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# A novel approach for determining the minimum feed in nanochannels processing via molecular dynamics simulation

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ABSTRACT

A novel approach based on molecular dynamics (MD) simulation has been proposed for the first time with the focus on quantifying the minimum feed (MF) in atomic force microscope (AFM) based nanochannel fabrication. This approach involves a coarse-to-fine criterion to determine MF so that regular nanochannel patterns can be obtained. The method is first introduced step by step and then confirmatory test is performed to demonstrate the capability of this contour-based method. MF judging studies are also performed systematically in which they vary in the aspects of scratching depth, tip angles, and tip shapes. Dislocations generation, surface quality, and scratching forces in the initial and subsequent scratches are investigated in detail. This method can overcome the drawbacks of high cost and low efficiency in experimental studies. Furthermore, our method sheds light on the manufacturing technique of nanochannels, which can help to obtain the surface morphologies with higher quality than traditional approaches.



## 1. Introduction

As the scaling-down revolution has brought us, nanostructures especially nanochannel arrays have stimulated great interest due to their extensive application in nanometer scale devices. Wire grid polarizer (WGP), whose performance can be significantly improved by reducing the nanochannel pitch below 140 nm, could be possibly applied in microdisplay-based projection systems [1]. Deposition of target material into a template with nanochannel arrays can be one of viable approaches for fabricating nanotubes and nanowires [2]. The semiconductor industry has also been pushing high-precision nanochannel fabrication to manufacture ever-shrinking transistors and high-density integrated circuits (ICs) [3]. Introducing biomolecules into nanochannels is an effective way for studying the biosensing process and developing the nanochannel array-based bioanalytical devices [4]. Yet, the key to these components in nanometer scale leads to a basic problem: nanochannels fabrication. The state-of-art methods for nanochannel arrays fabrication include, to name a few, electron-beam lithography (EBL), nanoimprint lithography (NIL), femtosecond laser machining, and AFM-based nanoscratching [5–8]. AFM-based nanoscratching is the most notable approach due to its advantages of high resolution, low-cost, material flexibility, and ease of operation.

In order to fabricate desired nanochannel patterns by AFM-based nanoscratching, some critical issues have been addressed for such demanding and industrially relevant process. Some researchers focused on developing theoretical prediction models for nanoscratching with expected depths [9,10]. Effects of parameters such as normal loads, reciprocal times, and scratching speed were also elucidated [11,12]. As representatives of the leading-edge research, all these researches are inspiring. However, the issue of producing nanochannels by necessary feed still remains to be solved. The feed, also known as pitch, is defined in terms of the distance between two adjacent parallel nanochannels. Unsuitable scratching feed would lead to failure of integrate nanochannel formation and required surface quality [13]. From the view of manufacturing, feed is critical for improving the machining efficiency and special attentions are needed. As mentioned before, the performance of nanodevices and ICs can be greatly improved by high-density nanostructures and minimizing the feed provides a solution for the ever-shrinking-scale nanomanufacturing. Therefore, numerous experiments were carried out to evaluate the influence of scratching feed on nanochannels formation [11,14]. However, traditional experimental method is crippled by high cost and time consumption. A deeper understanding of nanoscratching mechanisms still remains as a challenging problem. Thus, another research methodology superior to experiment is imminently required.

In nanoscale processing, traditional continuum mechanisms are not suitable for analysis since the deformation is inherently atomic. As a consequence, many attempts have been made to effectively

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emulate nanoscratching process by molecular dynamics (MD) simulation. For instance, Yan et al. investigated the influence of feed on scratching depth and surface quality, and proposed a proper feed for machining non-interfering parallel nanochannels [15]. Promyoo et al. conducted MD simulations to probe the minimum distance between two nanochannels so that interference can be avoided [16]. Fang et al. demonstrated a clear relationship between the scribing feed and the resultant force. They also revealed the effects of feed on surface roughness [17]. Nevertheless, the explicit and stringent criterion for judging the minimum feed is not established and therefore, the minimal feed in their study is subjective and inaccurate. Meanwhile, Zhu et al. performed MD simulations to investigate how the tip geometrical parameters influence the nanoscratching process [18]. However, no pioneering work is presented for the investigation of minimum feed under different working conditions such as tool geometries, scratching depth or other influence factors. Since our literature survey does not furnish any particular method, judgment of the minimum feed is particular in demand.

Therefore, in this article, we develop a methodology to determine the minimum feed (MF) in nanochannel arrays processing. The proposed coarse-to-fine approach starts from a coarse identification which provides a range including MF, and the process is carried onto the fine subdivision stage based on the contour-based angle measurement method. Details of the MF judging method are systematically elaborated by one example. Then MFs for different scratching depths, tip angles, and tip shapes are investigated based on our method. The scratching forces, surface deformation and dislocations generation are also compared in each condition. This coarse identification and fine subdivision method is desirable for obtaining MF in uniform nanochannel manufacturing process and could greatly benefit the nanofabrication industry.

