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Investigation of the shape transferability of nanoscale multi-tip diamond tools in the diamond turning of nanostructures

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ABSTRACT

In this article, the shape transferability of using nanoscale multi-tip diamond tools in the diamond turning for scale-up manufacturing of nanostructures has been demonstrated. Atomistic multi-tip diamond tool models were built with different tool geometries in terms of the difference in the tip cross-sectional shape, tip angle, and the feature of tool tip configuration, to determine their effect on the applied forces and the machined nano-groove geometries. The quality of machined nanostructures was characterized by the thickness of the deformed layers and the dimensional accuracy achieved. Simulation results show that diamond turning using nanoscale multi-tip tools offers tremendous shape transferability in machining nanostructures. Both periodic and non-periodic nano-grooves with different cross-sectional shapes can be successfully fabricated using the multi-tip tools. A hypothesis of minimum designed ratio of tool tip distance to tip base width (L/W_f) of the nanoscale multi-tip diamond tool for the high precision machining of nanostructures was proposed based on the analytical study of the quality of the nanostructures fabricated using different types of the multi-tip tools. Nanometric cutting trials using nanoscale multi-tip diamond tools (different in L/W_f) fabricated by focused ion beam (FIB) were then conducted to verify the hypothesis. The investigations done in this work imply the potential of using the nanoscale multi-tip diamond tool for the deterministic fabrication of period and non-periodic nanostructures, which opens up the feasibility of using the process as a versatile manufacturing technique in nanotechnology.

1. Introduction

Recently, great interest has been shown in the fabrication of periodic micro/nano structures over large scale due to their increasing applicability in diverse research fields including optics and electronics, cell biology, bioengineering, and medical science [1–3]. The advances in current nanofabrication techniques, including optical and electron beam lithography, focused ion beam (FIB) milling, nanoimprinting, and femtosecond laser machining, have boosted the development of new platforms and methodologies to produce nanostructures of targeted functions. However, these methods fail to meet the increasing interest in commercializing functional nanostructured devices due to their inherent limitations, particularly the complex processing step, low processing efficiency, and high operational costs. These limitations have created substantial interest in developing cost-effective scale-up manufacturing approaches.

Diamond turning using multi-tip single crystal diamond tools, as a new machining technique, shows powerful capacity in the fabrication of micro/nano structures [4–7]. In recent decades, various kinds of micro multi-tip tools (with tool tip dimensions ranging from 15 to 100 μm) fabricated by the FIB milling technique were successfully applied to form well-ordered micro grooves [4,5], arrays [6], and diffraction gratings [7]. Recently nano-gratings with the pitch as low as 150 nm were fabricated using a nanoscale multi-tip diamond tool through the diamond turning operations [8]. The effect of feed rate and the alignment issues on machining accuracy associated with the use of separate single-tip tool can be completely eliminated when using nanoscale multi-tip tools [9]. Owing to the unprecedented merits of high throughput, one-step, and highly flexible precision capabilities, this technique has led to the hope for breaking the technical bottleneck for the scale-up manufacturing nanostructures.

Nevertheless, the formation mechanism of the nanostructures as well as the relationship between the geometry of nanostructures pre-fabricated on the tool tip and the form accuracy of nanostructures replicated on the work substrate remain unclear, which has become a significant barrier to the realization of the deterministic

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Table 1
Dimensions of nanoscale multi-tip diamond tool models (a = 3.567 Å).

	Tip distance (L)	Tip angle (θ)	Tip base width (W_f)
T1	3a, 6a, 9a, 12a, 14a	0°	9a
T2	3a, 6a, 9a, 12a, 14a6a	14.0°16.3°, 14.0°, 11.8°, 9.46°, 7.13°	9a 9a
T3	3a, 5a, 7a, 9a, 12a	0°(left tip); 14.0°(right tip)	9a
T4	4a, 6a, 7a, 9a, 12a	0°	9a (left tip); 6a (right tip)

nanomanufacturing capability. As the nanostructures are formed synchronously within a single cutting pass, the interactions of the deformed layers created by each tool tip might alter the material removal mechanism [9] and result in unpredictable processing defects. Although a few reports can be found in the literature, preliminarily describing the high form accuracy and throughput of this technique [4–8], no experimental or theoretical research work has been found which investigated the dependence of the form accuracy of machined nanostructures on the tool geometrical parameters. The characterization of the shape transferability of this technique is needed before the standardization and commercialization of nanocale multi-tip diamond tools.

