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Analysis micro-mechanism of burrs formation in the case of nanometric cutting process using numerical simulation method

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Burrs (exit failure), being one of the important factors influencing the final precision of workpiece, have been widely studied. Today, with the development of manufacturing technology, the depth of cut falls into the range of nanometer or sub-nanometer, there may be some different disciplines dominating the burrs generation process. Molecular dynamics (MD) method, which is different from continuous mechanics, plays an important role in describing microscopic world. Take the example of single crystal copper, this paper carries out MD analysis micro-mechanism of burrs generation process. The results show that the burrs geometry depends on the type of workpiece (ductile or brittle). The depth of cut is decreased in the case of positive burrs generation process while the depth of cut is increased in case of negative burrs generation process.

burr, molecular dynamics, micro-mechanism

1 Introduction

Burrs are always generated in the workpiece at the exit end of the cut in most machining operations. Burrs can modify the nature of chip formation and the associated force, stress, and strain both in the workpiece and tool. This can have a detrimental effect on the chipping and fracture of brittle cutting tools, such as ceramics, cemented carbides, in interrupted cutting of high-strength materials at high speeds or feeds. While there are numerous studies on the entry and exit effects on the tool fracture, relatively few studies were focused on the micro-mechanism of burr formation in the workpiece. Presently, with the development of computer and semiconductor industry, the manufacturing precision has been improved to nanometer or sub-nanometer level. There may be new discipline dominating in this regime and influencing the burrs formation process. New powerful theoretical toolkit should be adopted to study the micro-mechanism of burrs formation process.

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Although macroscopic continuum mechanics has been perfectly developed in engineering design and has played an important role in the mechanical industry, it cannot be applied to solids or liquids in the atomic or molecular state. MD simulation studies, in general, were initiated in the 1950s by Alder and Wainwright in the field of statistical mechanics. Since then, MD simulation has been applied to a wide range of fields including crystal growth, diamond synthesis and so on. However, its application to machining is of only recent origin. In the late 1980s, a group at Lawrence Livermore National Laboratory of USA conducted pioneering studies on MD simulation of nanometric cutting of copper with a diamond tool. This work led other researchers[1], particular from Japan[2], and in the present author's laboratory in China[3−6], to explore and extend MD simulation of nanometric cutting to many practical machining applications. This investigation about burrs formation process using MD simulation method may be a contribution to burrs research work under the conditions of ultra-precision manufacturing technology (UMT).

As burrs have an important effect upon UMT, people conducted much work about burrs formation in the workpiece as well as in the tool. Lucca[7] carried out research on the formation of exit failure of different materials under different machining conditions. The results showed that the exit chip separation process is a ductile shear type failure of workpiece due to elastic constraint at the boundary. The depth of exit separation chamfer is reported to equal the depth of cut. The exit chip separation angle is reported to lie in 20°—25° range for each material. The behavior of foot formation process is reported to be different for various materials. Ko et al.[8] proposed quantitative fracture model of burr formation for orthogonal machining. They think that the fracture strain should be used to explain burr formation, and they adopted McClintock's ductile fracture criterion to determine the fracture location. Finally they employed modified milling machine with scanning electron microscope to observe the burr formation all the time. Sangkee et al.[9] constructed finite element model to investigate burr generation process. Firstly, they carried out finite element simulation of two-dimensional orthogonal cutting and validated it by experimental observation. Subsequently, they constructed three dimensional finite element model of drilling burr formation process. With this model, they studied the mechanism of burr formation and employed the simulation results in the process of reducing of burrs. Kim[10] developed an analytical model for drilling burr formation based on observation of plastic deformation of low alloy steel. Their model is applicable to ductile workpiece which do not undergo fracture. Their model is deduced from the principle of energy conservation and metal cutting theory, and the experimental results showed good agreement with their model.

Today, most research about burrs formation is limited in the range of experimental study, which cannot trace the dynamic process of generating burrs. Numerical simulation technology, especially molecular dynamics method, has the ability of describing micro-initialization of burrs in the atomic level and thus can provide basic principle for the reduction of burrs. Taking single crystal materials as an example, this paper carries out MD simulation of burrs formation mechanism in the nanometric cutting process.

2 The kinds of burrs

Generally speaking, no matter turning, milling, or drilling, etc., there may be burrs generated at the exit edge which is shown in Figure 1. Based on generation mechanism, Gillespie[11] proposed another criterion about burrs sorting (Figure 2).

