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Molecular dynamics simulation and experimental investigation of the geometrical morphology development of injection-molded nanopillars on polymethylmethacrylate surface

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ABSTRACT

Injection molding is one of the most promising techniques to fabricate polymeric parts with functional surface nanostructures in large numbers. The replication fidelity of nanostructures directly affects their efficiency. In this study, molecular dynamics (MD) simulation and experimental trial for injection molding nanopillars on polymethylmethacrylate (PMMA) surface were constructed in both injection and packing phases. The filling process was investigated by analyzing the snapshots, densities and gyration radiuses. Influences of packing parameters on geometrical morphology were studied. Results showed that the central area of nanopillars was almost voided during the injection phase and polymer melt could barely flow into nano-cavity. Only the edge area was filled in injection phase and circular structure was observed on the top surface in the experiments. Complete filling was mainly achieved in packing phase. PMMA molecules were stretched along the sidewall and gradually enriched due to the nonbonded interactions. Molecules near the cavity surface were highly oriented along the flow direction. The circular structures were increasingly obscure with a higher packing. PMMA melt was adsorbed on cavity surface because of the lyophilicity of nickel mold insert. Experimental study provided consistent regulation with MD simulation in geometrical morphology development of injection-molded nanopillars on PMMA surface.

1. Introduction

Products with surface nanostructures have a wide application in the field of surface Raman spectroscopy [1], high efficient solar cell [2], super hydrophobicity or self-clean surface [3], and lab-on-chip device [4]. It is undoubted that there will definitely be a huge market potential to commercialize the idea of preparing surface micro/nano-structure in mass production. Polymer material is one of the most widely used materials for its advantage on relatively low price, excellent compatibility, easy handling and processing with special feature. Polymethylmethacrylate (PMMA), sometimes called acrylic glass, is a commonly used polymer material and is an economical alternative with good mechanical strength and moderate properties. Currently, there are generally two kinds of methods in preparing surface nanostructures, bottom-up and top-down technology. For polymer materials, nanomolding technology is an effective choice that belongs to the top-down method. Polymeric surface nanostructures can be manufactured by nano-imprint lithography, injection molding and hot embossing [5–7]. Among these, micro injection molding technology is regarded as one of the cost-effective technologies to produce polymer items in large numbers. Sub-micrometer structures or even surface structures in nanometer scale have been successfully fabricated by injection molding [8–11].

Injection molding technology is used to produce polymeric product with regular size for scientific or industrial purposes. When the feature size of surface structure goes down to the nanometer, significant differences in molding process and the corresponding mechanism can be observed. Compared to traditional injection molding, the replication quality of nanostructures is very sensitive to the variations of processing parameters and feature sizes [12,13]. The nanostructures on their surface not only contribute to harden the polymer melt filling into the nano-cavity, but also lead to a decrease in cooling rate of polymer melt because of the rapid heat transfer from polymer melt to cold mold. Due to the increase of the surface to volume ratio, proper filling of the polymer material into the nano-cavity becomes more difficult. It is known that the replication quality of injection-molded nanostructures

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is of great importance to the final efficiency of the polymer device. Therefore, further investigations on the filling mechanism and the geometrical morphology development are in urgent required.

Although experimental researches have been done to analyze the influences of processing parameters and flow behaviors in nano-injection molding process, the development time for polymeric product with surface topography would be substantially decreased if sufficiently robust simulation results allow the determination of the replication quality, influenced by changes in geometries and molding parameters [14]. These simulation results mainly based on the continuum mechanics have provided valuable guidance in understanding polymer flow behavior but also presented the limitations for the analysis of microscale system [15–17]. Once the simulation scale is down to nanometer, continuum mechanics fails to predict the system behavior accurately because of the drastic properties changes in nanoscale compared with those in macroscale [18]. Because of the obvious particle characteristics in nanoscale, the flow behaviors of polymer melt during the whole injection process are highly affected by those factors that would be ignored in conventional injection molding process, including wall slip, surface interaction, and intermolecular forces and so on.

Molecular dynamics (MD) simulation has attracted great attention for the analysis in nanoscale. It can study the physical movements of atoms and molecules that are allowed to interact for a fixed period, giving a view of the dynamic evolution. MD method is widely used to analyze the mechanical behavior of polymer [19], interface interactions [20], nanometric cutting [21], nano-imprinting lithography [22] and etc. However, few literatures can be found on the topic of MD studies on polymer filling into nano-cavity, especially in injection molding process. Mori et al. studied the filling process of epoxy resin into a nano-sized pore formed on aluminum surface and observed the deformation of metallic nanopore [23]. Pina-Estany et al. established a model system by taking the simulation results in macro-scale into the MD simulation during the injection process [24]. Those researches simplify the MD process by simulating the whole process under the injection velocity or pressure. Meanwhile, the influences of packing process on the filling mechanism and the geometrical morphology development of injection-molded nanostructures are still unknown. Comparative work by both MD simulation and experiment will surely help to guide the injection molding process for a better replication quality of surface nanostructures, in spite of the fact that it would be a complicated task to have a comprehensive analysis because of the scale effect [25]. However, MD simulation generally focuses on the smaller scale. The simulation work with the same geometry size as that in the experiment trial would be a huge time-consuming process. Despite the gaps of time-scale and size-scale between the MD method and experimental research, the MD simulation can not only provide insight view of the movement behavior of polymer molecule but also qualitatively estimate the morphology development in nanoscale.

