Molecular dynamics simulation of dewetting of ultra-thin liquid film with artificial dry patches SUSUMU KONO, ICHIRO UENO, Department of Mechanical Engineering, Faculty of Science and Technology, Tokyo University of Science — Large scale molecular dynamics simulations of dewetting of ultra-thin liquid films on a solid substrate are carried out. In case of thin film of nanometer-scale thickness, the liquid film is ruptured spontaneously which is called spinodal decomposition. The instability generates the dry patches in the film. The dewetting process begins from the several dry patches. Finally, the liquid film varies to droplets on the substrate. In the present study, we focus on the dry patch distribution in the liquid film, and investigate the depending of the initial distribution of the dry patches on the final stage of the nanometer-scale droplet formation. First, the liquid film composed by LJ fluids covered solid substrate with the preset dry patches. Then the dewetting behavior based on the artificial dry patches distribution is observed. As a result, it is found that there exists a sharp threshold of the initial radius of the artificial patch to realize the spontaneous rupture. This threshold depends on the initial film thickness, contact line curvature and LJ liquid-solid parameter. In comparing with usual dry patches distribution due to spinodal decomposition to artificial one, the final droplets formation also depends on initial dry patches distribution.

1Research Institute for Science and Technology (RIST), Tokyo University of Science

Susumu Kono
Dept of Mechanical Engineering, Faculty of Science and Technology,
Tokyo University of Science

Date submitted: 02 Aug 2013

Electronic form version 1.4