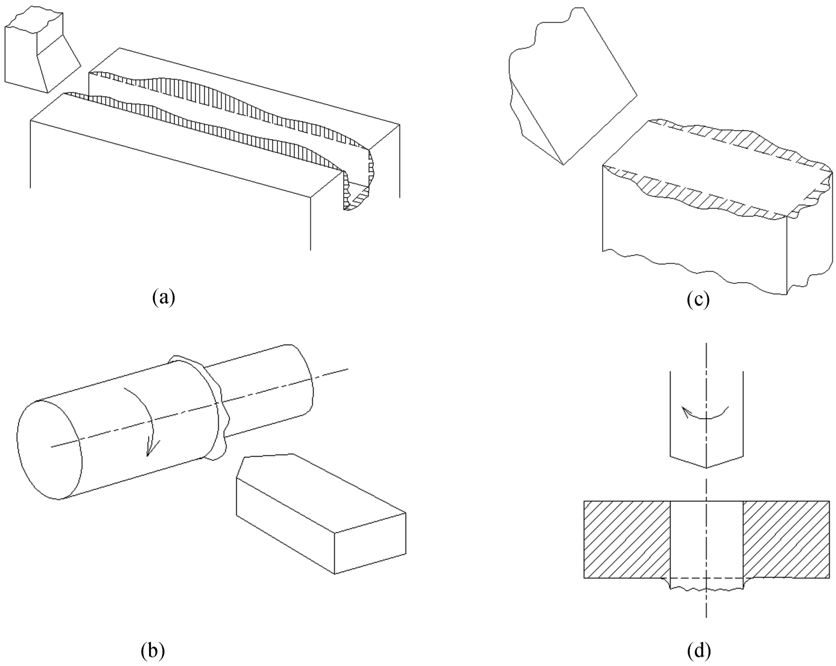

Figure 1 Generated burrs under different manufacturing process. (a) Broaching; (b) turning; (c) milling; (d) drilling.

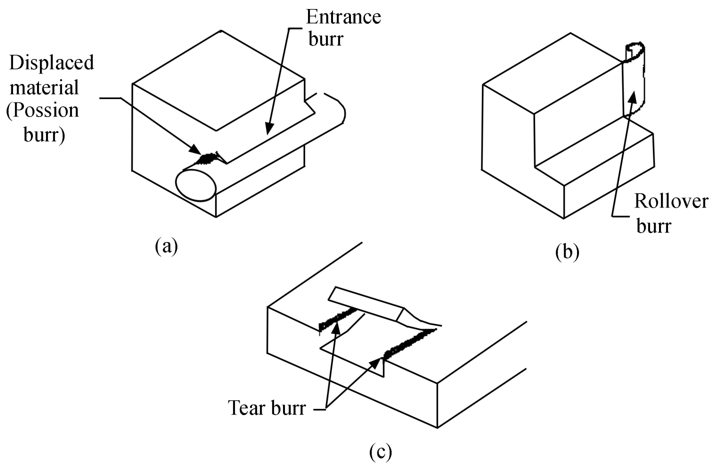

Figure 2 Types of burrs[11]. (a) Possion burr; (b) rollover burr; (c) tear burr.

3 MD simulation methodology

Because of adjusting technique parameters, the experimental study of burrs is time consuming while this work can be easily realized using computer simulation method. The simulation model employed in this paper is shown in Figure 3. No boundary atoms are placed at the exit of workpiece in order to generate burrs. The potential function adopted in the simulation is Morse potential. Two different kinds of fcc materials, namely, ductile material and brittle material are compared to investigate the effect of ductile on the burrs generation process. The parameters used in this paper are given in Table 1, and corresponding potential function graph is shown in Figure 4. This paper carries out MD simulation the effect of technique parameters (ductile, tool angle, depth of cut) on the of burrs generation process.

