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An atomistic investigation on the mechanism of machining nanostructures when using single tip and multi-tip diamond tools

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ABSTRACT

In our previous work, a scale-up fabrication approach to cost effectively manufacturing nano-gratings over large area has been developed through diamond turning by using a multi-tip diamond tool fabricated by Focused Ion Beam. The objective of this study is to gain an in-depth understanding of the mechanism of machining nanostructures on single crystal copper through diamond turning when using a single tip and a multi-tip nanoscale diamond tool. For this purpose atomistic models of a single tip tool for multi-pass cutting and a multi-tip tool for single-pass cutting were built, respectively. The nature of the cutting chip formation, dislocation nucleation and propagation, cutting forces, and temperature distribution during nanometric cutting processes were studied through molecular dynamics (MD) simulations. Results show that nanostructure generation process at steady cutting stage was governed by a strong localization of the dislocation movement and the dynamic equilibrium of chip-tool contact area. Except the apparent improvement of machining efficiency that proportional to the tool tip numbers, the nano-grooves generated by multi-tip tool also have higher center symmetry than those machined by single tip tool. While the average tangential cutting force per tip were calculated all around 33.3 nN, a larger normal cutting force per tip being 54.1 nN was observed when using a multi-tip tool. A concept of atomistic equivalent temperature was proposed and used to analysis the important features of temperature distribution during the machining process. The advantage, disadvantage and applicability of diamond turning using multi-tip tool were discussed in comparison with those of using single-tip tool. The findings suggest that diamond turning using multi-tip tool might be more applicable than using single tip tool when apply to scale-up fabrication of periodic nanostructures.

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1. Introduction

In recent years, the design and fabrication of periodic nano-structured surface have drawn great interest in diverse research fields including optics and electronics, solar energy, cell biology, bioengineering and medical science [1–3]. Numerous nanofabrication technologies including optical and electron beam lithography, focused ion beam (FIB) milling, nano-imprinting, femtosecond laser machining have been developed up to date to produce small quantities of nano-structured device/materials. However, these methods do have their own limitations such as high operational costs due to the need of clean room operation, low efficiency, or requiring complex multi-step for production, or not capable of the fabrication of 3D nanostructures. Lack of new cost effective scale-up manufacturing approach has become a significant barrier to industry, especially SME's realizing 3D ultra precision nanostructures (nanometer level tolerance) for many applications.

Diamond turning using multi-tip single crystal diamond tools is a new promising approach to the fabrication of micro/nano structures [2,4,5]. The technical feasibility of diamond turning using multi-tip tools (with tool tip dimensions ranging from 15 μm to 100 μm) has been successfully demonstrated by researchers through ultra-precision turning/scratching operations for the fabrication of periodic micro groves [6], arrays [7], and diffraction gratings [5]. Recently, new progress was made by Sun et al. by whom nanoscale multi-tip diamond tools with pitch at 100 nm have been successfully fabricated by focused ion beam [2]. Through ultra-precision diamond turning operation, nano-gratings were successfully generated on nickel sample without observing tool wear after hundreds of meters cutting distance [2].

However, lack of support from systematic theoretical study has seriously hindered the advance and industrialization of this

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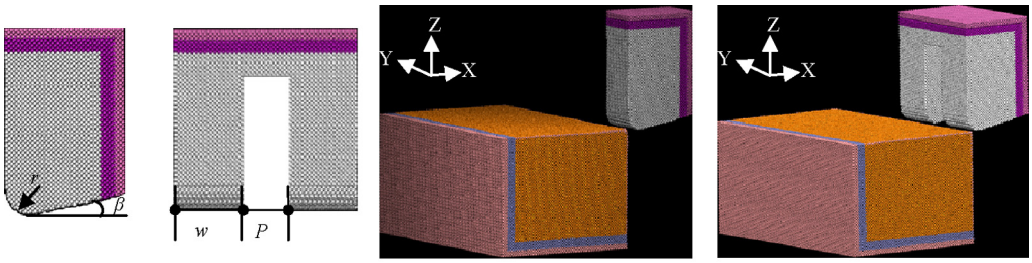

(a) Tool geometry (b) Single tip model (c) Multi-tip tool model

Fig. 1. Models of MD cutting simulation.

technique. The machining mechanisms of nanostructures when using multi-tip tool has not been fully understood up to date. As the tools and the machined structures are in a range of sub-microns or even nanometers, the influence of surface effects such as material side flow and elastic recovery on the integrity of machined nanostructures cannot be ignored. In addition, some critical questions are also needed to be addressed including the evaluation of the advantage, disadvantage and applicability of this novel technology. However, we cannot get quick answers through experiment work due to the limitations of the current real-time detect equipment. On the other hand, molecular dynamics (MD) simulation provides a solution for this problem which will be further reviewed in next section. Undoubtedly, the theoretic results obtained through simulations will provide valuable feedback and guidance for further development of this new technique.

