 ICCES, vol.13, no.2, pp.33-33

An Investigation into Atomic Scale Forming Mechanism and Friction Characteristics in Direct Nanoimprint by Molecular Dynamics Simulation

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Summary

Molecular dynamics (MD) simulation has been demonstrated as a promising method to analyze formation and friction mechanisms of the nanoimprint process. Especially, it provides a useful tool for investigating critical issues that are generally difficult to be examined by the experiment because of cross talks among influential factors or attainability of direct measurement. This study utilized the friction mechanism to explore the factors that would affect the quality of mold replication in the direct nanoimprint. Those factors included mechanical properties of thin films, interaction force between mold and thin-film materials, and surface roughness of the mold, etc. First, we set up the simulation model for various linewidth-to-pitch ratios of the mold as well as for different film thicknesses. The imprinting and friction forces during imprinting and demolding stages were calculated, respectively, to analyze the relations between the factors and forming results. Furthermore, because of the dissimilar cohesion energy between the mold and the thin film, which would make apparent difference in adhesion behavior after demolding, silicon and nickel molds were both constructed to examine how they would affect the forming properties of the aluminum thin film. Finally, since the material properties, surface roughness of the mold, springback phenomena and the deformed region pulled up by the friction force would affect the imprinting process, we proposed the formation height as an index for qualitatively evaluating the quality of formation affected by these factors in the nanoimprint simulation in an attempt to achieve better pattern transfer.

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