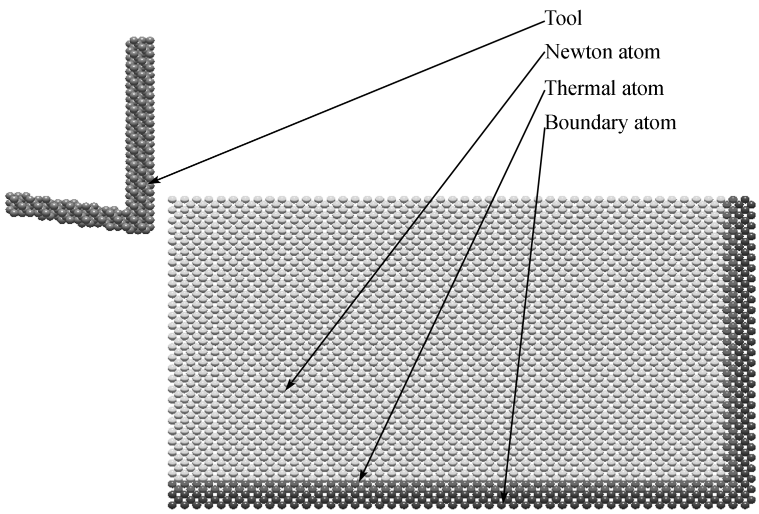

Figure 3 MD simulation model.

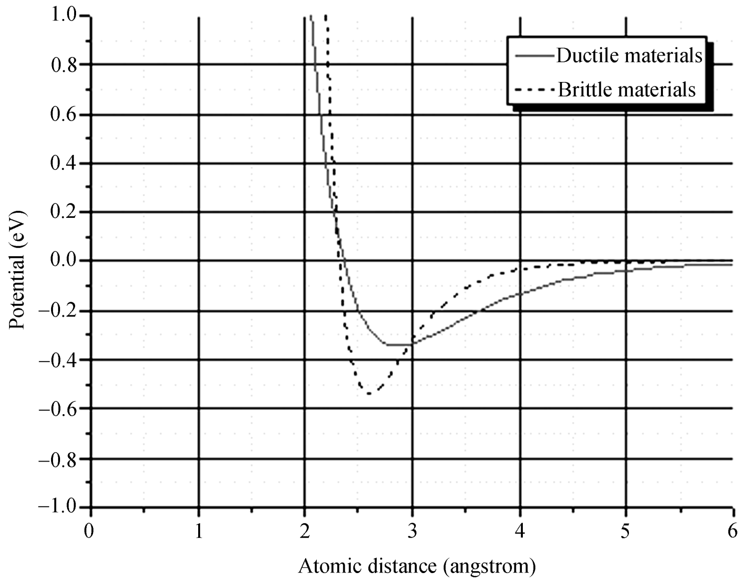

Figure 4 MD simulation model.

Table 1 Simulation parameters

Workpiece materials	Brittle (B); Ductile (D)
Crystal structure	fcc
Crystal lattice (Å)	3.62 (D); 3.17 (B) (1 Å＝10^{-10}m)
Potential function	Morse
Potential parameters	D: 0.34 eV; α: 1.359 $Å^{-1}$; r_{eq}: 2.87 Å (D) D: 0.54 eV; α: 2.47 $Å^{-1}$; r_{eq}: 2.6 Å (B)
Workpiece dimension (Å)	50×30×50
Tool dimension (Å)	30×50×50
Tool property	rigid body
Tool radius	sharp
Tool rake angle	–40°, –20°, 0°, 10°, 20°, 30°
Depth of cut (Å)	5, 10, 15
Speed (m/s)	300 (D); 200 (B)
Temperature (K)	293

3.1 Effect of depth of cut

Figure 5 shows the MD simulation results of burrs formation process at different depth of cut. The tool rake angle is 0°, while the relief angle is 10°. The burrs geometry is similar under different conditions, but the dimension of the burrs is increased with the increasing depth of cut. When the depth of cut falls in the range of angstrom level, the generated burrs are basically positive and the burrs are mainly generated by shear force. The generated burrs dimension is small compared with workpiece in the conventional manufacturing while the burrs cannot be ignored in the case of