2. The state-of-the-art MD simulation study on nanometric cutting

MD simulation studies, in general, were initiated in the late 1950s by Alder and Wainwright in the field of statistical mechanics [8]. Since 1980s, the feasibility of using MD simulation method to study nanometric cutting processes has been demonstrated by many researchers [3,9–15]. In the following part, only classical models and results pertaining to the studies of nanometric cutting of copper are selected and briefly reviewed.

Since 2000's MD simulations studies on nano-scratching of copper by a pin diamond tool have been reported by Fang (2000), Kim (2005) and Yan (2006, 2008) etc. Fang and his co-workers [9] have identified the frictional coefficient and forces as a function of the pin angle. Kim et al. [10] reported that in the nano-indentation and scratching process, the nucleation of the dislocation plays more important role in determining the abrupt drop during stick-slip than subsequent propagation of partial dislocations. Yan et al. [11] have simulated the multiple scratching processes of using an atomic force microscope (AFM) tip and investigated the effect of the feed rate on the deformation of the machined surface. A deformation criterion relating the single-atom potential energy variation to atom lattice deformation was further explored and the simulation results showed that four states exist between AFM pin tool and the workpiece surface [12]. Moreover, MD models were also built successfully to investigate the role of friction and tool wear in nanometric machining of copper, such as the work done by Ye et al. [3], Maekawa et al. [13], Lin and Huang [8] etc. Recently, large scale MD model with model size up to 10 million atoms has been performed by Pei et al. [14] to study the "size effect" existed in nanometric cutting of copper. Using this model, they further quantified the effect of processing parameters on cutting force and lattice defects [15]. These studies have made significant contributions toward our understanding of the mechanics of nanometric cutting of copper. However, until now no experimental work or simulation model has been found to investigate the cutting process and the machining mechanism for nanostructures by using multi-tip diamond tools.

Therefore, the main purpose of the present paper is to carry out MD simulations to study the nanometric cutting process and to reveal the mechanism of machining nanostructures using multi-tip nanoscale diamond tool. In order to benchmark the advantage and disadvantage of diamond turning using multi-tip nanoscale tools, a comparison between using single tip and multi-tip nanoscale tools in nanometrc cutting has been made from the aspects of cutting forces and temperature distribution during the machining process. Of course, the simulation may have their own limitations including the need to run at very high cutting speeds, but this may not be a serious limitation as long as we are interested in the general nature of the process without consideration of the speed effects.

3. MD simulation

3.1. Geometric model for MD simulation

To avoid the size effect induced by using period boundary condition [14], two large scale nanometric cutting models with free boundary condition in all directions were built, respectively (as shown in Fig. 1(b) and (c)). The geometry of the cutting tools is shown in Fig. 1(a). The tool-tip width is $15a$ ($a = 3.567$ Å) with the tool rake angle α being 0° and the tool clearance angle β being 12°. To save the computational time, a double-tip nanoscale diamond tool with a pitch of $10a$ is employed in this paper to represent the multi-tip nanoscale tool. Both of the single tip and multi-tip nanoscale diamond tool are created based on perfect diamond crystal structure. Unlike previous research, where the diamond tool is treated as a rigid body, the tools built here are deformable body so as to track the cutting force and temperature distribution in the tool. Since the radius of cutting edge of diamond tool is usually larger than the minimum depth of cut in nanometric cutting, in our large-scale MD simulations, all of the tools are built with round cutting edge with an edge radius of $5a$ instead of a sharp cutting tool.

The workpiece has a dimension of $50a_0 \times 80a_0 \times 40a_0$ ($a_0 = 3.615$ Å) and consists of boundary layer and thermostat layer with thicknesses of $2a_0$ and $3a_0$, respectively (as shown in Fig. 1(b) and (c)). Copper is chosen as workpiece material because of its high machinability when using diamond turning, particularly suitable for the fabrication of master tools used in roll-to-roll manufacturing [6]. The three orientations of the workpiece are [1 0 0], [0 1 0] and [0 0 1] in the X, Y and Z directions.

3.2. Potential functions for MD Simulation

There are three different atomic interactions in the MD simulation: (1) the interaction between copper atoms (Cu—Cu) in the workpiece; (2) the interaction between diamond atoms (C—C) in

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