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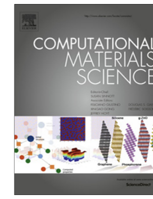

Effects of recovery and side flow on surface generation in nano-cutting of single crystal silicon

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ABSTRACT

The effects of the recovery and side flow on the surface generation, as well as the stagnation region, phase transformation in nano-cutting of single crystal silicon are investigated by means of molecular dynamics. In this study, the workpiece material would experience two cutting processes in the conditions where the recovery and subsurface damage of the former cutting trace could be and not be taken into consideration. Therefore, the combined effects of the side flow and recovery on the surface generation are decoupled and investigated respectively. The results show that the side flow of the material increases the generated surface roughness making it deviate from the theoretical value. The recovery left on the former cutting trace enlarges the size of side flow and further increases the surface roughness indirectly. But the overall surface roughness is decreased by the effect of recovery. Comparing the effects of the side flow and the recovery on the generated surface roughness, the side flow plays a more important role in surface generation of nano-cutting process. Therefore, the suppression of the side flow is an effective way to improve the generated surface roughness in nano-cutting. The phase of single crystal silicon in machined subsurface is transformed to amorphous and bct5-Si phases. A larger stagnation height would make more materials phase transformed.

1. Introduction

Nano-cutting is one of the deterministic and efficient machining methods in producing the functional parts with nanometric surface roughness and sub-micrometric form accuracy or with micro/-nanometric feature size [1–3]. In nano-cutting process, the ideally generated surface is affected by the feed rate f and the nose radius R_n of the cutting tool. The theoretical surface roughness, PV (peak-to-valley) value, is formulated as $PV = R_n - \sqrt{R_n^2 - (f/2)^2} \approx f^2/8R_n$ [4]. By increasing the tool nose radius R_n and decreasing the feed rate f, the theoretical surface roughness could attain nanometric, and even sub-nanometric scale. However, the effects of tool geometries [5–9], material properties [10,11] make the generated surface roughness deviate from the theoretical value. The recovery and the side flow of materials which have been investigated by many researchers, are two factors affected by tool geometries and material properties in causing the deviation.

The combined effect of the recovery and the side flow was referred as the swelling effect by Cheung et al. [12], in 2000. They thought larger swelling effect would make greater and deeper marks generate on the machined surface and further increase the generated surface roughness. Sata et al. [13] experimentally investigated the swelling of brass and medium carbon steel in cutting processes, and found that larger swelling would generate on the surface of softer materials. Cheung [12] and Kong et al. [14] thought the amount of the recovery which is determined by the forces on the clearance face and Young' modulus of the workpiece material, would cause a wavy machined surface. In 2015, Schaal et al. [15] experimentally investigate the influence of cutting edge radius on the recovery in metal cutting. Results showed that the recovery for the sharp tool is lower than that of the blunt tool. The variation of the recovery is in coherence with the change of surface roughness [15]. To predict the surface roughness affected by the recovery in nano-cutting processes, Zong et al. [16] introduced an additional term to the roughness formulation proposed by Grezesik [17]. It is formulated as

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$$PV = \frac{f^2}{8R_n} + \frac{h_m}{2}\left(1 + \frac{R_n h_m}{2}\right) + k_1 r_\beta \frac{H}{E} k_2 \quad (1)$$

where k_1 is a coefficient relating to the recovery affected by the tool nose radius and rake angle, k_2 is a coefficient affected by the maximal uncut chip thickness (UCT) and tool edge radius, h_m is the minimum UCT, H and E are the Vickers hardness and Young's modulus. In 2016, He et al. [18] considered the contribution of the recovery to the machined surface roughness. Based on the proposed prediction method, the contribution of the recovery to Al6061 is $0.9162h_m = 0.3207r_\beta$, where r_β is the tool edge radius.

In 1971, the side flow which is the plastic deformation of workpiece material at a direction opposite to the feed direction in cutting process, has been investigated by Pekelharing et al. [19]. The side flow was thought to be a result of the interactions between cutting tool and workpiece material [20]. In 1999, Kishawy et al. proposed two mechanisms about the formation of side flow [9]. The first one is the squeeze between the machined surface and the tool flank face especially when the UCT is smaller than the minimum UCT. The second one is the trailing edge notch induced high temperature and pressure makes the material flow to the side. Ge et al. [21] found that the severe worn tool edge caused an increase of surface roughness due to the side flow. The side flow of material has been taken into account to predict the machined surface roughness [16,18,20,22]. In 2006, Liu et al. [20] established a relationship between the roughness due to side flow R_p and the rheological factor x, which is formulated as

$$R_p = k_1 \ln x + k_2 \quad (2)$$

$$x = \frac{E\cot\theta}{\bar{\sigma}_y e} \quad (3)$$

where $\bar{\sigma}_y$ is the average flow stress, e is defined as the ration of the average flow stress with and without strain gradient strengthening, k_1 and k_2 are two coefficients need to be calibrated via actual cutting tests.

