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Modeling and simulation of the probe tip based nanochannel scratching

Z. Guo [a], Y. Tian [a,b,*], X. Liu [b], F. Wang [a], C. Zhou [a], D. Zhang [a]

[a] Key Laboratory of Mechanism Theory and Equipment Design of Ministry of Education, Tianjin University, Tianjin 300072, China
[b] School of Engineering, University of Warwick, Coventry CV4 7AL, UK

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ABSTRACT

This paper presents the theoretical modeling and numerical simulation of the probe tip based nanochannel scratching. According to the scratching depth, the probe tip is modeled as a spherical capped conical tip or a spherical capped regular three side pyramid tip to calculate the normal force needed for the nanochannel scratching. In order to further investigate the impact of scratching speed, scratching depth and scratching direction on the scratching process, the scratching simulation is implemented in LS-DYNA software, and a mesh-less method called smooth particle hydrodynamics (SPH) is used for the sample construction. Based on the theoretical and simulated analyses, the increase of the scratching speed, the scratching depth and the face angle will result in an increase in the normal force. At the same scratching depth, the normal forces of the spherical capped regular three side pyramid tip model are different in different scratching directions, which are in agreement with the theoretical calculations in the d_3 and d_4 directions. Moreover, the errors between the theoretical and simulated normal forces increase as the face angle increases.

1. Introduction

Nanochannels have wide applications in microfluidics technology, such as rapid DNA sequencing, drug delivery, battery and nanofluidic transistor [1]. Among various methods of nanochannel fabrication, probe tip based micro/nano scratching has been widely applied [2–6]. In the nanochannel scratching, the sample is usually mounted on a piezoelectric actuated micro/nano positioning stage, which has many excellent advantages including fast response time, large mechanical force and high positioning precision, there have been many investigations on the modeling and control of this kind of stage [7]. As the cutting tool, the probe tip is pressed into the sample with a desired depth, and then through the motion control of the precision positioning stage, the nanochannel can be fabricated on the sample surface.

Various kinds of probe tip models have been developed in the past few years. According to the tip geometry, they can be mainly categorized into spherical tips [8–10], conical tips [11,12] and pyramidal tips [13–15]. The spherical tip is usually with a diameter in the micron scale, which is not appropriate for the nanochannel fabrication. For the conical tip and pyramidal tip, it is impossible to obtain an ideal sharp tip due to manufacturing errors and tip wear, thus, these tips are usually modeled as a conical or pyramidal base with spherical cap. If only the spherical cap is involved in the operation for the surface topography measurement and scratching, the tip is still modeled as a sphere. However, in the scratching with large depth, the tip base will dominate the scratching process, so the tip base must be considered in such kind of application. Although the spherical capped conical model has been widely used, but it cannot substitute the pyramid structure. Geng proposed the spherical capped pyramidal tip model for the AFM tip, and the tip-sample interface was analyzed for single scratching [13], but the calculation of the horizontal projected area is complicated. Besides the AFM probe tip, the Berkovich probe has also been used for scratching investigation, but the scratching direction was not be considered [14–16], this kind of tip has regular pyramidal structure, which has many special geometry property compared with the general pyramidal structure, such as equilateral triangle of horizontal cross-section.

As a supplementary means for theoretical analysis, the numerical simulation usually acts as the role of guiding the experiments, and shows the possible phenomenon in the actual experiment. Molecular dynamics (MD) is an efficient method for the investigation of the micro/nano scratching, and which has been adopted by many researchers. Zhu et al. investigated the effect of the scratch-

* Corresponding author at: Key Laboratory of Mechanism Theory and Equipment Design of Ministry of Education, Tianjin University, Tianjin 300072, China.
E-mail address: meytian@tju.edu.cn (Y. Tian).

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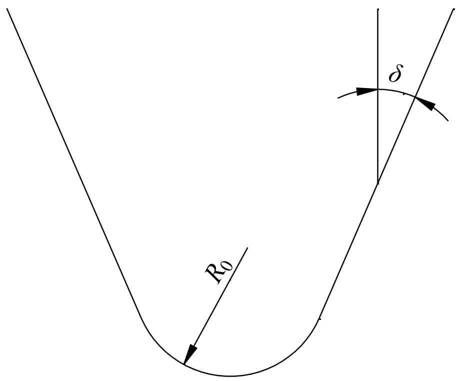

Fig. 1. Spherical capped conical tip model.

ing velocity on the scratching process in reference [17–19]. Zhang explored the subsurface deformed layers in AFM-based nanometric cutting process through molecular dynamics simulation [20]. Yan studied the effect of feed on the nano-scratching process using MD simulation [21]. Zhang examined the influence of double-tip scratch on nano scratching process via MD [22]. Fang researched the nanoscratch behavior of multi-layered films with MD [23]. However, in all these simulations, the scratching depth was less than 10 nanometers, since a larger scratching depth will result in a very long simulation time. Thus, MD is not an appropriate method for the simulation of dozens even hundreds nanometer scratching depth.

