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Microscopic properties of a nanocrystal aluminum thin film during nanoimprint using quasi-continuous method

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ABSTRACT

In this article, we perform a multi-scale simulation of nanoimprint on a single-crystal aluminum thin film using the quasi-continuous method. The effects of contact stiffness between the stamper, thin film, and imprint orientation on the microstructure of the nanocrystal aluminum are examined. Results show that for a smaller value of contact stiffness, plastic deformation occurs relatively late. However, early plastic deformation is found when the stamper imprints perpendicular to the plane (111). In addition, to explore the effect of offset on the microstructure of a single-crystal aluminum thin film during the multi-imprint process, we perform a secondary imprint with an imprint depth of 10 Å. The effect of the first nanoimprint process on the secondary process can be found to be negligible when the offset is larger than 100 Å. However, we do not obtain a good pattern for a 50-Å offset. Therefore, for simulation cases, we suggest that the appropriate offset between the two imprints is 100 Å.

1. Introduction

Nanoimprint lithography (NIL) is an attractive fabrication method for the development of nanophotonic, nanoelectronic, and nanosensing devices owing to its advantages of low cost, high resolution, and high throughput [1–4]. In addition, NIL is an emerging technology in advanced semiconductor lithography because it has the characteristics required in the semiconductor industry.

Although NIL is a useful method for fabricating fine-scaled patterns on polymers [5], the direct nanoimprint of crystalline metals is still not feasible due to formability limitations at the nanometer scale. With the rapid development of computer technology over recent years, molecular dynamics (MD) have been very effective in exploring the physical properties of nanostructured materials, recognizing microscopic mechanisms, and offering insights into microscopic behaviors [6–8]. Using MD, imprint on metal thin films has been previously investigated [9–14]. For example, Fang et al. [9] studied the nanoimprint behavior of Cu–Ni alloys through MD. They found that with increasing Ni content of the Cu–Ni alloy, the spring-back phenomenon was more obvious after the punch was retrieved during the nanoimprint process, thereby inducing a smaller residual stress within the specimens. He et al. [12] performed MD to elucidate the deformation mechanisms of aluminum thin films during the nanoimprint process.

NIL is also an easy and inexpensive method for fabricating the nanopatterns of large area [15–16]. Multi-scale MD approaches [17] are more suitable than traditional MD techniques for understanding the detail characteristics and observing the physical phenomena in large-area patterns during the NIL process. Among multi-scale methods, the quasi-continuous (QC) method [18] is the most successful development for modeling and exploring the mechanical deformation of nanocrystalline solids, which is a mixed atomistic and continuum algorithm for investigating certain contact problems. Such problems are best suited to the application of the QC method since only the atoms near the contact region are needed for the calculations in multi-scale materials. The method has been proven effective in dealing with large-scale simulations, such as nanoindentation, without compromising simulation precision [19–22]. For instance, Shan et al. [19] performed the multi-scale simulation of surface step effects on nanoindentation using the QC method and demonstrated the precision of the method. Mei and Ni [22] investigated the anisotropic behavior of nanoscale adhesive contact when a Ni tip indents into single-crystal Cu substrates. They proposed that to reduce wear, nanoadhesive contact between a Ni tip and the Cu substrate with the same orientation should be avoided.

In general, the mechanical properties of thin films, such as the Young's modulus and hardness, are characterized by the nanoindentation test, and the nanoimprint process is then used to fabricate the

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nanopatterns. In addition, reciprocating nanoimprint on a piece of work may be employed to fully utilize the material. In this article, we use the QC method to study the imprint microstructure on a single-crystal aluminum thin film. To explore the effect of offset on nanopattern fabrication, imprints are performed twice.

2. Simulation method

In this article, the QC method [18] is used to study the deformation behavior of nanocrystal aluminum during the nanoimprint process. The method represents a coupling between the continuum mechanics and the atomistic simulations to determine the mechanical response of the crystalline material.

The simulated models consist of both a stamper and a nanocrystal aluminum thin film. The stamper is assumed to be a rigid body. The similar assumption is also made in the previous studies using the QC method [23–24]. The nanoimprint is performed by lowering the stamper to mechanically deform the aluminum thin film. The time step is 0.2 Å. The two types of force applied by the stamper on the aluminum thin film are explored: a uniform force applied directly on the boundary and a variation force that models the stamper and aluminum atoms through a simple repulsive potential [25–26]. To study the effect of orientation, the three types of crystal orientation are examined in the first imprint. A description of these orientations is listed in Table 1. The stamper is imprinted into the direction along the orientations I, II, and III. In addition, three offsets of 50, 100, and 150 Å are used in the second imprint. The simulation conditions for the second imprint are the same as those for the first imprint.

A schematic illustration of nanoimprint by a stamper on a nanocrystal aluminum thin film is shown in Fig. 1(a). Numbers 1 and 2 denote loading and unloading, respectively, along the y-direction for the first imprint, while numbers 4 and 5 are the same for the secondary imprint. Number 3 represents the offset, along the x-direction, between the first and secondary imprints.