Additionally, some fundamental issues related to nanometric cutting processes using the single tip diamond tool have been effectively investigated using molecular dynamics (MD) simulations method. Numerous MD nanometric cutting models were built to emulate the material removal process [10–12] and to study the effect of tool geometry on the machined surface quality [13–15]. Recently the difference in machining nanostructures between using single tip and multi-tip diamond cutting tools has also been reported [9,16]. These studies have made a great contribution towards the in-depth understanding of the dynamic behaviour of materials under different nanometric cutting conditions. However, no pioneering research work has been developed, for nanometric cutting, to investigate the shape transferability of nanoscale multi-tip diamond tools with different tool geometries.

This article therefore reports systematic research on the shape transferability of nanoscale multi-tip tools with different designed tool geometries. A hypothesis of a minimum designed ratio of tip distance to tip base width (L/W_f) of the nanoscale multi-tip tool is proposed based on a theoretical study of the effect of tip distance, tip angle, and the tip configuration on the quality of machined nanostructures. Nanometric cutting experiments using nanoscale multi-tip diamond tools are then conducted to verify the hypothesis. The potential of using nanoscale multi-tip diamond tools for the deterministic scale-up fabrication of period and non-periodic nanostructures are discussed in the subsequent section.

2. MD simulation

2.1. Geometric models for MD simulations

In order to fully explore the shape transferability of nanoscale multi-tip diamond tools, four categories of diamond tool used to machine periodic and non-periodic nanostructures were studied. The cross-sectional shapes of the tools and the tip configurations are shown in Fig. 1a–d (L is defined as the tip distance; θ is the tip angle; W_a and W_f are used to represent the width of the top and the bottom of the tool tip, respectively). For the purpose of concision, the four types of multi-tip tools are generally labelled as T1, T2, T3, and T4 in this article. All of the tool models built here are based on a deformable body with a round cutting edge radius r of 5a (a = 3.567 Å), a tool rake angle α of 0°, and a tool clearance angle β of 10° (as shown in Fig. 1e). To save computational time, the tools were built with a double-tip to represent the multi-tip tool. The cutting processes of using 21 diamond tools with different combinations of cross-sectional geometrical parameters (listed in Table 1) are simulated in this research.

The MD nanometric cutting model using multi-tip single crystal diamond tool is developed as shown in Fig. 1f. The copper workpiece has dimensions of $50a_0 \times 80a_0 \times 40a_0$ (a_0 = 3.615 Å). It consists of the boundary layer and the thermostat layer with thicknesses of $2a_0$ and $3a_0$, respectively. The three orientations of the workpiece are [1 0 0], [0 1 0], and [0 0 1] in the X, Y, and Z directions, respectively.

2.2. Potential functions for MD Simulation

The embedded atom method (EAM) potential proposed by Foiles et al. [17] was used to describe the interactions between the workpiece atoms which can be expressed as:

$$E_{\text{eam}} = \sum_i F^i \left[\sum_{j \neq i}^{n} \rho^i(r^{ij}) \right] + \frac{1}{2} \sum_{ij, i \neq j} \phi_{ij}(r^{ij}) \quad (1)$$

where the E_{eam} is the total energy of the atomistic system which comprises summation over the atomistic aggregate of the individual embedding energy F^i of atom i and the pair potential ϕ_{ij} between atom i and its neighbouring atom j. The lower case Latin superscripts i and j refer to different atoms, r^{ij} is the distance between the atoms i and j, and $\rho^i(r^{ij})$ is the electron density of the atom i contributed by atom j.

For interactions between C–C atoms, the Tersoff potential [18] was adopted and computed as follows:

$$V_{ij} = f_C(r_{ij}) \left[f_R(r_{ij}) + b_{ij} F_A(r_{ij}) \right] \quad (2)$$

where V_{ij} is the bond energy of all the atomic bonds, i, j label the atoms of the system, r_{ij} is the length of the ij bond, b_{ij} is the bond order term, f_R is a two-body term, f_A includes the three-body interactions, and f_C merely represents a smooth cutoff function to limit the range of the potential.

The Morse potential function [11] was used to describe the interaction between Cu–C and the total energy E_{tot} is expressed as:

$$E_{tot} = \sum_{ij} D_0 \left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right] \quad (3)$$

where r is the instantaneous distance between atoms i and j. The cohesion energy D, the elastic modulus α, and the equilibrium bond distance r_0 are 0.087 eV, 5.14 Å^{-1}, and 2.05 Å, respectively.

2.3. MD simulation setup

Due to the limitation of computational power, a high cutting speed was adopted as other researchers to speed up the MD simulation. In this study all of the cutting tools were applied along the minus X direction at a constant speed of 200 m/s with a depth of cut of 2.5 nm. Two nano-grooves were formed synchronously by a single cutting pass. MD simulations were implemented by using