Molecular dynamics study on fracture of Si mold in nanoimprint for glass film

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In nanoimprint lithography (NIL), the mold patterns are frequently suffered from damages during the repeating pattern transfers. The defects in the mold cause a serious problem in mass production of the devices using NIL. Figure 1 shows a scanning electron micrograph of typical damage in Si mold after several imprints. The Si mold fractures along {111} planes.

The advantage of the molecular dynamics (MD) analysis is to investigate the behavior of the materials in atomic level in NIL. Recently, several MD simulations of NIL have been investigated.[1,2]

To elucidate the fracture mechanism of the mold during NIL processes, a comprehensive analysis involving three factors should be conducted: mold deformation, resist deformation, and the interaction between them. However, previously reported continuum mechanics and molecular dynamics simulations have neglected the mold deformation. At present, few researchers have performed comprehensive analyses of NIL processes. In this study, we newly developed a simulation system for the comprehensive analysis of NIL including mold deformation.

The simulation model for the nanoimprinting process includes a single-crystal silicon mold and a glass film. Figure 2 shows cross-sectional views of MD simulation of NIL process. In this case, a mold has {100} top surface and {110} front face. The pattern is successfully transferred and the mold does not fracture.

Figure 3 shows (a) a cross-sectional view at breaking point and (b) a schematic illustration of configuration of {111} planes in the mold. In this case, a mold has {110} top surface and {110} front face. The mold fractures along a {111} plane in the pressing process. This result agrees with the experiment shown in Fig. 1.

Our simulation result shows the behaviors of the fracture of the mold are strongly associated with the configuration of the {111} planes in the mold.

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1) J. H. Kang, et al., Tribology. Lett. **25**, 93 (2007).
2) K. Tada, et al., Jpn. J. Appl. Phys. **47**, 2320 (2008).

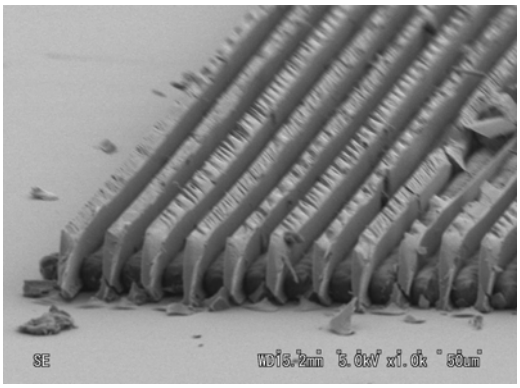

Fig 1: Scanning electron micrograph of typical damage in Si mold after several imprints.

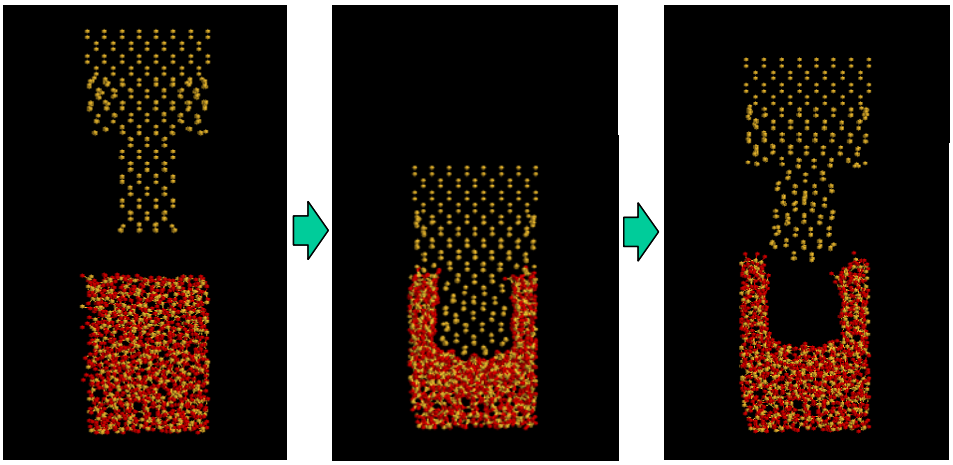

Fig 2: Cross sectional views of MD simulation of NIL process.

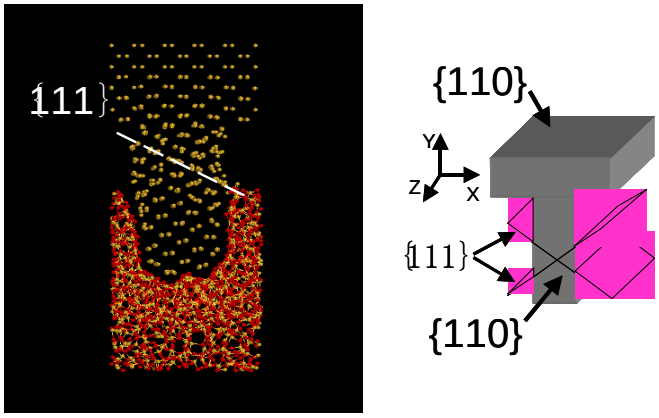

Fig 3: (a) Cross-sectional view at breaking point and (b) schematic illustrations of configuration of {111} planes in the mold.