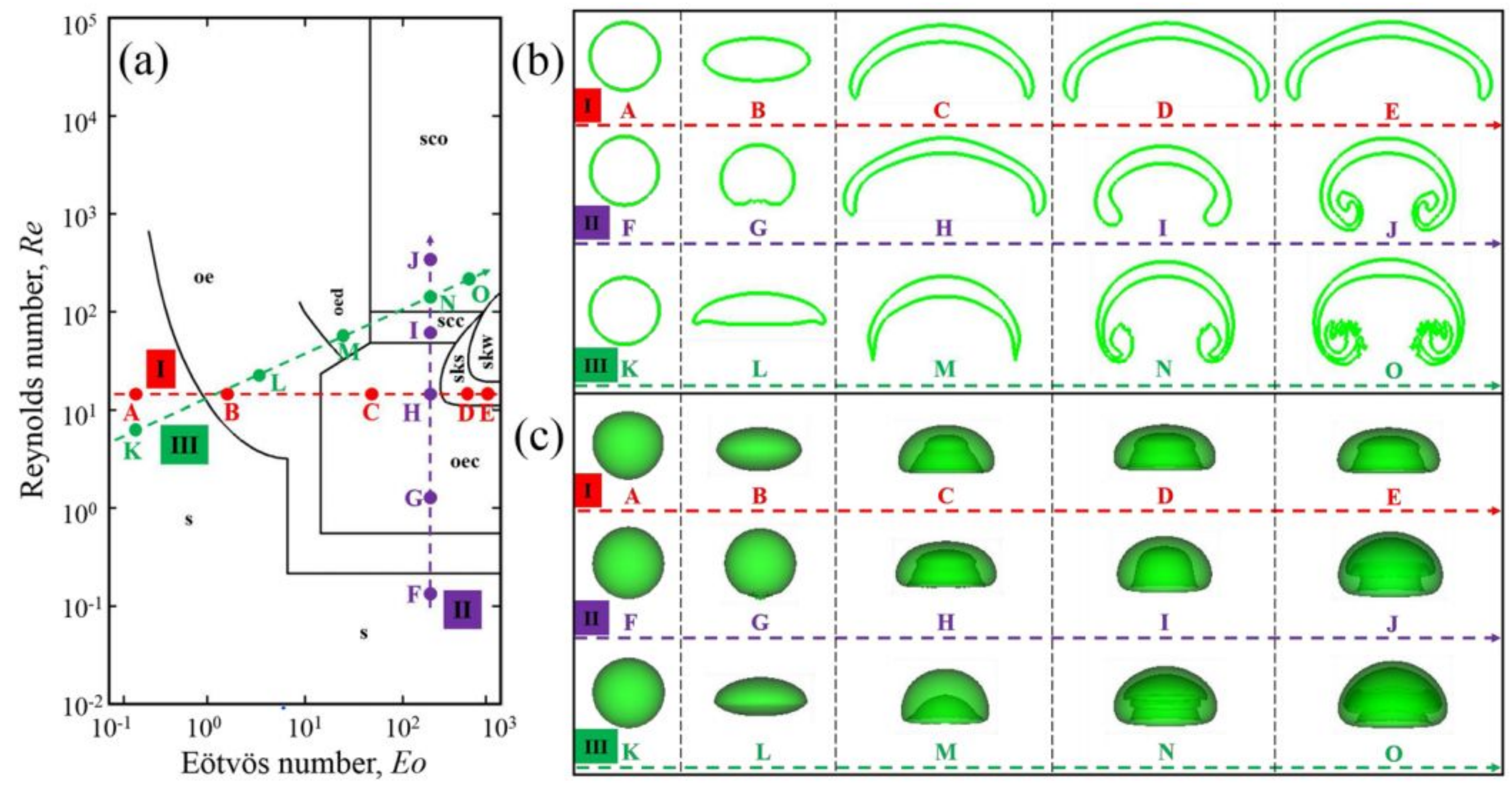


Fig. 4. Regime map of observed bubble shapes in a liquid [2]. S, Spherical; OE, oblate ellipsoid; OED, oblate ellipsoidal (disk-like and wobbling); OEC, Oblate ellipsoidal cap; SCC, Spherical cap with closed, steady wake; SCO, spherical cap with open, unsteady wake; SKS, skirted with smooth, steady skirt; SKW, skirted with wavy, unsteady skirt.

Analysis - Looking at Fig. 4., a bubble with a radius of 0.3cm, Re and Eo values of [4.335*10^3] and [2.976*10^0] respectively, would have a shape similar to B, an oblate ellipsoid. Looking at Fig. 5, it is evident that our model replicates the predicted behaviors of rising bubble shape, according to [1].