In 2014, Zong et al. [16] introduced a scale coefficient k_3 relating to the side flow to the surface roughness prediction formulation. In determining the value of the coefficient k_3, the feed rate and tool nose radius are considered. In 2015, He et al. [22] thought the side flow is one of the uncertain components. The surface roughness influenced by it is predicted empirically by a radial basis function (RBF) neural network. In 2016, a new prediction model was proposed by them [18]. The side flow induced increment of surface roughness is formulated as $w = k_d k_t k_f h_m b_D$, where b_D is the effective cutting width, k_d is a scale coefficient determined by the material properties of workpiece, k_t and k_f are two variable coefficients relating to the tool nose radius and feed rate respectively.

However, the experimental investigation on the recovery and side flow on the surface generation in nano-cutting is high-cost and time consuming. The effects of these two factors always couple with each other and make it is difficult to distinguish their own respective influences on surface generation by experiments. Therefore, the prediction model taking consideration of these two factors could not be constructed precisely. Numerical methods, such as the finite element method (FEM) [23] and the molecular dynamics (MD) simulation [24,25] could give a straightforward result and distinguish the respective effect of the recovery and side flow. In 2006, Kishawy et al. investigated the formation of side flow by 3D thermo elasto-viscoplastic FEM. They found that more side flow is generated with higher nose radius and lower feed which happens to be the way to decrease the theoretical surface roughness [23]. In nano-cutting, MD simulation is a powerful method in investigating the material removal and surface generation mechanisms [26–29]. In 2017, Lai et al. [24] investigated the surface generation on partially overlapped nano-cutting of single crystal germanium and found that the side flow would increase the height of the tool marks left on the machined surface, therefore, causing the increment of the machined surface roughness. Recently, Xu et al. [29] investigated the crystallographic orientation effect on surface generation of aluminum in nano-cutting by MD simulations. They found that small minimum UCT accompanied with small recovery height and contact length between the flank face and workpiece material generated a better surface quality. After that, side flow effect on surface generation in nano-cutting of aluminum was also investigated by MD simulations [25]. The results showed that materials tending to flow to the side are at or under the stagnation region. In the nano-cutting process, they are extruded by the tool edge to form the side flow. The position, shape and size of the stagnation region which are determined by the material properties and tool edge geometry would influence the side flow of nano-cutting process. Small tool edge radius and positive rake angle would decrease the size of side flow [25].

Above all, the effects of the recovery and side flow on surface generation in cutting process have been widely investigated. However, the experimental methods could not give their own respective effects on surface generation. The prediction model of the surface roughness is derived from the machined results indirectly and based on some assumptions without precise verification. The simulation methods could give a direct and visualized result. Especially when using the MD simulations, the coupled effects of the recovery and side flow on the surface generation in nano-cutting could be decoupled and investigated respectively. In this study, MD simulations are applied to investigate the effects of the recovery and side flow on the surface generation in nano-cutting. Six cutting directions are employed to obtain the anisotropy of the single crystal silicon in nano-cutting. Besides that, the phase transformation of silicon under the action of the tool edge is also discussed. This study contributes to a better understanding of the surface generation in nano-cutting processes.

2. Methods

The side flow and recovery in nano-cutting of single crystal silicon are investigated by employing MD simulations. The cutting model, as shown in Fig. 1, consists of a rigid diamond tool and a silicon workpiece. Detailed information about the cutting model is displayed in Table 1. In order to limit the computation time to an acceptable value, the tool nose radius R_n is set as 15 nm and the tool edge radius r_β is set as 5 nm. The rake angle and the clearance angle of the cutting tool are 0° and 12.5°. The size of the workpiece is 45 nm × 20 nm × 50 nm and it contains about 2,250,000 atoms. To simulate an ideal cutting trace left on the workpiece surface, part of the workpiece is cutting off by a cylinder with radius of 15 nm which is equal to the tool nose radius R_n. Therefore, at the first cutting as shown in Fig. 1, the side flow in nano-cutting could be investigated in the condition where the recovery and subsurface damage of the former cutting trace is ignored. At the second cutting, the generated surface would be influenced by the first trace in which the recovery and subsurface damage could not be ignored. Base on the proposed cutting model, the coupled effects of the side flow and recovery on the surface generation could be decoupled. Their effects could be investigated respectively and systematically.

In the cutting model, atoms of workpiece are defined as three parts: boundary layer, thermostat layer and Newtonian layer. Atoms in boundary layer are fixed at space to prevent the unexpected movement under the action of cutting force. The thermostat layer is kept at a constant temperature of 293 K to imitate the heat dissipation in nano-cutting. The rest atoms which would be cut by