Detrimental Nanoscale Gas Defects in Manufacturing-Based Nanoimprint Processes

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One of the main goals in today's nanoimprint lithography (NIL) research is to develop the processing approaches that can improve the performance and yield of NIL systems, therefore making NIL suitable for manufacturing commercially viable device products. Among various NIL methods, UV-curable nanoimprint lithography (UV-NIL) based on in-situ liquid resist dispense has been adopted as an important candidate manufacturing technology for patterning functional nanostructures over large areas [1]. However, the current UV-NIL processes still suffer seriously from gas bubble defects, which have significantly hindered the industrial applications associated with mass production [2, 3]. Several previous works identified the formation mechanisms of microscale bubble defects and sought to establish the routes for eliminating such microscale bubbles through the gas dissolution into liquid resist [2-4]. However, these previous works cannot provide a solid scientific explanation for the experimentally observed long-term retention of nanoscale gas bubble defects in UV-NIL resists and the insolubility of such nanoscale bubbles in liquid resists.

Here, we present a nanoscale computational fluidic dynamics (CFD) study on the formation and evolution mechanisms of nanoscale gas defects in liquid resists. This study indicates that the formation of detrimental nanoscale gas defects is attributed to the pinning of resist spreading edges at the topographical nanostructures/nanoparticles or flat contaminants on the mold/substrate surfaces. Such pinning-induced nanoscale gas defects, after formation, undergo an evolution process governed by the net effects of the edge pinning and the gas dissolution (or molecular diffusion) into the liquid resist. Such an evolution of nanoscale gas defects results in a prominent drop of the gauge pressure inside the defects and therefore a significant reduction of the gas dissolution rate. Such a nanofluidic mechanism can explain the long-term retention of nanoscale gas bubble defects in UV-NIL resists. In addition, this work also implies that electric field pulses applied in the liquid resist could effectively release the pinned gas bubbles from the pinning sites and ultimately eliminate such nanoscale gas defects.

Fig. 1 (a) displays the SEM images of representative nanoscale gas bubble defects formed in imprinted resist films. Even in a resist layer pressed by a flat mold without topographic nanostructures, similar nanoscale defects can be still formed (**Fig. 1 (b)**). All such nanoscale gas bubble defects feature a shallow hemispherical shape. **Fig. 2** displays the time-dependent simulation (2D cross-sectional view) result of the profile evolution of a nanoscale gas defect pinned at a contaminant area on the mold. Due to the pinning effect, the defect finally relaxes to a hemispherical shape with significantly reduced Laplace pressure, which is highly consistent with the SEM-observed profile of typical real nanoscale gas defects in the cured resist, as shown in **Fig. 1 (b)**. Our simulation work further implies that electric field pulses applied in the liquid resist (before curing) could generate electrohydrodynamic forces acting on the interfaces between gas defects and pinning sites, capable of releasing the gas defects back to the resist, as shown in **Fig. 3**. Once released, the gas defects are expected to have a significantly enhanced Laplace pressure, leading to a quick dissolution of the gas defects into the liquid resist.

This nanofluidic simulation work identifies the scientific mechanisms responsible for the formation of detrimental nanoscale gas defects in NIL processes and provides important insights for the ultimate elimination of such defects.

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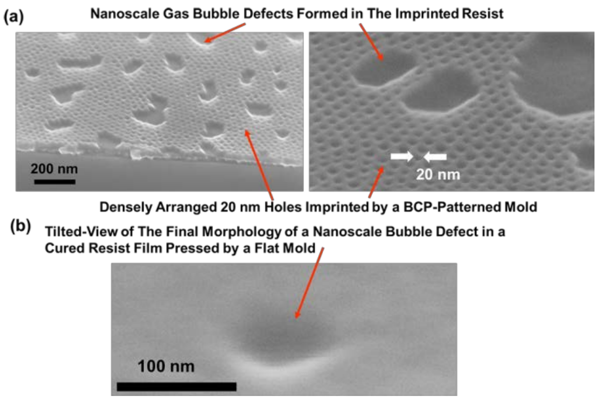

Fig. 1 SEMs of (a) nanoscale gas defects in a cured resist film (here, the densely arranged 20 nm holes are desirable structures imprinted by a block-copolymer mold and (b) tilted view of the final profile of a nanoscale gas bubble defect. All such nanoscale gas bubble defects feature a shallow hemispherical shape.

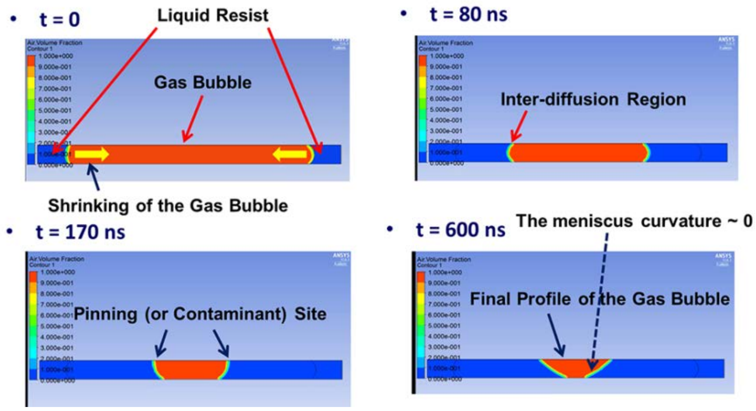

Fig. 2 Time-dependent simulation (2D cross-sectional view) of the profile evolution of a gas bubble defect pinned at a contaminant region on the mold.

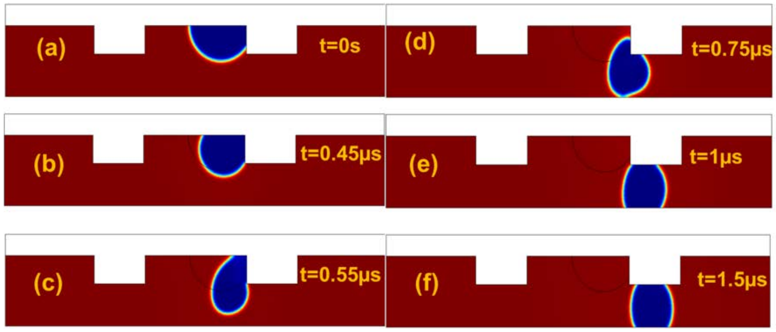

Fig. 3 Time-dependent simulation of the kinetic evolution of a nanoscale gas defect that is initially pinned at topographical nanostructures (before resist curing) and subsequently subjected to an electric field pulse. Such an electric field pulse could result in the release of the gas defect from the pinning site and effectively eliminate the defect.

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