The stamper is cylindrical with a diameter of 20 Å, and is periodic in the z-direction. The dimensional scales of the aluminum thin film are approximately 2000 Å × 1000 Å in the x-direction and y-direction, respectively, as shown in Fig. 1(b). The region of atoms imprinted by the stamper is treated with mesh refinement. The area outside of the imprinted region is treated with mesh coarsening to reduce the calculation time. In addition, in the simulation of the aluminum thin film, the atoms consist of local and non-local atoms, as shown in Fig. 1(c). The local atoms represent a continuum region and undergo only a near-homogeneous deformation; their energies are calculated from the local gradient of deformation based on the Cauchy–Born rule. The non-local atoms are subjected to an external compression force and show severe plastic deformation. They are essential for revealing the atomistic nature. The so-called ghost force arises due to the asymmetry in calculating the energies at the interface between the atomistic and continuum regions. The ghost force will lead to error of the solution. A recalculation method [27] of the correction force is used in order to improve the accuracy of the solution in transition region. In the calculation process, it will update automatically according to certain criteria.

3. Results and discussion

3.1. First nanoimprint with different contact stiffnesses

For the first nanoimprint, the relationship between the load and the displacement with different loading conditions in orientation II is studied. The load–displacement curves for the cases of uniform force, k = 1, and k = 20 for $\frac{1}{2}kr^2$, as shown in Fig. 2. A uniform force implies that the applied force exerted by the stamper is uniform on the aluminum thin film. On the other hand, the repulsive potential depends on the contact stiffness (k) and distance (r) between the stamper and the aluminum thin film. This potential can be expressed as $\frac{1}{2}kr^2$. Therefore, the force applied on the thin film varies with the parameters k and r.

Table 1
Imprint orientation.

	X	Y	Z
Orientation I	[$\bar{1}$10]	[111]	[$\bar{1}\bar{1}$0]
Orientation II	[111]	[$\bar{1}$10]	[$\bar{1}\bar{1}$2]
Orientation III	[100]	[010]	[001]

The three load–displacement curves increase linearly up to depths of approximately 6.5, 7, and 7.5 Å for the cases k = 1, uniform force, and k = 20, respectively, suggesting that the deformation reaches an elastic limit. However, after these indentation depths, at the 35th step, the three curves experience an abrupt drop, corresponding to a sudden decrease in load. This indicates the dislocation nucleate in this step, which also alters the microscopic structure and increases the hardness of the

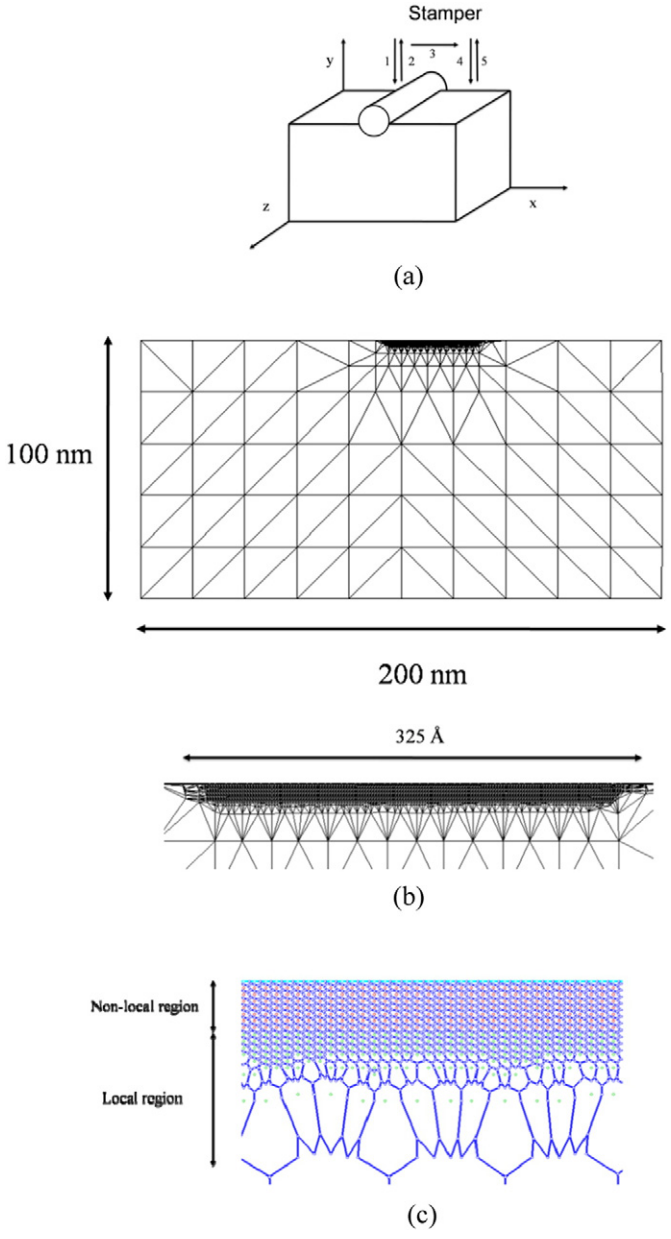

Fig. 1. The schematic illustration of nanoimprint on a nanocrystal aluminum thin film.