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Ultra-Precision Cutting of Monocrystalline Calcium Fluoride at Elevated Temperatures

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Brittle materials such as calcium fluoride (CaF_2) have been widely employed in the manufacturing industry due to their excellent mechanical, physical, optical and electrical properties. But, manufacturing of brittle materials faces many challenges from technical to economic aspects. To obtain a smooth and damage free surface of brittle materials, traditional machining processes such as grinding, lapping and polishing are commonly used, which is very costly and extremely time consuming. Ultra-precision ductile mode cutting is thereafter an alternative way to achieve such high quality and crack free surfaces of brittle materials. Although ductile mode cutting of CaF_2 is possible, it has been shown to exhibit microstructural changes which has an adverse effect on the machined surface quality. In this paper, a novel approach has been proposed for machining of CaF_2 at elevated temperatures to enhance the plasticity of the substrate material thus reducing or eliminating the subsurface damage completely. To this end, a realistic molecular dynamic (MD) simulation model has been developed to provide an atomistic insight into the machining process with an appropriate choice of valid interatomic potential. Based on this model, MD simulations have been carried out to study the nanoscale cutting of single crystal CaF_2 at both room temperature and elevated temperature.

1. Introduction

In today's modern technological era, many vital components are made up of hard and brittle materials which require stringent ultra-precision machined surface with tolerances approaching the atomic length scale to fulfil their functionalities [1-4]. Calcium fluoride (CaF_2) is a transparent colorless single crystal with a fluorite-type crystal structure having extremely high permeability, good refractive index and excellent color aberration compensation ability ranging from 125 nm (ultraviolet) to 12 μm (infrared) wavelength. As such, CaF_2 is not only an optical substrate material for dark-field imaging systems but also an indispensable lens substrate material for large-scale semiconductor lithography systems, more especially when 193 and 157 nm lithography systems were developed. CaF_2 is becoming the most commercially important material within the optics community lately. Specific applications for CaF_2 include 193 nm excimer laser components, chromatic aberration correction of 193 nm stepper lens systems, and stepper lenses for future 157 nm systems [5].

Calcium fluoride (CaF_2) have been widely employed in the manufacturing industry due to their excellent mechanical, physical, optical and electrical properties. But, manufacturing of brittle materials faces many challenges from technical to economic aspects. To obtain a smooth and damage free surface of brittle materials, traditional machining processes such as grinding, lapping and polishing [6] are commonly used, which is very costly and extremely time consuming. Therefore, ultra-precision cutting is thereafter an alternative way to achieve such high quality and crack free surfaces of brittle materials [7]. Although ductile mode cutting of CaF_2 is possible, it has been shown to exhibit microstructural changes which has an adverse effect on the machined surface quality. In this paper, a novel approach has been proposed for machining of CaF_2 at elevated temperatures to enhance the plasticity of the substrate material thus reducing or eliminating the subsurface damage completely.

2. MD Simulation of Nanometric Cutting of CaF_2

A 2-D molecular dynamics (MD) model used in this study is shown in Fig. 1. The geometrical details and process parameters are shown in Table 1. The cutting tool in the model is assumed as a rigid body. The workpiece is divided into three unique zones: Newtonian, thermostat and boundary zones. The boundary atoms are assumed to remain unaffected or rigid during the simulation and were kept fixed in their initial lattice positions, thus it reduces the boundary effects and maintains the symmetry of the lattice. Fig. 2 shows the snapshots of chip formation made by MD simulation of cutting processes at different undeformed chip thickness and varying temperatures under the conditions listed in Table 1.

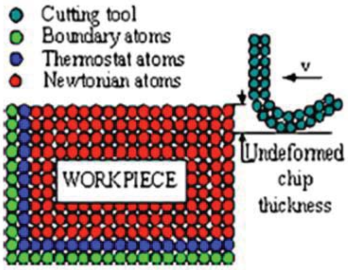
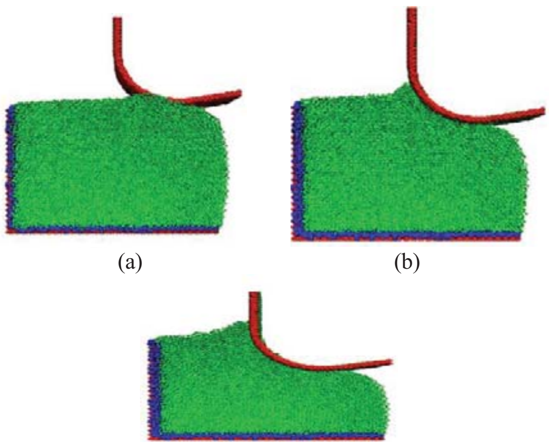


