

DEFORMING FREE SURFACE OF SOLUTION DRIED ON A SUBSTRATE WITH CIRCLE-PATTERNED BANK STRUCTURE: NUMERICAL STUDY

J. FUKAI¹, J. WANG¹ and S. HIRONAKA¹

¹Kyushu University, Fukuoka, JAPAN

Email: jfukai@chem-eng.kyushu-u.ac.jp

A mathematical model describing drying behavior of a solution droplet deposited on a flat surface was proposed to predict the morphology of the formed solid film. The model includes the fluid dynamics, heat transfer, and mass transfer, and also considers wettability of the substrate and deformation of the free surface [1].

This model is applied into the system where a solution dries on a substrate with circle-patterned bank structure (Figure 1). The radius (a) and height (b) of a hollow cylinder are $2.25 \mu\text{m}$ and $45 \mu\text{m}$, respectively. N, N'-bis(3-methylphenyl)-N, N'-bis(phenyl)-benzidine (TPD) is chosen as a typical organic semiconductor. Anisole is chosen as solvent. Initial mass fraction of solute is 0.02. Contact angle (Ψ_c) is assumed to be 60° .

The effect of solutal Marangoni forces on drying behavior is mainly discussed. Figure 2 shows time variation of liquid frame. R and Z are defined as r/a and z/a , respectively. Dashed lines represent the results for the case where Marangoni forces are neglected. The free surface keeps a near-spherical cap during drying. The center of the free surface reaches near the bottom of substrate when the droplet volume decreases to 50% of the initial volume (i.e. $V/V_0=0.5$). On the other hand, solid lines represent the results where Marangoni forces are considered. At $V/V_0 < 0.6$, Marangoni flows near the meniscus largely deform the whole of the free surface. The deformation develops the effective convective flows to transfer the solute mass as shown in Figure 3, which depicts the time variation of area density profile of solute. It is found that the shape of density profile at $V/V_0 = 0.2$ is similar to the experimental morphology of the solid film formed under the same condition [2].

Consequently, the present calculations reveal that solutal Marangoni flows play an important role in formation of solid film.

REFERENCES:

1. Fukai J., Harada T. and Ishizuka H. 'A new mechanism of coffee-ring formation deduced from numerical simulations with considering deformation and wettability' *J. Chem. Eng. Jpn.*, accepted
2. Sakanoue K., Harada H., Ando K., Yahiro M. and Fukai J. 'Surface planarization effect of siloxane derivatives in organic semiconductor layers' *Thin Solid Films*, **2015**, 212-219

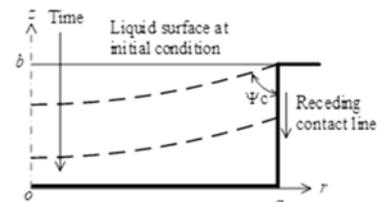


Figure 1 Computational domain

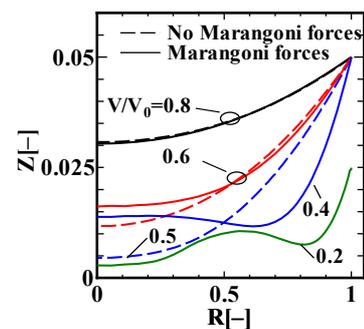


Figure 2 Change in free surface profile with time

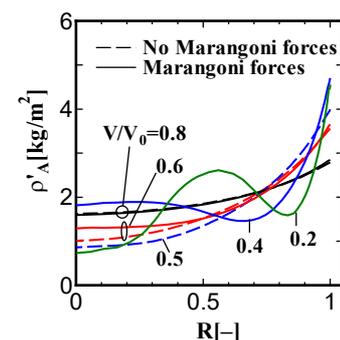


Figure 3 Change in area density profile with time