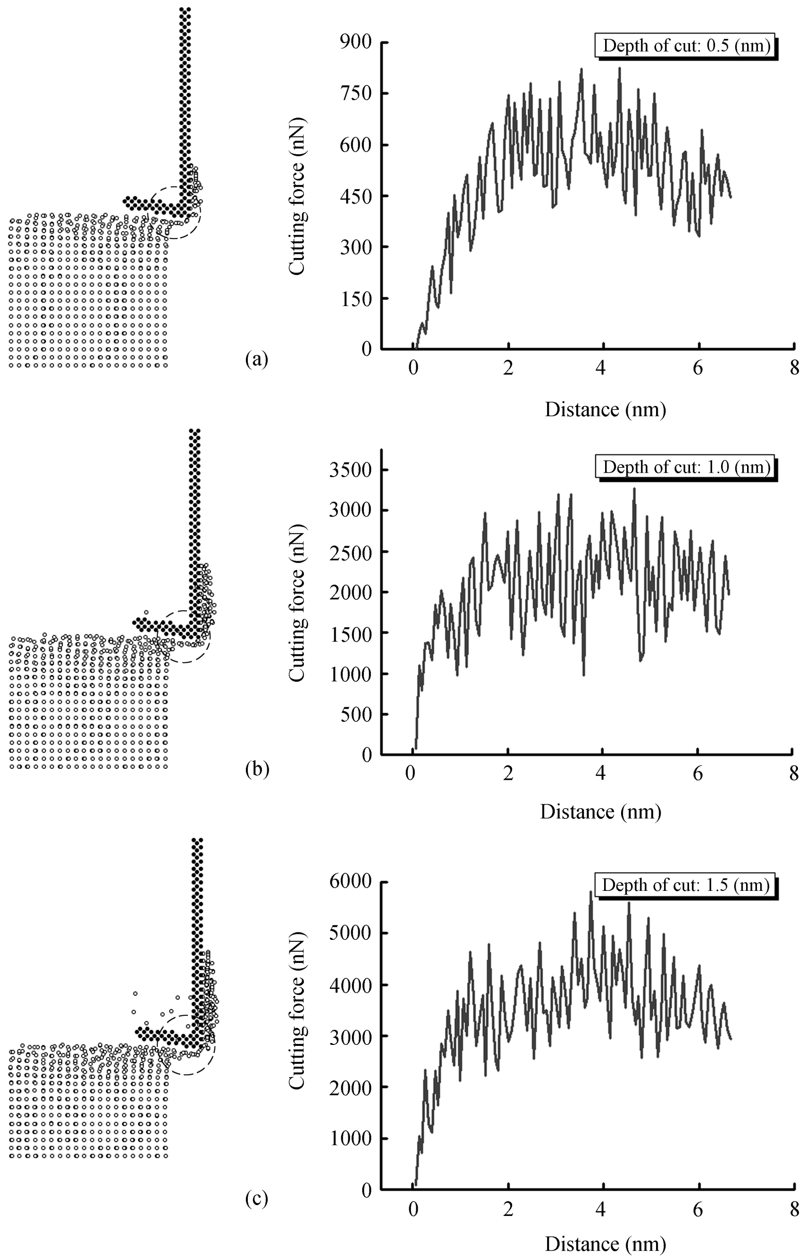

Figure 5 MD simulation generated burrs under different depth of cut. (a) Depth of cut: 0.5 nm; (b) depth of cut: 1.0 nm; (c) depth of cut: 1.5 nm.

nanometric manufacturing technology. The cutting force increases with the increasing depth of cut because the interacting atoms increased in this process. The dislocation is generated continuously in the cutting process, the generated dislocation accumulated and formed potential barrier which increases the difficulty of further plastic deformation and thus decreases the cutting force. The cutting force is reduced after the tool passes by, and no more dislocation is generated. The piled up dislocation begins to release, which reduced the cutting force.

3.2 Effect of tool angle

Figure 6(a)—(e) shows the MD simulation of generated burrs with different rake angles. The results demonstrate that increasing of rake angle results in decreasing of the burrs dimension. This can be explained by the fact that small rake angle can reduce the compressing effect and then reduce the plastic deformation. When the tool passes the exit of workpiece, most of materials are removed in the form of chip.