Fig. 1 Schematic model of nanometric cutting of CaF_2

Table 1 Geometrical and process parameters used in MD simulation

Work material	Monocrystalline CaF_2
Workpiece dimensions	45 nm x 22.5 nm x 6 nm
Cutting edge radius	7 nm
Depth of cut	3.5 nm, 4 nm, 5 nm and 6 nm
Cutting orientation and cutting direction	Case 1 : {111} <-110> Case 2 : {110} <001>
Rake angle and clearance angle	0° and 10°
Workpiece temperature	300 K, 325 K, 350 K, 400 K
Cutting Speed	100 m/s
Potential energy function	Born Huggins-Meyer (BHM)
Time step	1 fs



(a) (b)

(c)

Fig. 2 Snapshots of the MD simulation at depth of cut (a) 3.5 nm (b) 5 nm and (c) 6 nm.

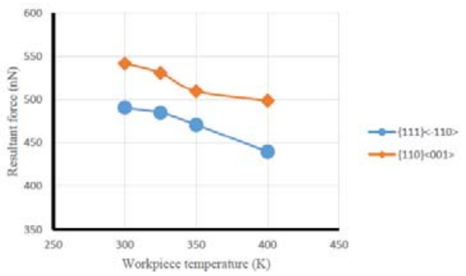


Fig. 3 Resultant force as a function of temperature and crystal orientation.

Fig. 3 shows a comparison between the different crystal orientation and cutting direction. It can be seen clearly that the {111} <-110> crystal set up is the easiest cutting combination as compared to the {110} <001>. MD simulation results shows that work material plasticity is enhanced when machining at elevated temperatures as compared to that at room temperature irrespective of the cutting directions. So that there is a cutting force reduction when cutting of CaF_2 at elevating the workspace temperatures. Higher workpiece temperature elevated, deriving a smaller cutting force.

3. Experimental Setup

Experimental verification was conducted on an ULG-100 Toshiba 4-axis ultra-precision machining system. CaF_2 single crystals with a dimension of 10 mm × 10 mm × 5 mm were used as the workpiece having a crystal orientation of {111}, and a smooth surface finish of less than 2 nm as well. No further surface treatments were required before the cutting experiments. The workpiece was mounted on a prefaced aluminum blank using a heat-softening glue. A round monocrystalline diamond tool with a nose radius of 0.8 mm, rake angle of -10° and relief angle of 10° was used to cut CaF_2 single crystals. Electrical heating was used to realize an elevated temperature and an infrared camera was used to monitor the workpiece temperature as shown in Fig. 4. Fig. 5 shows the measured CaF_2 single crystal temperature of 100.2°C. A Kistler dynamometer 9251B1 with Type 5051A amplifiers was used to measure the cutting force.

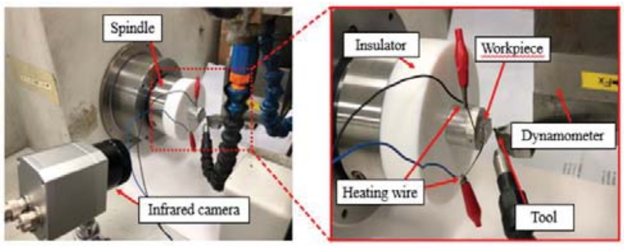


Fig. 4 Experimental set-up for machining of CaF_2 single crystal at elevated temperatures

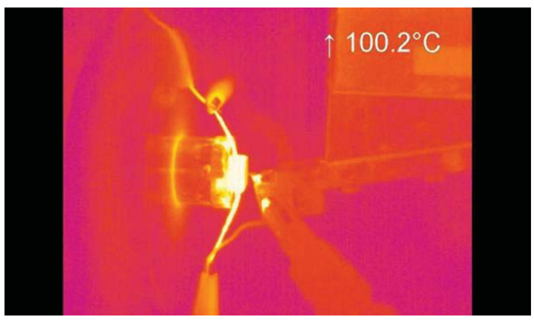


Fig. 5 Infrared camera reading indicating temperature obtained for 100°C under hot machining

