Atomic step pattering in nanoimprint lithography : Molecular dynamics study

Kazuhiro Tada[1], Masaaki Yasuda[2], Yasuyuki Akita[3], Yumiko Miyake[3], Hiroaki Kawata[2], Mamoru Yoshimoto[3] and Yoshihiko Hirai[2]

[1]Toyama National College of Technology, Toyama 939-8630, Japan

[2]Graduate School of Engineering, Osaka Prefecture University, Osaka 599-8531, Japan

[3]Tokyo Institute of Technology, Yokohama 226-8503, Japan

e-mail address; tada@nc-toyama.ac.jp

Resolution limit of Nanoimprint lithography (NIL) is one of the most impressive interests in both scientific and industrial points of views. Single-nanometre resolution has been demonstrated using polymer material.[1] On the other hand, inorganic materials must have advanced resolution due to fine unit structure.[2] Akita et al. demonstrated atomic step replication of glass material.[3]

In our previous study[4], a theoretical study of resolution in NIL has been carried out based on molecular dynamics (MD) simulation. The ultimate resolution in the glass NIL has been proved to be 0.4 nm for L & S pattern.

In this study, atomic scale formability with nanoimprint atomic stepped mold is investigated through a MD simulation for inorganic SiO_2 glass material.

Figure 1 shows a schematic diagram of the numerical simulation systems. Periodic boundary conditions are applied to horizontal direction. A single-crystal Si mold is pressed into a SiO_2 glass. Born-Mayer-Huggins potential, which includes three-body term[5], is adopted to describe the interactions between atoms in the SiO_2 glass. Morse potential[6] is used to simulate the interfacial behavior between the Si mold and the SiO_2 glass. The Si mold is assumed as a rigid body.

Figure 2 shows snapshots of MD simulation of NIL using atomic stepped mold with w = 2.0 nm and h = 0.6 nm (a) before pressing and (b) after releasing.

Figure 3 shows the Fourier transformation of glass surface pattern (a) before pressing and (b) after releasing using the mold with w =2.0 nm and h = 0.6 nm. Before pressing, the spectrum contains a broad range of frequency components all around. On the other hand, after releasing, low frequency components corresponding to the mold step width 2.0 nm are enhanced.

This transformation shows that atomic step is successfully transferred to glass materials in NIL.

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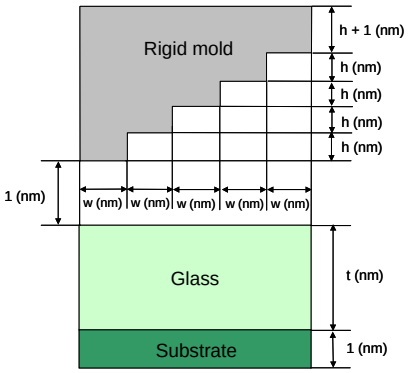

Figure 1: Schematic diagram of numerical simulation systems.

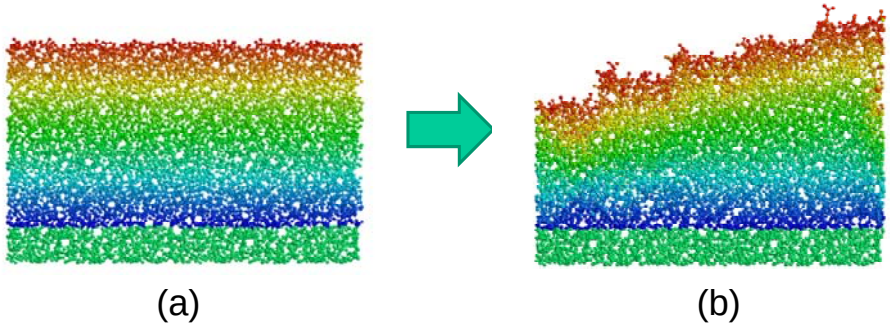

Figure 2: Snapshots of MD simulation of NIL using atomic stepped mold with w = 2.0 nm and h = 0.6 nm (a) before pressing and (b) after releasing.

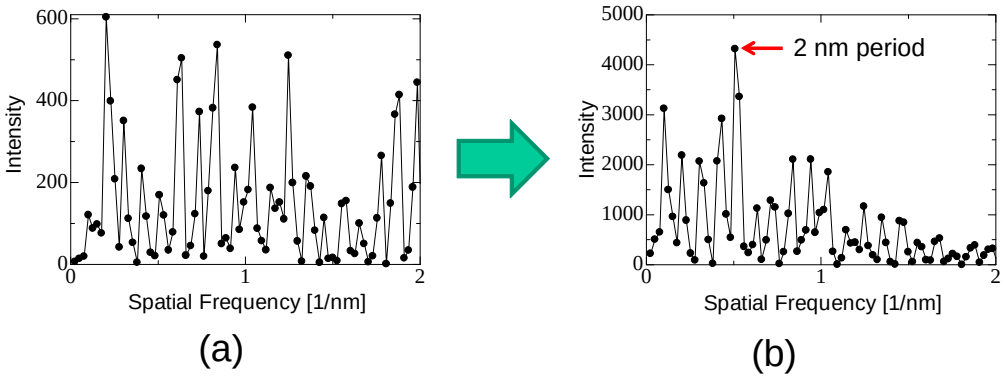

Figure 3: Fourier transformation of glass surface pattern (a) before pressing and (b) after releasing using the mold with w =2.0 nm and h = 0.6 nm.