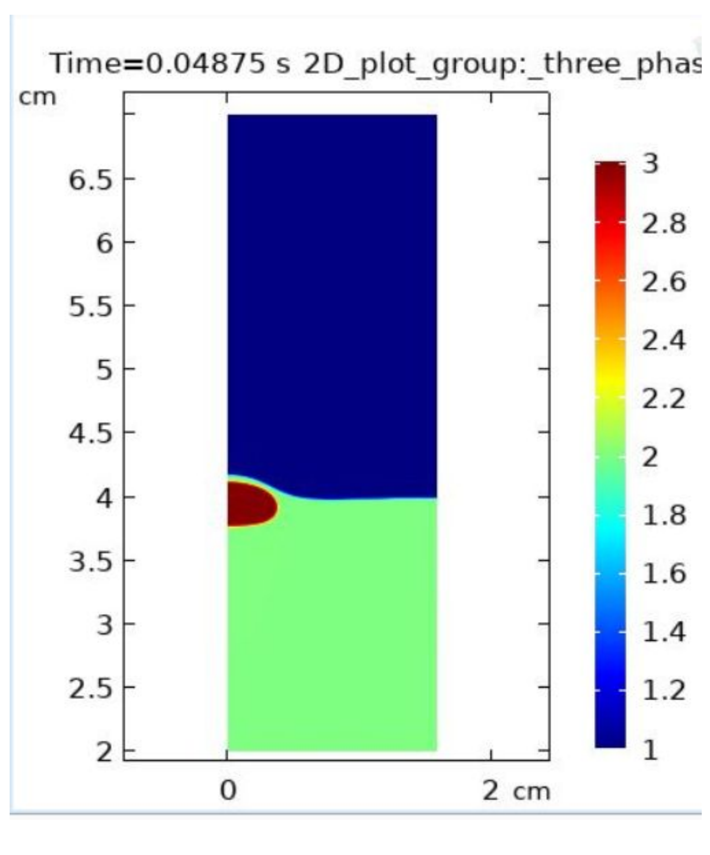
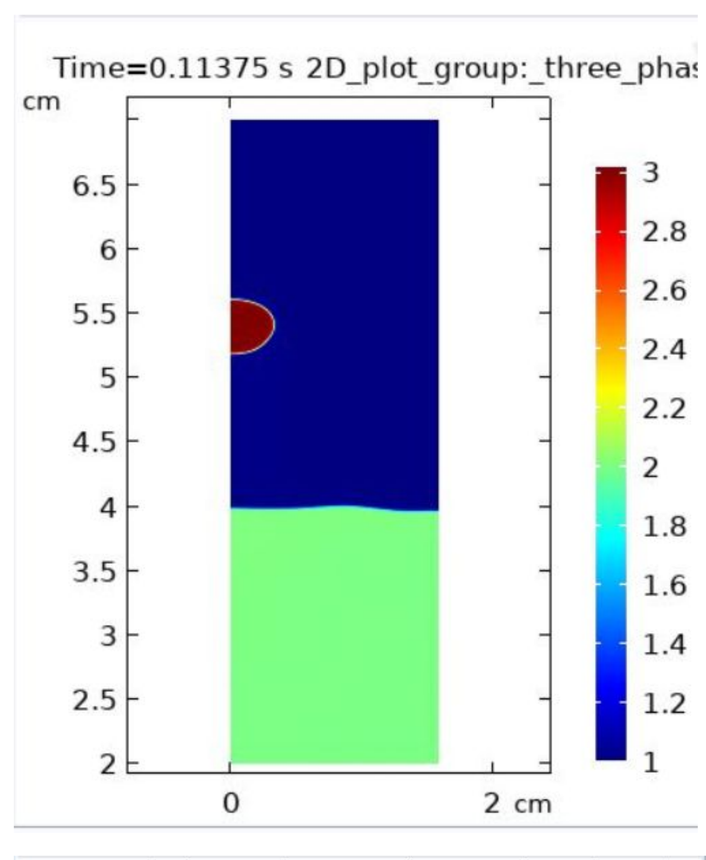


Fig. 5. Two instances of a rising bubble with an initial radius of 0.3cm.