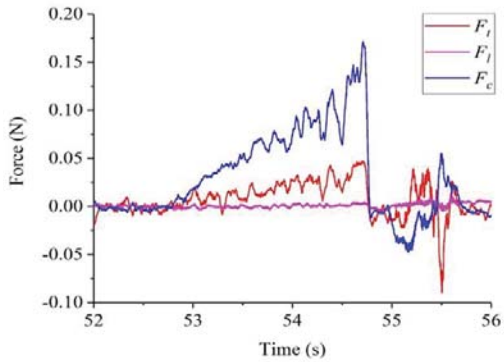
The micro cutting experiments were performed on the {111} CaF_2

single crystals at both room temperature of 23°C and an elevated temperature of 100°C. The experiments aimed to uncover the influence of temperature on the anisotropic effect of CaF_2 single crystals. Table 2 gives the cutting conditions used in the experiment.

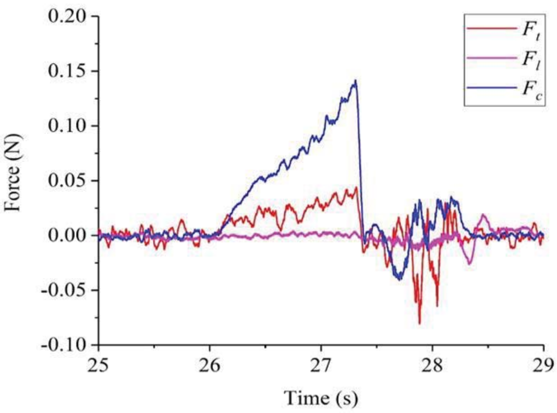
Table 2 Cutting conditions used at both room temperature and elevated temperature.

Spindle Speed	1200 rpm
Feed rate	1 mm/min
Depth of Cut	5 µm
Coolant	Oil mist

4. Experimental Results and discussion



(a) Cutting forces measured at room temperature of 23°C



(b) Cutting forces measured at an evaluated temperature of 100.2°C

Fig. 6 Cutting forces measured for cutting of CaF_2 single crystals at (a) room temperature and (b) evaluated temperature of 100°C.

The cutting force measured for cutting of CaF_2 single crystals at room temperature of 23°C and the elevated temperature of 100.2°C are shown in Fig 6 (a) and (b) respectively. It shows the variation of the cutting forces and thrust forces obtained from the experiments. Experimental results show that there is a slight reduction in thrust force when cutting at the elevated temperature compared with that at room temperature. That is well agreed with the MD simulation results, which indirectly indicated the enhancement of work material plasticity at elevated temperatures. It should be noted that CaF_2 has a high thermal expansion rate compared to other brittle materials, which would derive a loss of form accuracy in ultra-precision machining of CaF_2. This is to be expected as the workpiece is difficult to be deformed at low temperature. At high temperatures however, interatomic bond distances increase which leads to a decrease of the workpiece interatomic bonding energy, and consequently a decrease of the work piece's strength. It also must be noted that temperature variation at room temperature (23℃) and the selected variable at elevated temperature (100.2℃) may not be significant enough to expect a large reduction in the cutting forces, because it is difficult for CaF_2 having a temperature stabilization beyond this point during this experiment.

5. Conclusions

In this paper, a molecular dynamics (MD) model has been developed as a tool to study the nanoscale machining of single crystal CaF_2. A realistic MD simulation model has been shown to model the CaF_2 substrate at both room temperature and elevated temperature with the usage of an appropriate valid interatomic potential. The MD simulation results indicate that for machining of single crystal CaF_2 the thrust force decreases as the temperature increases irrespective of the cutting directions. This decrease in thrust force at elevated temperatures has shown to compare well with the experimental results that there is a slight trust force reduction when machining of single crystal CaF_2 at 100.2°C. It demonstrates that machining of single crystals at elevated temperatures is a better proposition by enhancing the crystal plasticity in order to reduce or eliminate subsurface damage for machining of CaF_2 single crystals.

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