Capstone Laboratory Projects on the Numerical Study of the Instability of Miscible and Immiscible Thin Fluid Layers on Substrates

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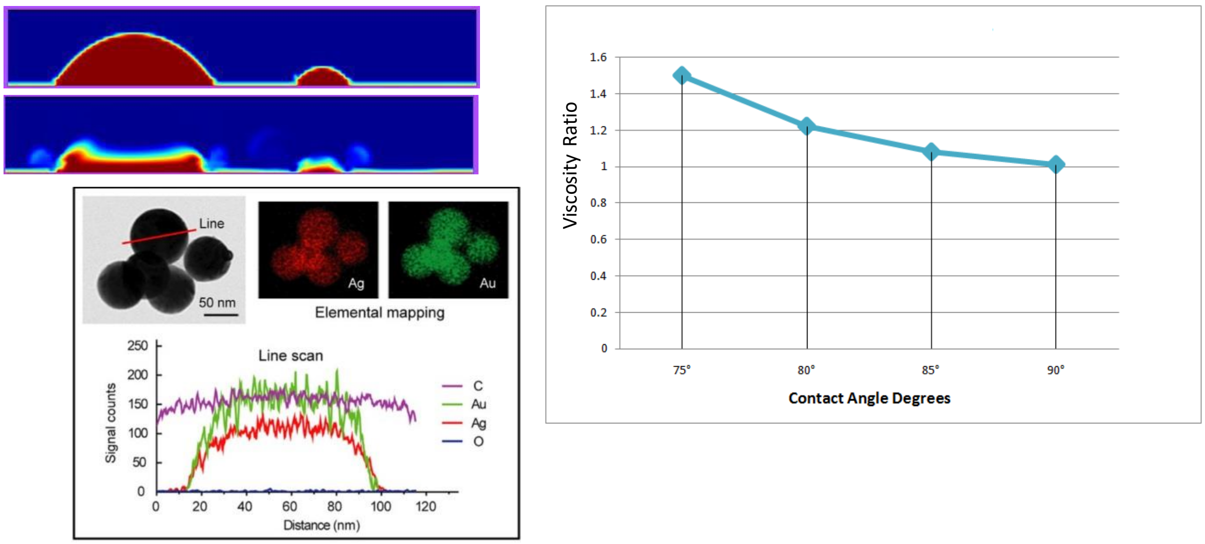
This capstone project involves the study of the fluid dynamical problem of thin bilayer films. There has been a recent experimental study on the Ag-Au bimetallic nanoparticles produced by the laser dewetting of Ag/Au bilayer films on a substrate. The aim of this activity here is to develop a physical understanding of final properties of bimetallic systems, and to enhance the knowledge of the structure and morphology of the nanoparticles. Of particular focus of this study here is to analyze the differences in the composition and the final size distribution of the nanoparticles using direct numerical simulations. While there are many parameters involve in the problem setting, here we only focus on changing the relative thickness of each layer, changing the relative viscosity of each layer, as well as relative viscosity of the surrounding, and finally varying the equilibrium contact angle.

Numerical study of the instability of miscible and immiscible thin fluid layers on substrates: This part involves a numerical study of the evolution of thin layers of miscible liquids, in contact with the immiscible surrounding fluid, toward equilibrium shapes. The understanding of competing forces for such systems is currently poor. This study aims at unraveling such mechanisms using direct numerical simulations. The final goal is to study the structural evolution and final morphology of nanometric bilayers consisted of miscible liquids. This findings will help us understand how to control the synthesis of alloy metallic nanoparticles. The specific goal is to study the fluids dewetting process when there are two layers of various thicknesses, with different viscosity components, and see the how changing these properties may affect the profile of the fluid as it dewets. We have implemented our state-of-the-art numerical framework that solves the full Navier–Stokes equations and tracks the interface based on the Volume-of-Fluid method, to study the compositional structure of thin bilayer films. Our preliminary numerical results reveal some novel and controllable mechanisms of the dynamics of bilayer thin films, that are unstable due to the presence of destabilizing van der Waals forces. Specifically:

- In the absence of a second layer, the instability of the thin film follows closely the predictions of the linear stability analysis.
- By making the second (bottom) layer slightly more viscous than the top layer, while the bilayer still remains unstable, the nonlinear instability leads to the formation of a secondary droplet, suggesting that even a small spatial variation of the viscosity can significantly alter the instability characteristic length scales (see Fig. 1(a)).
- For moderate thicknesses of the bottom layers, the formation of the secondary droplet is independent of the thickness ratio.
- There appears to be a correlation between the viscosity ratio and contact angle defining the threshold for the formation of a secondary droplet (see Fig. 1(c)).

We will perform further numerical simulations to reach definite answers in particular regarding the above findings when comparing various film lengths, layer sequence, and the surrounding viscosity. We have also achieved some very interesting results regarding the compositional structure of the bilayer system. Our preliminary numerical results reveal that the obtained final droplets have a composition of the two layers over the whole volume of the droplets (see Fig. 1(a) bottom panel), showing qualitatively similar distribution illustrated by the experimental results from [Applied Surface Science 434 (2018) 1293–1299].



(c)

(b)

Figure 1: (a) Final drop formation as a results of the instability of a bilayer liquid film; the bottom layer is only slightly more viscous than the top layer. The top panel show the whole droplet, as well as the secondary droplet, and the bottom panel shows the compositional structure of the final drop distribution. (b) Experimental results from [Applied Surface Science 434 (2018) 1293–1299], showing similar findings regarding the drop formation of an Ag 5 nm/Au 5 nm film observed after irradiation by a single pulse laser. (c) The threshold for the formation of the secondary droplet (symbols), showing the viscosity ratio of the bottom layer to the top layer as a function of the contact angle.

Future Work

To numerically illustrate the fabrication of particles with varying com- positional distribution. We will continue this direction by the involved undergrad students who are currently working on the project. This re- search direction is expected to lead soon to a preparation of a manuscript.