Study on the Mechanism of Chip Formation in Nanometric Cutting of CaF_2 by Molecular Dynamics

G.B. Xiao[1], S. To[1*] and M.J. Chen[2]
[1]*State Key Laboratory in Ultra-precision Machining Technology, Department of Industrial and Systems Engineering, The Hong Kong Polytechnic University, China*
[2]*School of Mechanical Engineering, Harbin Institute of Technology, China*

[*]*Sandy.To@polyu.edu.hk*

Abstract

Molecular dynamics (MD) simulations are performed to study the nanometric cutting process of CaF_2. The results show that the relative orientation between cutting direction and slip system {100}<011> has great influence on the mechanism of chip formation. When their relative orientation favours slipping of atoms on the slip system, slipping on the slip system becomes the main mechanism of chip formation. Otherwise, amorphous phase transformation and shearing in the amorphous region is primarily responsible for chip formation. When tool rake angle becomes negatively larger, shearing in the amorphous region plays a greater role in chip formation.

1 Introduction

CaF_2 is a very excellent material for optical imaging systems and deep ultraviolet photolithography systems [1]. The single-point diamond turning of CaF_2 [1, 2] has caught much interest in recent years for its capbility to produce complex surfaces. The previous studies are mostly based on experiments and the mechanism of chip formation is not well understood. In this paper, Molecular dynamics is adopted to study the mechanism of chip formation in the nanometric cutting process of CaF_2.

2 Methodology

The MD model of nanometric cutting of CaF_2 is shown in Figure 1 a). A thin sheet of CaF_2 atoms is used to apply external force on the workpiece instead of a real tool. The dimension of the workpiece is 32.8nm×4.4nm×9.8nm. The total number of atoms in the specimen is around 110,000. The cutting depth is 3.3nm and the cutting speed is 50m/s. The temperature of the model is set as 20℃. Five cutting orientations were adopted as shown in Figure 1 b), c) and d). Five different tool rake angles are adopted for the cutting orientation of (011)$\langle 0\bar{1}1\rangle$, which are 0°, -10°, -20°, -30° and -45° respectively. A method previously proposed by the authors [3] is adopted to identify those slipping atoms in the cutting region.

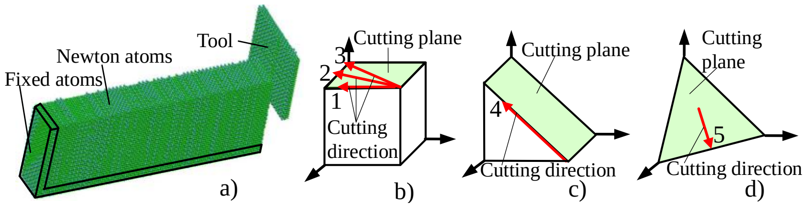

Figure1:(a) MD model for nanometric cutting of CaF_2 and adopted cutting directions, which are (b) $\langle 0\bar{1}0\rangle$, $\langle \bar{1}\bar{2}0\rangle$, $\langle \bar{1}\bar{1}0\rangle$, (c) $\langle 0\bar{1}1\rangle$ and (d) $\langle 11\bar{2}\rangle$ respectively.

3 Results and discussion

3.1 Influence of cutting orientation on chip formation

The simulation results are shown in Figure 2. For every cutting orientation, the entire workpiece, the slipping atoms in the cutting region and the corresponding cutting orientation and slip planes are shown in sequence. It can be seen that the chip size and material flowing direction is different for different cutting orientations, indicating that crystal anisotropy has great influence on chip formation.

In Figure 2 a) and e), the chip formation is mainly due to the amorphous phase transformation and subsequent shearing in the amorphous region. At the same time, there is also some slipping process along the slip system. To the contrary, in Figure 2 b), c) and d), slipping along the slip system is the main mechanism for chip formation. The difference can be explained by the different relative orientation between cutting direction and slip system. The cutting orientation $\langle 0\bar{1}0\rangle$ is perpendicular to the slip plane and thus it is difficult for the material to slip along the slip plane (Figure 2a),. In Figure 2 b), c) and d), the cutting orientation is inclined to the slip plane and thus it is easier for the material to slip along the slip system. The cutting orientation $\langle 11\bar{2}\rangle$ does not favour slipping on slip system, because slip vector of CaF_2 is (001)$\langle \bar{1}10\rangle$ and thus it is opposite to the cutting direction (Figure 2e).