Smooth particle hydrodynamic (SPH) is a mesh-less method based on Lagrangian method, which is firstly proposed by Gingold and Monaghan in 1977 to solve the astrophysical problems [24], but with the development of the method, it has been widely used in fluid simulation and solid mechanics for the advantages in dealing with the large distortions [25,26]. Furthermore, the method has been successfully applied in micro machining simulation in recent years [27–29]. Zhao studied the effects of cutting process on residual stress distribution, and the effects of residual stress on mechanism using SPH method [27], the cutting depth is from 300 nm to 900 nm. And then still with SPH method, his team further investigated the residual stress on sequential scratching with smaller scratching depth from 50 nm to 150 nm [28]. Cao compared the conventional scratching with the ultrasonic-assisted scratching on the material removal process, two scratching depth 70 nm and 2 μm were simulated with SPH [29].

In the tip based nanochannel scratching, the normal force is an important parameter because it directly decides the scratching depth, so this paper focuses on the theoretical calculation and the simulation of the normal force. Among various probe tips, the three side pyramid probe tip is the most popular for the good machining ability, thus a spherical capped regular three side pyramidal tip model is chosen to model this kind of tips in large scratching depth. The geometrical model of the spherical capped conical tip and the spherical capped regular three side pyramidal tip are firstly introduced in this paper, and then the horizontal projected areas of the tip-sample interfaces are analyzed in Section 2. The SPH simulation model are constructed in section 3, the effects of the scratching parameters (scratching speed, scratching depth and scratching direction) and the face angle of the probe tip on the scratching process are simulated and discussed in Section 4.

2. The probe tip model and the horizontal projected area of the tip-sample interface

In this section, two probe tip models are presented, one is spherical capped conical tip model and the other is spherical capped regular three side pyramidal tip model. The scratching depth considered in this paper is from 20 nm to 200 nm, and the spherical cap radius is assumed to be 90 nm. When the scratching depth is less than 60 nm, only the spherical cap takes part in the scratching, the former tip model has a complete spherical surface in this range, so it is selected for the simulation in this scratching range. When the scratching depth is larger than 60 nm, the probe base will dominate the scratching, the latter tip model is more similar with the actual three side pyramid probe tip in geometric features, so it is selected for the simulation in this range of scratching depth.

2.1. Geometrical model

A spherical capped conical tip model has been widely applied in the analysis of the tip-sample interface [10,11], which is shown in Fig. 1, where R_0 is the spherical cap radius and δ is the half angle. In precious paper, both the spherical cap and the conical base are used for the scratching, but in this paper only the spherical cap is selected for the small scratching depth under 60 nm, the cone part is seen as the assumptive probe tip base, so the value of δ does not affect the scratching process and the tip-sample interface.

For the large scratching depth from 60 nm to 200 nm, a spherical capped regular three side pyramidal tip model is presented, as shown in Fig. 2(a). The point A is the hypothetical apex, and the triangle ΔBCD is the critical horizontal section interface between spherical cap and pyramid base. The arcs $\hat{BC}$, $\hat{CD}$ and $\hat{BD}$ are the intersection of spherical surface and pyramidal surfaces, which are assumed to be tangent to the pyramidal edges. Fig. 2(b) and (c) are the section of triangle ΔAO_1O_3 and ΔAO_1C, respectively, where O_1 is the center of spherical cap surface with a radius R_0, O_3 is the center of arc $\hat{BC}$ with a radius r_0. In order to facilitate the scratching analysis, three angles α, β and γ are defined as face angle, edge

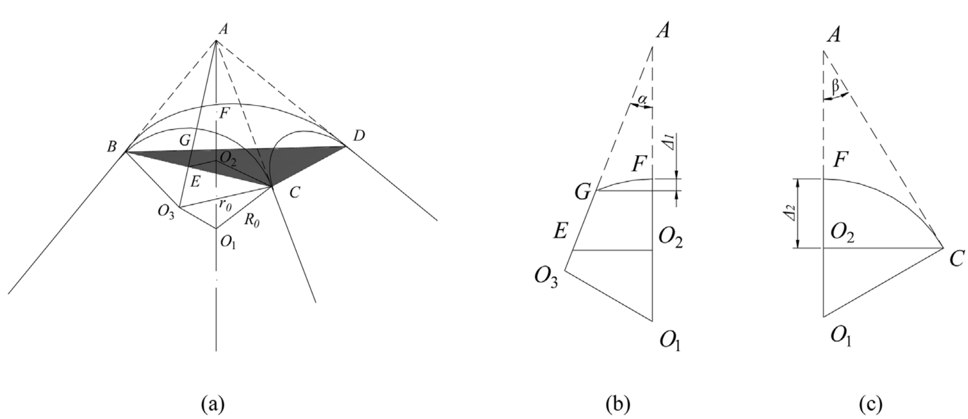

Fig. 2. (a) Spherical capped regular three side pyramidal tip model; (b) Section of the triangle ΔAO_1O_3; (c) Section of the triangle ΔAO_1C.

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