PROCESS EFFECTS ON NANOIMPRINT LITHOGRAPHY BY MOLECULAR DYNAMICS SIMULATION

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Introduction

Nanoimprint lithography needs high precise instrument to perform the process. By using computer code, a more detail process simulation can be conducted to understand the deformation details of photo resists under varied conditions such as different temperature state, different stamp width to depth ratio, different imprint speed and different adhesion state. Among these computational methods, Molecular Dynamics (MD) becomes an important one. However, it needs suitable computer resources, such as computation scheme, computation speed and random access memory for a several hundreds nanometer scale of nanoimprint lithography process.

Methodology

Molecular Dynamics Modeling

The materials being simulated by MD can be modeled according to the common single crystal structures, such as BCC, FCC, HCP and diamond-like structures. For current study, the stamp fabricated from silicon wafer was modeled according to diamond-like structure. There are five molecules in a chain in the Self-Assembled Monolayer (SAM) for anti-adhesion layer; the first one is CH_2 which is connected onto the surface of silicon stamp, while the end free one is CH_3. The simulation time step is 10^{-15}sec. Several long chains were used to represent $(CH_2)_n$ molecules connected with each other. The Lennard–Jones (LJ) potential energy was used to describe the interaction energy between the molecules in different polymer chains, while the Finitely extensible nonlinear elastic (FENE) potential was used to simulate the interaction energy between two neighbor molecules in the same polymer chain. Bond length stretching energy and bond angle bending energy were used to describe the interaction behaviors between two molecules in the same SAM chain [1]. A polymer chains of $(CH_2)_n$ with FENE potential was nanoimprinted by a stamp with self-assembled monomer (SAM) anti-adhesion layer as shown in Fig. 1. The width and depth of stamp are 18 nm and 9 nm, respectively.

Results and discussion

Effects of Anti-adhesion Layer

Two cases of nanoimprint lithography with process parameters, such as 18nm in stamp width, 0.5 in stamp depth to width ratio, 300K in homogeneous temperature state and 1,000m/s in imprint velocity were studied. The first case is stamp without SAM layer whose result is shown in Fig. 2(a). Due to the sever adhesion behavior between silicon stamp and FENE polymer chains, after withdraw of stamp, the FENE polymer material failed to shape a preferred geometry. The second case is stamp with SAM layer whose result is shown in Fig. 2(b). It's obviously clear to find out that when there are some SAM layers between stamp and FENE, the pattern transformation from stamp to FENE material is successful although formability is not 100% good enough. Figure 3 depicts the load-displacement relation for the above two cases. The needed force to deform FENE material with SAM layer in stamp is larger than that without SAM layer, because in the former case the SAM layer will also deform and it takes some forces to cover this deformation.

Temperature Effects

MD simulations at three different temperatures which are 0K, 300K and 450K were conducted to understand the temperature effects on the nanoimprint lithography process of FENE material when stamp was coated with anti-adhesion layers. Polymer chains of FENE material at 0K was perfectly imprinted after unloading of stamp as shown in Fig. 4(a) since the FENE polymer chains at this temperature behaved no motivation energy. When temperature was increased to 300K, the motivation energy of both the FENE polymer chains and anti-adhesion layers were increased. After unloading, the FENE polymer chains depicted a good cavity and the coated anti-adhesion layers contacted with stamp densely as shown in Fig. 4(b). When temperature was increased to 450K, the motivation energies of both materials were increased largely. After unloading, although the FENE polymer chains depicted a cavity pattern, the cavity and the coated anti-adhesion layers were loose and unstructured as shown in Fig. 4(c).

