

# Investigation of Ultra-Precision Machining Using Molecular Dynamics Simulation and Experiments on Single Crystal Silicon

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**ABSTRACT:** Ultra-precision machining is an advanced method for production of materials with nanoscale surface roughness. It is widely used in the manufacturing of precision components for defense, aerospace, optics, and electronics industries. For this feature, only a few industrial countries have access to this technology. Due to the high precision of this technology, many factors can affect the final surface quality. Machine components, machining conditions, tool geometry and material, environmental condition, workpiece material as well as vibration, are among the factors that are reviewed in this article. Afterwards, the effect of cutting depth on machining mechanism and surface quality is investigated using molecular dynamics investigation. The results revealed that when the ratio of cutting depth to tool edge radius becomes lower than 0.5, the effective rake angle would be bigger than the nominal rake angle. Furthermore, under this condition, the dominant machining mechanism is extrusion, which is different from the micro cutting mechanism. Finally, a series of experiments was conducted to study the impact of the undeformed chip thickness on the chip morphology and surface topography. For this purpose, field emission scanning electron microscopy, 2D ultra-precision point autofocus probe as well as white light interferometer were exploited. The results indicated that at the lower relative tool sharpness, chip edge tearing occurs. Besides, by increasing this parameter to 100 nm, silicon nano-ribbons is created.

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## 1- Introduction

Ultra-Precision Machining (UPM) is an advanced method by which 0.1-1  $\mu\text{m}$  form accuracy and 1-10 nm surface roughness is achievable [1]. Nowadays, the trace of this process could be found in lots of products. For instance, camera lenses, laser scanners, medical and defense sensors as well as contact lenses are all cases which this technology has been used. Using this method, ductile mode machining of brittle materials such as silicon is possible; which increases the surface integrity [2]. Since a lot of parameters could affect the surface roughness in this process, many researches have been done on the relationship between these factors and the final surface finish. Some studies have tried to provide an ideal model between different kinds of surface roughnesses [3] and machining variables [4]. However, most of the researches have focused on two areas of simulation [5] and empirical experiments [6].

In the current study, a set of molecular dynamics simulations was conducted to examine the effect of tool edge radius on the cutting mechanism and surface quality. Moreover, this parameter was experimentally investigated. In this regard, chip morphology as well as surface topography were studied.

## 2- Methodology

### 2-1- Molecular dynamics simulation

Due to the submicrometer undeformed chip thickness in

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UPM process, it is impossible to use finite element method for simulations. The reason for this is the limitation of continuum mechanics in the nano and atomic-scale dimensions. Molecular Dynamics (MD) is an alternative approach for nanometric studies, such as UPM. This method based on interatomic interactions and their motion equations.

Fig. 1 indicates the schematic model used in MD simulations. Single crystal diamond cubic silicon workpiece with the cutting plane of (001) is defined. Additionally, for machining, a 3-nm diamond tool in the cutting direction of [0 -1 0] is used. The interaction between Si-Si and Si-C particles are described by Tersoff potential function [8].

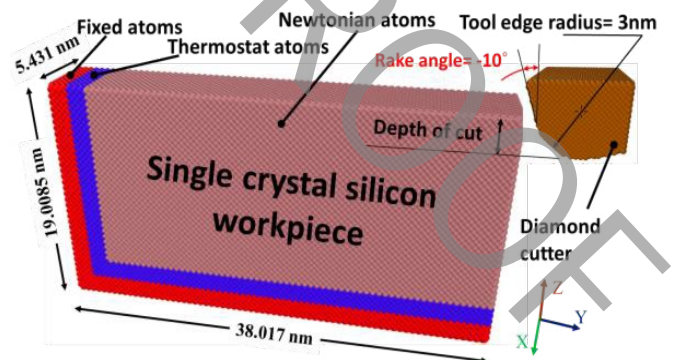


Fig. 1. Schematic of molecular dynamics model for ultra-precision machining of silicon substrate.

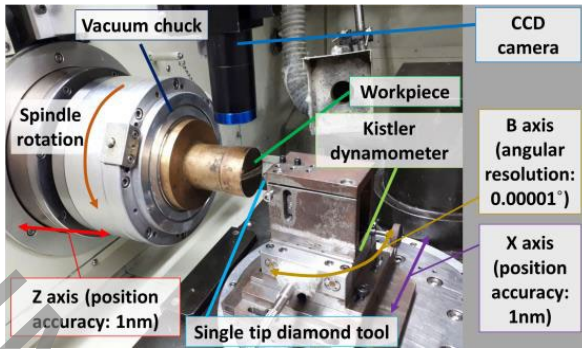


Fig. 2. Interior view of the 3-axis control ultra-precision machine.

### 2-2- Empirical experiment

A 3-axis ultra-precision machine (NACHI ASP-15, Japan- Fig. 2) was used for machining a p-type single crystal silicon wafer with plane orientation (110). Furthermore, a single crystalline diamond tool (Tokyo Diamond Corp., Japan) with the nose radius of 10 mm, edge radius of 100 nm as well as rake and clearance angle of  $0^\circ$  and  $8^\circ$ , respectively, was employed. The machined surfaces were examined by an ultra-precision point autofocus 2D probe (with the precision of 100 nm) and a white light interferometer. Finally, a Field-Emission Scanning Electron Microscope (FE-SEM, Model Inspect F50) was used to observe the sample surfaces.