The main purpose in this paper is to propose a better understanding of the flow behaviors that effected by the movements of polymer molecules during the filling process of nanostructures. In this study, MD simulations and experimental trials for injection molding nanopillars on PMMA surface were constructed respectively. Previous experimental and analytical studies from other research groups shown that the filling was mainly done in the packing stage[15,26]. Therefore, the whole process was divided into two phases, injection phase and packing phase. The filling process of PMMA melt was studied to observe the flow behavior and the geometrical morphology development for both phases. For simulation work, the effects of cavity width on the filling process of polymer molecules were investigated by analyzing the snapshots, densities in nano-cavity and gyration radius variations at different filling stages. Meanwhile, the influences of processing parameters, including packing pressure and packing time in packing phase on the geometrical morphology of the nanopillars were investigated comparatively. Wetting behaviors of PMMA melt on mold surface were introduced to explain the morphology forming mechanism of injection-molded nanopillars.

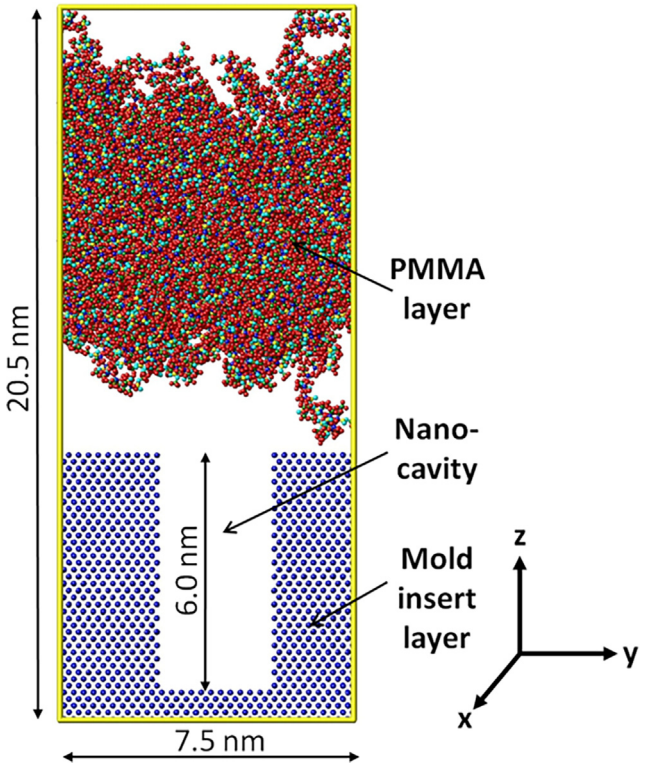

Fig. 1. Atomistic model of MD simulation.

2. Simulation model and methodology

2.1. Model constructing

The MD simulation model in a cuboid of 7.5 nm × 7.5 nm × 20.5 nm, consisted of an isotactic PMMA layer and a mold insert layer, as shown in Fig. 1. The PMMA layer was constructed in a configuration with 2000 MMA monomers in total, with the molecular weights of 5000. The mold insert layer was composed of nickel atoms, which has FCC structure with (1 0 0) plane. One rectangle nano-cavity was located in the upper of the nickel layer. The depth was 6.0 nm and the width of nano-cavity varied from 1.5 to 3.0 nm. Periodic boundary conditions in both x and y direction were utilized for approximating a large system, while the non-periodic and shrink-wrapped boundary condition in z direction was set, so that the heights of PMMA atoms were able to shrink in injection molding process. All the atoms were encompassed in z direction and the interaction between the top PMMA chains and the nickel atoms at the bottom could be avoided. The initial density of PMMA system was set to be 1.18 g/cm^3 at a temperature of 298 K (25 °C). In order to get access to the actual processing condition, energy minimization and subsequent anneal treatment were done to optimize the molecule structure of PMMA layer.

In injection molding process, polymer must be heated to melt temperature. After that, the melt was injected to the cavity and then kept under pressure before demolding. In the study, PMMA layer was firstly heated up to the temperature of 513 K (240 °C) and then relaxed for 50 ps in a constant particle number, volume and temperature (NVT) ensemble. The temperature of mold insert layer was kept at 383 K (110 °C), a bit higher to the T_g of PMMA. The whole nickel atoms were restrained by setting each component of force to zero. Finally, the interface model was made by assembling two layers together and exported as a source data file.

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