Imprint Speed Effect

Due to MD computation of FENE materials and anti-adhesion layers involved a lot of particles' interactions the imprint speed of stamp is normally increased to reduce the needed computation time. Therefore, it is interested to know the imprint speed effect on nanoimprint lithography. Three different imprint speeds were first studied, such as 1000m/s, 100m/s and 10m/s; while the other conditions are 3nm of stamp width, 3nm of stamp imprint depth and at 0K. Figure 5(a)~(c) depict the MD simulation results at these three imprint speeds which all show good nanoimprint patterns. However, the spreading patterns of SAM (anti-adhesion) layers are quite different. In high speed, 1000m/s, the SAM layers have high momentums, therefore, they don't deform when imprinting into FENE material, as shown in Fig. 5(a). In low speed, 10m/s, the SAM layers spread into a flat geometry, as shown in Fig. 5(c). In 1000m/s, when stamp contacts with FENE material, the imprint force increased dramatically and when stamp imprinted gradually, the needed force decreased. However, in 100m/s or 10m/s, the trends of load-displacement curves are quite different to case of 1000m/s. The needed forces in both cases increased slowly when stamp imprinted gradually which will reach peak values in the end of loading stage.

Four additional cases with different imprint speeds of MD simulation, such as 700m/s, 600m/s, 400m/s and 200m/s were conducted to find out the marginal speed which can distinguish the trend of load-displacement curve between high imprint speed and low imprint speed. Figure 6 depicts load-displacement curves of these seven cases, it's clear that the marginal speed is 400m/s. In Fig. 6, there is a force peak at stamp travel 5.4nm for imprint speed of 1000m/s, 700m/s, 600m/s, 400m/s. From observing the deformation pattern of SAM layers, in high speed the SAM maintain the former geometry while in low speed the SAM layers spread into a flat geometry.

Conclusions

The nanoimprint processes of polymer chains $(CH_2)_n$ with FENE potential were simulated by consideration of process variable effects. The case of stamp without SAM layer shows sever adhesion behavior. The deformation pattern of polymer chains in low temperature is better than in high temperature. The marginal speed which can distinguish the trend of load-displacement curve from high imprint speed to low imprint speed was also depicted.

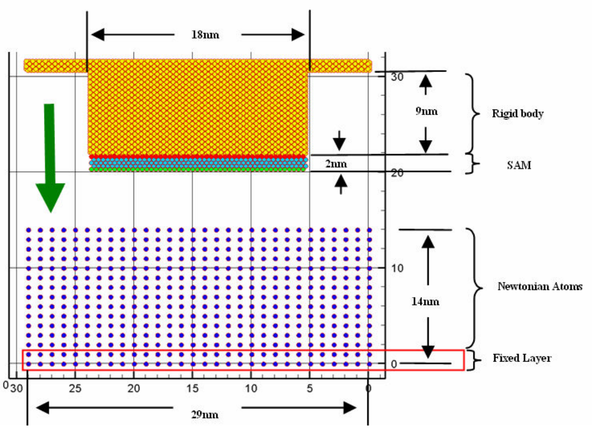
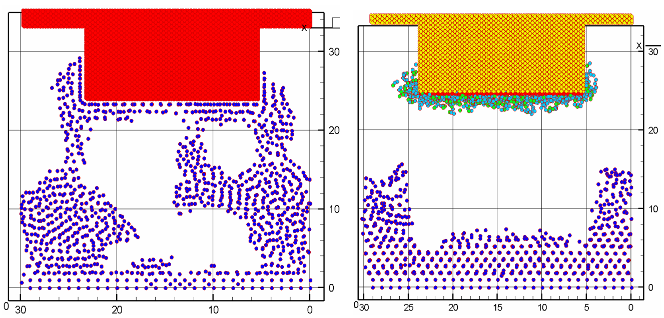


Fig. 1 Molecular dynamics model for nanoimprint lithography.



(a) without SAM (b) with SAM

Fig. 2 Two cases of nanoimprint lithography at 300K and 1,000m/s in imprint velocity.

