NUS National University of Singapore
Department of Mathematics
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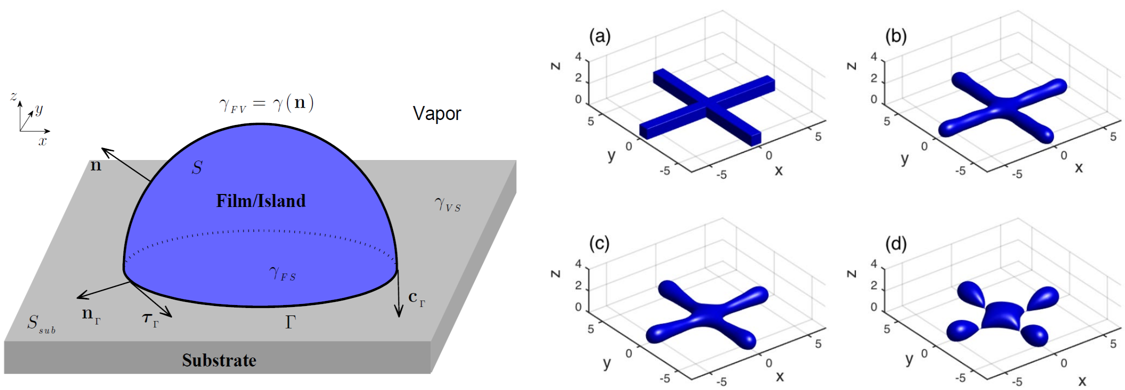
Research Highlight:
Modelling and Simulation for Solid-State Dewetting in Materials Science

Work of Professor BAO Weizhu

Solid-state dewetting is a ubiquitous phenomenon in thin film technologies since solid films are energetically unstable in the as-deposited state, and tend to dewet and form islands when heated to sufficiently high temperatures. The process is driven by surface and interface energy minimization and can occur via surface diffusion together with contact line migration. This phenomenon can either be deleterious, destabilizing a thin film structure, or advantageous, leading to the controlled formation of an array of nanoscale particles, e.g., used in sensor devices and microelectronic processing, catalysts for the growth of carbon nanotubes and semiconductor nanowires.

By adapting the thermodynamic variation method, Prof BAO Weizhu and his collaborators systematically derived sharp interface models for solid-state dewetting with isotropic/weakly anisotropic and strongly anisotropic surface energies in two dimensions and three dimensions [1, 2, 3]. In addition, a parametric finite element method (PFEM) [1, 4, 5] was proposed to solve the sharp interface models numerically, which is semi-implicit, energy-stable, efficient and accurate. Extensive numerical simulation results have been carried out to verify the sharp interface model and to demonstrate the efficiency and accuracy of the PFEM. Numerical results from the sharp interface model agree qualitatively with experimental results. The future goal is to investigate different experimental setups and to guide new experiments.



An illustration (left) and several snapshots in the evolution of an initially cross-shaped island (right) of solid-state dewetting of thin films on a flat substrate in three dimensions.

Reference:

[1] Q. Zhao, W. Jiang and W. Bao, A parametric finite element method for solid-state dewetting problems in three dimensions, SIAM J. Sci. Comput., 42 (2020), B327-B352.
[2] W. Jiang, Q. Zhao and W. Bao, Sharp-interface model for simulating solid-state dewetting in three dimensions, SIAM J. Appl. Math., 80 (2020), 1654-1677.
[3] W. Bao, W. Jiang, D. J. Srolovitz and Y. Wang, Stable equilibria of anisotropic particles on substrates: a generalized Winterbottom construction, SIAM J. Appl. Math., 77 (2017), 2093-2118.
[4] W. Bao, W. Jiang, Y. Wang and Q. Zhao, A parametric finite element method for solid-state dewetting problems with anisotropic surface energies, J. Comput. Phys., 330 (2017), 380-400.
[5] Q. Zhao, W. Jiang and W. Bao, An energy-stable parametric finite element method for simulating solid-state dewetting, IMA J. Numer. Anal., to appear (arXiv: 2003.01677).