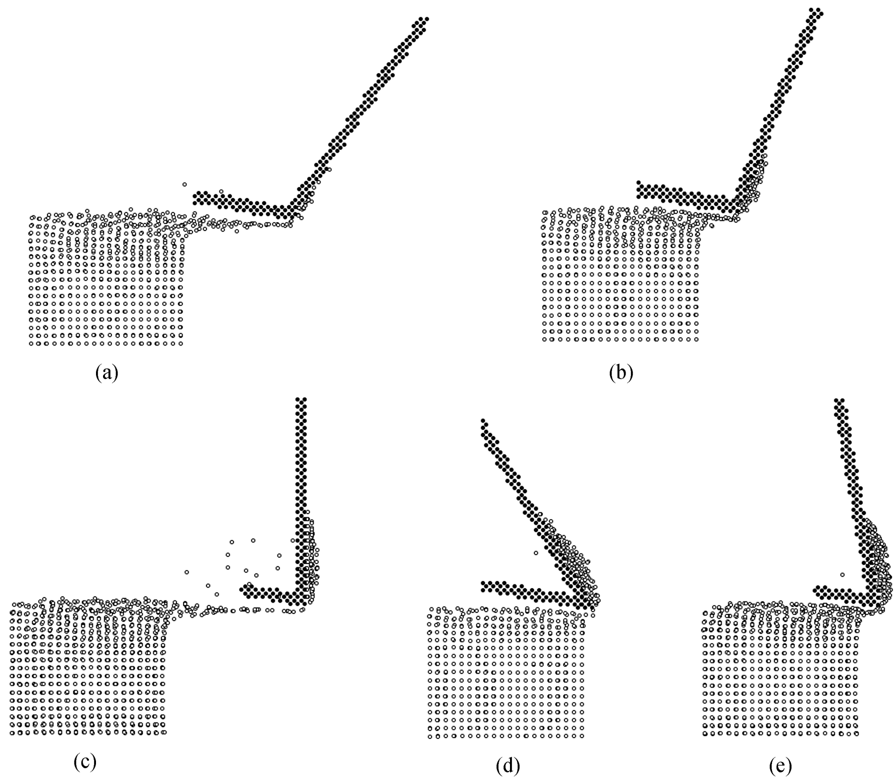

Figure 6 MD simulation burrs generation with different rake angles (depth of cut: 8 Å, ductile materials). (a) Rake angle: –30°; (b) rake angle: –20°; (c) rake angle: 0°; (d) rake angle: 20°; (e) rake angle: 30°.

3.3 Effect of materials type

Figure 7(a)—(e) shows MD simulation of burrs generation process in the case of nanometric cutting brittle materials. The result shows that when the rake angle lies in the range –30°—30°, the cracks are generated near the tool tip and extended to the internal of workpiece and formed negative burrs, at the same time the negative rake angle tool may generate a large hydrostatic pressure which results in large plastic deformation and amorphous layer, then deteriorating the surface roughness. While the rake angle lies in the range of positive value, the cracks near tool tip propagate parallel to the cutting direction and formed positive burrs. The normal pressure is small under this condition which results in little plastic deformation and better surface quality is acquired.