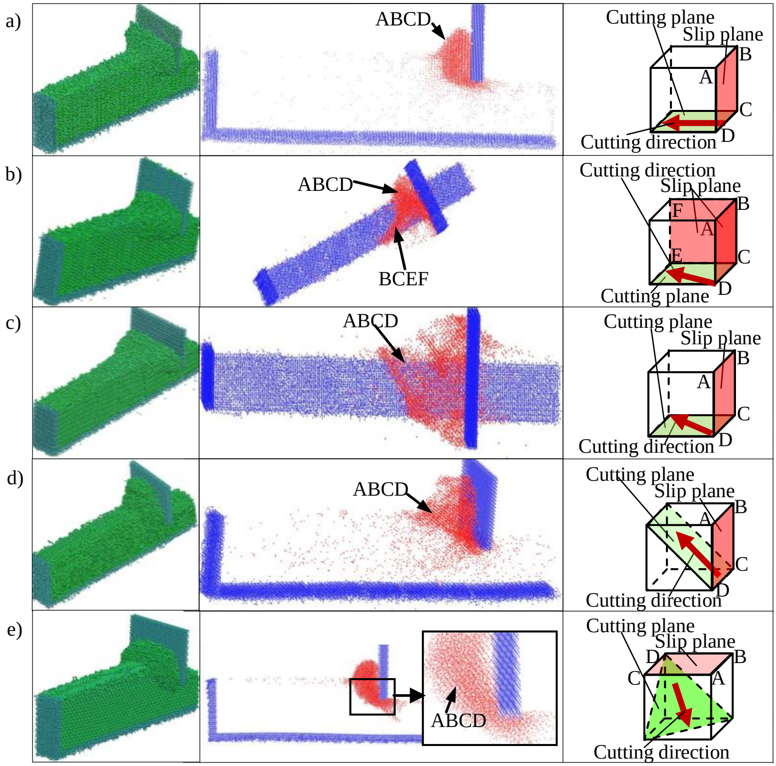

Figure 2: Simulation results in various cutting orientations (a) $<0\bar{1}0>$, (b) $<\bar{1}\bar{2}0>$, (c) $<\bar{1}\bar{1}0>$, (d) $<01\bar{1}>$ and (e) $<11\bar{2}>$.

3.2 Influence of tool rake angle on chip formation

Figure 3 shows the slipping atoms for cutting orientation (110)$<01\bar{1}>$ under various tool rake angles. The case for tool rake angle of 0° has already been shown in Figure 2 d) and thus it is omitted here. It can be seen that slipping on the slip system is the main mechanism of chip formation when tool rake angle is 0° and -10°, while amorphous phase transformation and subsequent shearing in the amorphous region is the main mechanism of chip formation under tool rake angle of -20°, -30° and -45°. This means that larger negative tool rake angle promotes the amorphous phase transformation and at the same time can impede the slipping on slip system. This may be caused by the higher hydrostatic stress under larger negative rake angle.

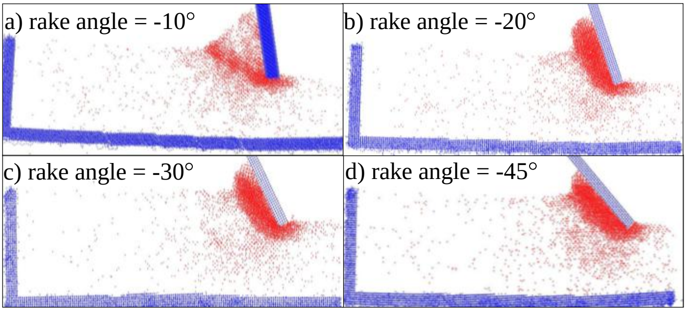

Figure 3: Slipping atoms in the cutting region under various tool rake angles (a) rake angle is -10°, (b) rake angle is -20°, (c) rake angle is -30° and (d) rake angle is -45°.

4 Conclusion

In this paper, MD simulations have been performed to investigate the influence of cutting orientation and tool rank angle on the chip formation. The results show that when the relative orientation between cutting direction and slip system favours slipping on the slip system, slipping on slip system is the main mechanism of chip formation. Otherwise, amorphous phase transformation and subsequent shearing in the amorphous region is a main mechanism of chip formation. As tool rake angle becomes negatively larger, amorphous phase transformation and subsequent shearing in the amorphous region plays a greater role in chip formation.

5 Acknowledgement

The authors would like to express their sincere thanks to the Research Grants Council of Hong Kong for their financial support of the research work .

References:

[1] JW Yan, JI Tamaki, et al, Int. J. Adv. Manuf. Technol. 24 (2004) 640-646.

[2] JW Yan, K Syoji, J Tamaki, J. Vac. Sci. Technol. B 22(1) (2004) 46.

[3] MJ Chen, GB Xiao, et al, J. Comput. Theor. Nanosci. 9 (2012) 1–7.