Three different undeformed chip thickness of 25, 50 and 100 nm were used to apply the same Relative Tool Sharpness (RTS) ratios in MD simulations (0.25, 0.5 and 1). A constant 5- $\mu\text{m}$  depth of cut was also used in all conditions. Besides that, the cutting speed was adjusted as 50 m/s. This was done by changing the spindle rotation rate at different cutting diameters.

### 3. Results and Discussion

Simulation results indicate that the dominant mechanism at RTS=0.25 is extrusion. By increasing RTS to 0.5, the shearing mechanism starts as the conventional machining. In this circumstance, more volume of the surface atoms is pushed toward the chip. This mechanism also continues up to RTS=1; and hence, there is no appreciable difference on the machined surfaces.

As demonstrated in Fig. 3 (a), owing to the minor

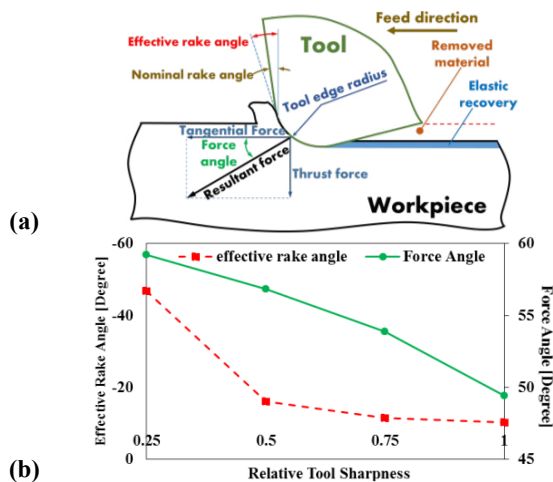


Fig. 3. a). Nanoscale cutting mechanism, b). Influence of RTS on effective rake angle and force angle.

undeformed chip thickness in the nanometric machining, the effective rake angle is different from the nominal rake angle. As can be seen in Fig. 3.(b), the bigger effective rake angles occur at the lower depths of cut. It is also observed that increasing the RTS to 1, results in changing the effective rake angle to the nominal rake angle ( $-10^\circ$ ). This is because of changing the material removal mechanism from nanometric to conventional machining. Under this condition, the rake face will be in contact to the particles into the material flow, instead of the cutting edge.

The results of force angle also show almost the same trend. In the extrusion mechanism, a large number of atoms in front of the tool was compressed beneath the cutting edge and makes the freshly machined surface. This highly hydrostatic pressure leads to the maximum value in the force angle. As the depth of cut increases, the more portion of the particles is transformed into the chip, which results in dropping the force angle.

Fig. 4 illustrates the FE-SEM micrograph of cutting chips at different RTS ratios. Although silicon has a brittle nature, continuous chip and consequently, ductile mode machining is seen at RTS=0.25. However, sporadic chip edge tearing is observed. Due to the variation along the undeformed chip thickness, the stress concentration is higher in the thinner edge and as a result, chip edge tearing takes place. By increasing RTS up to 0.5, the cutting chips are still continues, with the difference that there is no chip edge tearing. The continuous-form chips remain still at RTS=1. However, more magnification demonstrates that it is not quite continuous and nano ribbons are formed.

### 4. Conclusion

Ultra-precision Machining (UPM) process was explained in this study. Next, Molecular Dynamics (MD) simulations and empirical experiments were carried out on single crystal

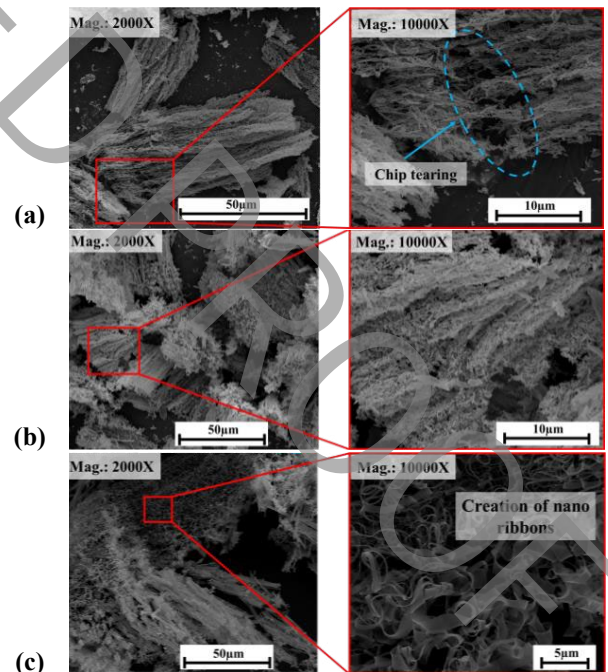


Fig. 4. FE-SEM micrograph of chips obtained at RTS of a. 0.25, b. 0.5 and c. 1.

silicon wafers. The main conclusions are as below:

- Although the ultra-precision machine tool is similar to the conventional machines, the movement mechanism of the machine tool, and consequently, material removal behavior vary with each other.
- Simulational results demonstrate that the least relative tool sharpness (RTS) for chip formation is 0.25. In this circumstance, extrusion mechanism is dominant and the effective rake angle increases dramatically.
- Despite the brittle nature of silicon substrate, the ductile mode cutting is achievable at the RTS ratios below than 1.
- Although the single crystal diamond was used as the cutting tool, different types of tool wear are still inevitable and result in non-uniformity on the machined surface. Tool adhesion is also seen on the cutting edge which results in various roughnesses along the machined surface.

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