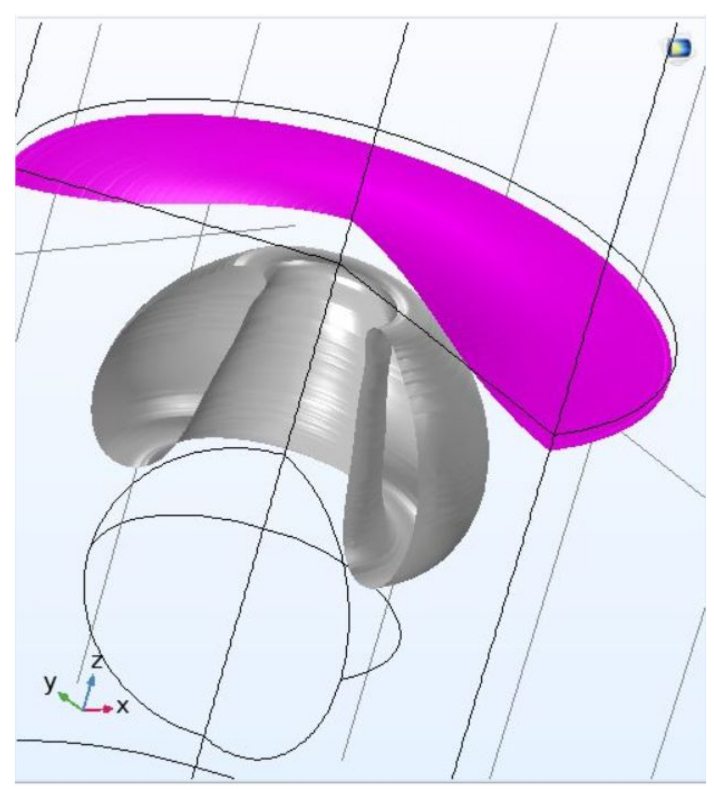
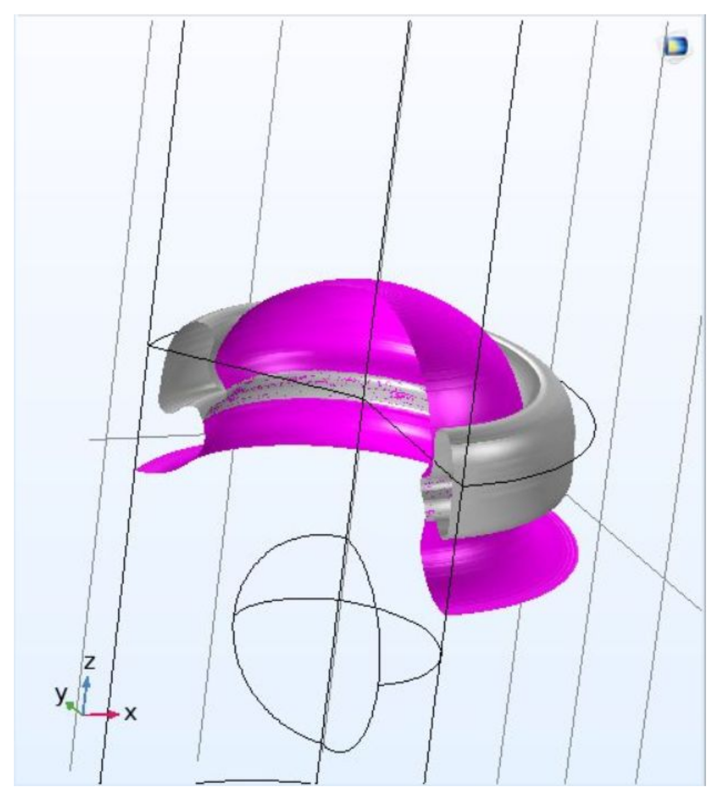


Fig. 6. A toroidal bubble forms from an initial radius of 1.5cm. Larger bubbles with larger Re and Eo values are split by a liquid jet due to a volumetric buoyancy force. The pink coloring represents the water-liquid gallium interface.



Conclusion - Here, we can deduce that larger bubbles will have more issues in the shapes it takes during its ascension, and that our focus should be directed towards working with smaller bubbles since their stability is more apparent.

References, Acknowledgments, & Support Information

[1] A. Zavabeti, J. Z. Ou, B. J. Carey, et al., "A liquid metal reaction environment for the room-temperature synthesis of atomically thin metal oxides," Science, vol. 358, no. 6361, pp. 332-335, Oct. 2017. Accessed on: June 15, 2021. [Online]. Available doi: 10.1126/science.aao4249

[2] A.Zhang, Z.Guo, Q. Wang, et al., "Three-dimensional numerical simulation of bubble rising in viscous liquids: A conservative phase-field lattice-Boltzmann study," Physics of Fluids, vol. 31, no. 6, pp. 1-19, June 2019. Accessed on: July 22, 2021. [Online]. Available doi: 10.1063/1.5096390

This work is funded by the National Science Foundation REU Site Grant: "Propelling California Community College Students through Engineering Research and Sustained Online Mentoring" (NSF Award 1757690) and supported by the Transfer-to-Excellence Summer Research Program at the University of California, Berkeley. This wouldn't have been possible without my Professor Zakaria Y. Al Balushi, Mentor Jiayun Liang, Senior Colleague Sara Susanto, Manager Nicole McIntyre and her Assistants, Tony Vo Hoang and Sam Mountain.

NSF