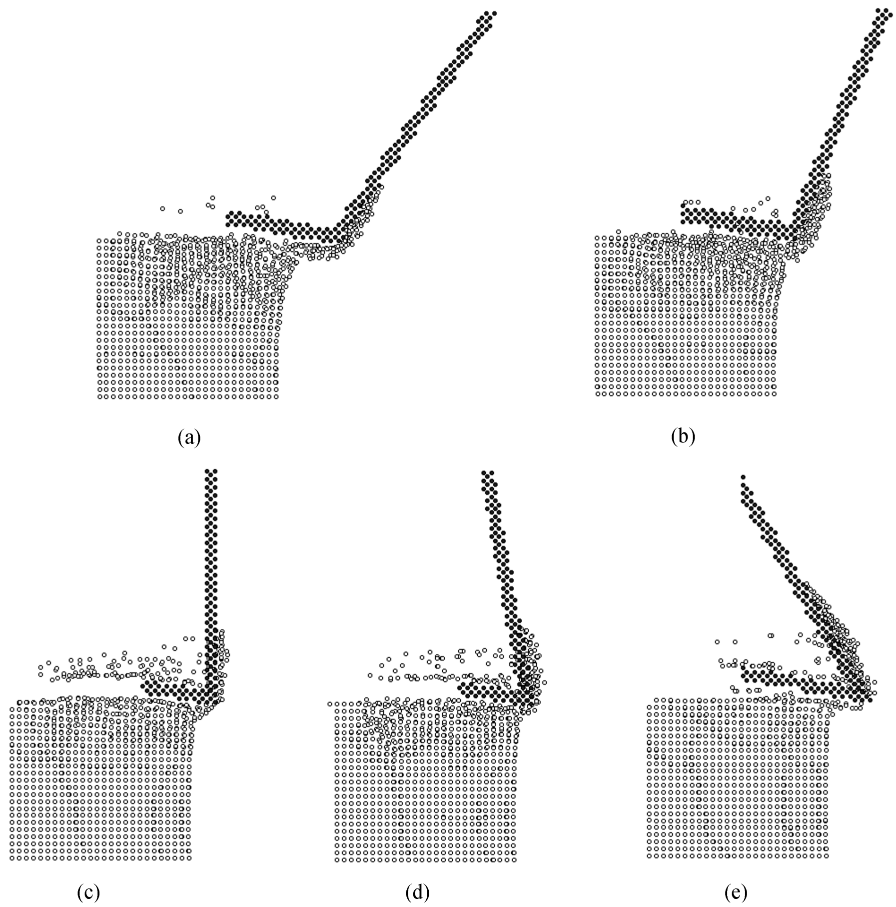

Figure 7 MD simulation generated burrs with brittle materials (depth of cut: 8 Å). (a) Rake angle: –30°; (b) rake angle: –20°; (c) rake angle: 0°; (d) rake angle: 20°; (e) rake angle: 30°.

Compared with cutting ductile materials, there exists a transition from negative burrs to positive burrs when cutting brittle materials. The negative burrs generated in the case of manufacturing brittle materials would interrupt cutting process and impact the tool thus shortening its using life. Clearly, the choice of adequate tool technique parameters is of great importance in reducing the burrs dimension.

4 Conclusion

Although many studies have been carried out about burrs formation in the conventional manufacturing process, the efforts on micro-mechanism of burrs generation are limited. Taking the single crystal copper as example, this paper investigates burrs generation mechanism in nanometer cutting process. After that we draw some conclusions:

(1) The MD simulation results show that there are five stages in the burrs generation process,

namely, stable cutting, initialization of burrs, development, initialization of crack, burrs generation. With the propagation of shear deformation, the uncut layer is removed in the form of chip while in the stable cutting stage the burrs begin to build. The energy needed to generate chip is transformed into the energy needed to generate burrs after the initialization of burrs. Finally, the plastic bending and the burrs are generated at the exit of materials (Figure 8).

(2) The burrs geometry depends on the workpiece type (ductile or brittle) as shown in Figure 9. When cutting ductile materials, the cracks propagate parallel to the cutting direction and form positive burrs; while cutting brittle materials, the cracks propagate into the workpiece and formed negative burrs. The negative burrs may result in abrupt fractured and impact tool tip thus shortening the using life of the tool.

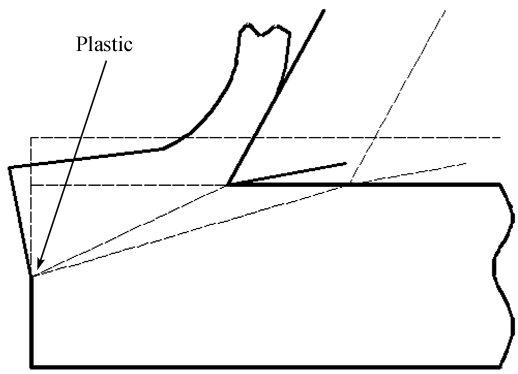

Figure 8 Initialization of burrs.

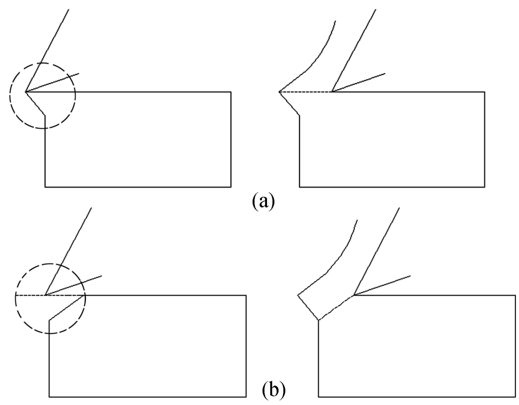

Figure 9 Geometry model of burr. (a) Positive burr; (b) negative burr.

(3) The depth of cut become changing since the initialization of burrs no matter generated positive or negative burrs. The depth of cut is decreased in the positive burrs formation process while the depth of cut is increased in the negative burrs formation process.

(4) Burrs formation process observed using MD simulation shows good agreement with that reported in the literature at macro and micro level based on extensive experiment [12,13]. Consequently, MD simulation can be used as an inexpensive tool for studying the process parameters before conducting extensive and expensive experimentation.

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