## 2. Simulation methodology

MD simulations in our study are conducted using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) developed by Plimpton [19].

### 2.1. Geometric model for MD simulations

Fig. 1 shows the schematic model used in MD simulations. The simulation model consists of two rigid diamond tips and a defect-free monocrystalline copper workpiece. The two diamond tips with identical geometry are utilized to imitate the first and second scratches. They are constructed with perfect diamond atomic lattice and are treated as rigid bodies for the high hardness. The copper workpiece assumed to be in perfect face center cubic (FCC) configuration contains 440,000 atoms within a size of $70a \times 50a \times 30a$,

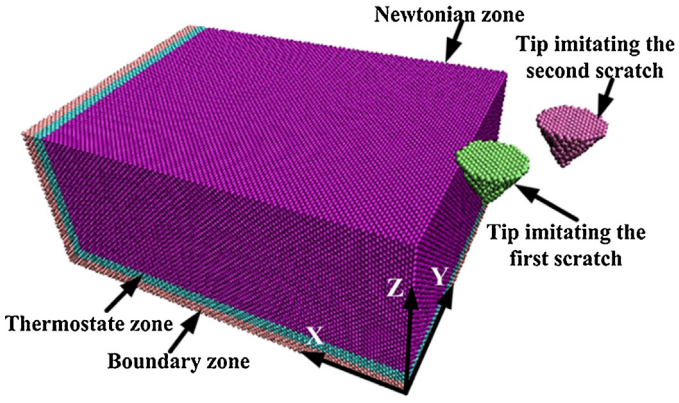


**Fig. 1.** MD simulation model.

where $a$ is the lattice constant of copper, $a = 0.3615$ nm. The crystal orientations of the workpiece along $X$, $Y$ and $Z$ axis are [100], [010] and [001]. The scratching is implemented on (001) surface along [−100] direction in all simulations.

When building the model, there are two alternatives for simulating the multi-scratch process. One is to use double tips to scratch the workpiece surface simultaneously (double-tip scratch) and another is to scratch the workpiece one after another (single-tip scratch). Previous studies have revealed that double-tip scratch can obtain two parallel nanochannels of high quality regardless of scratching feed, depth and orientation. However, the second scratch significantly influences the former nanochannel in the single-tip scratch [13,20]. In consideration of the real scratching process, single-tip scratch has more practical significance. Therefore, in our simulations, one tip initially scratches the workpiece surface along [−100] direction for a given length and then the tip is elevated along $Z$ axis to depart from the workpiece. Then, the second tip thrusts into the workpiece and also scratches along [−100] direction. Two tips are separated by a distance equivalent to feed in $Y$ direction. It should be noted that the feed could be smaller than radii summation of the two tips. In case of interference, tips are also separated by a few nanometers in $X$ axis, which can be seen clearly from Fig. 1.

The monocrystalline workpiece in MD simulations is divided into three different zones, namely: Newtonian zone, thermostat zone, and boundary zone. The relative position of the three zones is illustrated in Fig. 1. Eight layers of boundary atoms with fixed boundary conditions are placed at the bottom and left side of the workpiece and the thermostat atoms are placed in between the boundary zone and the Newtonian zone. The thermostat zone is employed to imitate heat dissipation in real scratching. The motion of atoms in the Newtonian and thermostat zones remains strictly within the limits of Newton's equation of motion. And the motion is determined by directly integrating the classical Hamiltonian equation of motion using Velocity-Verlet algorithm. The initial temperature of the workpiece is kept constant at 298 K by velocity scaling method [21]. Periodic boundary conditions maintained along $X$, $Y$, and $Z$ directions are adopted to enlarge the simulation scale, investigate the behavior of an isolate system, and avoid the boundary effect. All MD simulations are conducted in the *NVE* ensemble, where the system is isolated from changes in number of atoms ($N$), volume ($V$) and energy ($E$). The time step in simulations is usually on the order of femtosecond (fs), which is determined by the intrinsic inter-atomic vibration distance. In our current simulation, time step is set to be 1 fs to allow the system to reach the equilibrium configuration. Limited by our computational resource, a high scratching speed of 100 m/s is adopted in the simulation.

### 2.2. Potential functions for MD simulation

The selection of potential energy functions is crucial to the accuracy of MD simulations as they determine the credibility of the simulation results. On the other hand, the efficiency of MD simulations depends on the complexity of the potential energy functions. There are three types of atomic interactions: Cu–Cu interaction, Cu–C interaction, and C–C interaction. The embedded atom method (EAM) potential, which provides a more realistic description of metallic cohesion and avoids ambiguity inherited by the volume dependency, is employed to describe the interaction between copper atoms [22–24]. The total atomic energy of an EAM potential system can be expressed as:

$$E_{eam} = \frac{1}{2}\sum_{ij, i\neq j}\phi_{ij}(r_{ij}) + \sum_{i}F_i\left[\sum_{j\neq i}^{n}\rho_i(r_{ij})\right], \quad (1)$$