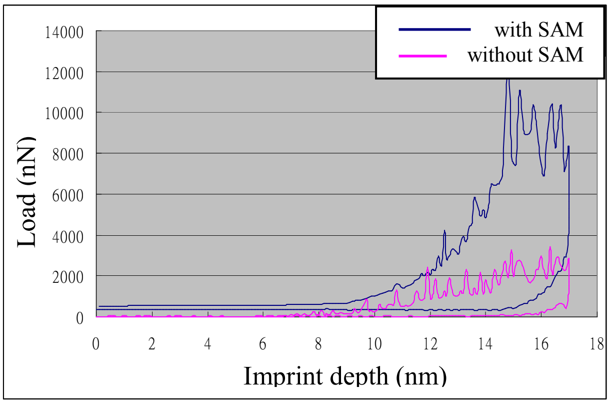
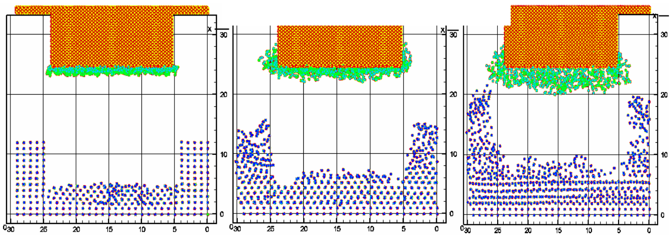
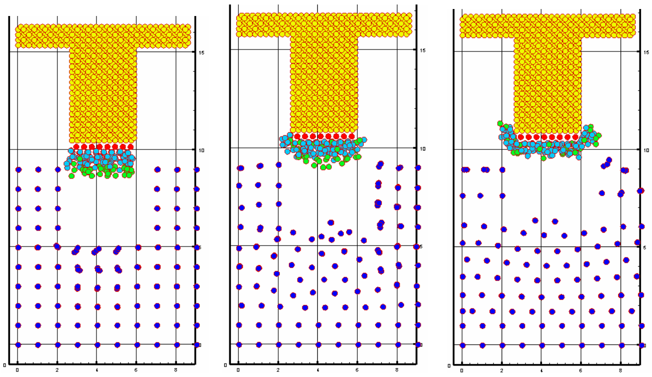


Fig. 3 Load-displacement relation with or with SAM.



(a) 0K (b) 300K (c) 450K

Fig. 4 Three cases of nanoimprint lithography.



(a) 1000m/s (b) 100m/s (c) 10m/s

Fig. 5 Three imprint speeds for cases of 3nm width, 3nm imprint depth, and 0K.

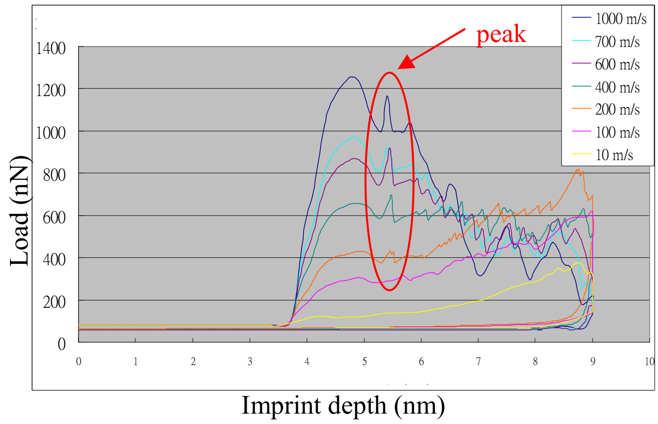


Fig. 6 Imprint speed effects on load-displacement relations for case of 3nm width, 3nm depth, and 0K.

Reference

1. Q. C. Hsu, C. L. Lin and T. H. Fang, 2008, "Study on Nanoimprint Lithography of the Polymer Chains $(CH_2)_n$ with Anti-Adhesion Layer on Stamp by Molecular Dynamics Method," Proceedings of the Sixth International ASME Conference on Nanochannels, Microchannels and Minichannels, 2008/6/23~25, Darmstadt, Germany, Paper No. ICNMM2008-62172.