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Modelling and experimental investigation on nanometric cutting of monocrystalline silicon

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Abstract

A new model to understand the behaviour of how materials are removed from workpiece in nano cutting is proposed. This model postulates that the mechanism of nanometric scale material removal is based on extrusion, which is different from the shearing mechanism in conventional cutting. It also explains why brittle materials are removed in ductile mode. Analytical results from molecular dynamics and nano indentation show good agreement with the proposed modelling. Experiments are conducted to verify the new model for nanometric cutting of monocrystalline silicon. The theoretical modelling and experimental verification present a good understanding of nano-scale material removal and provide an approach to fundamentally control the machining performance.

Keywords: Modelling; Brittle material; Micro machining; Nano cutting

1. Introduction

Mechanical cutting is one of the primary material removal processes as it has high economical value, process stability, and user-friendly operation. The machining performance and parts quality are essentially determined by the material removal scale. Material removal at nanometric scale is increasingly required in micro machining and ultra-precision machining to produce parts of intricate features and surface finish quality [1–19]. In conventional machining, the cutting mechanism is well established, i.e. the chip formation is mainly due to material shearing [20–22]. But the mechanism of nano-sacle cutting is still not clear. In recent years, many investigations have been conducted to study the cutting behaviour in nano-scale using molecular dynamics (MD) simulation [23–30] or material deformation behaviour using nano indentation [31–33]. However, little research has been done in establishing a nanometric cutting model.

In this paper, a model for cutting materials at nanometric scale is proposed. This extrusion model reveals that the nano-scale cutting mechanism is different from that in conventional machining. Molecular dynamics simulation and nano indentation analysis are applied to support the proposed mechanism. To verify the model, taper cutting experiments are conducted and nanometric monocrystalline silicon surfaces are generated.

2. Modelling of nano cutting monocrystalline silicon

2.1. Ratio of undeformed chip thickness to cutting edge radius less than threshold

In conventional machining, it is accepted that the mechanism of chip formation is due to the shearing effect in the cutting zone of the work materials [20–22]. Although this classic cutting model is being applied by researchers no matter how small the undeformed chip thickness is, there is no evidence showing that the work material is removed by shearing in nanometric cutting. An obvious fact is that when cutting brittle materials in ductile mode, no sheared chips were found when the undeformed chip thickness is reduced to few nanometres or less.

Unlike in conventional cutting, where the depth of cut is significantly large compared to the cutting edge radius, in nanometric cutting this edge effect can no longer be

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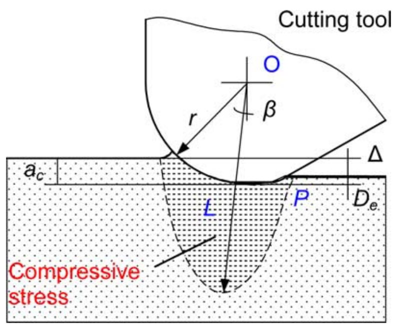

Fig. 1. Schematic illustration of nanometric cutting model at ratio of undeformed chip thickness to cutting edge radius less than the threshold.

neglected. Regardless of the nominal rake angle, either it is positive, negative, or 0°, the effective rake angle is always negative, as is apparent in Fig. 1. The negative rake face produces the necessary compressive stress to enable plastic deformation to occur in front of the cutting edge. With a decrease in the ratio of undeformed chip thickness, a_c, to cutting edge radius, r, there could be a stagnation point S (threshold). When the ratio is decreased below the point S, chip formation does not occur but elastic and plastic deformation do as shown in Fig. 1, where r is the cutting edge radius. After the work material has passed the lowest cutting edge point L, the elastic portion D_e springs back. The plastic deformed portion Δ leads to a lasting deformation behind the point P, and β is the angle from the vertical direction to the resultant force direction. The compressive stress distribution depends on the resultant cutting force. The ratio is associated with the material property, tool geometry and machining conditions.

2.2. Ratio of undeformed chip thickness to cutting edge radius greater than threshold

In the case of the ratio of undeformed chip thickness to cutting edge radius being above the stagnation point S, the material below the point S undergoes an elastic and plastic deformation as shown in Fig. 2. After the work material has passed the lowest cutting edge point L, the elastic portion D_e springs back. The plastic deformed portion Δ leads to a lasting deformation behind the point P. The material above the point S is extruded to form chips.

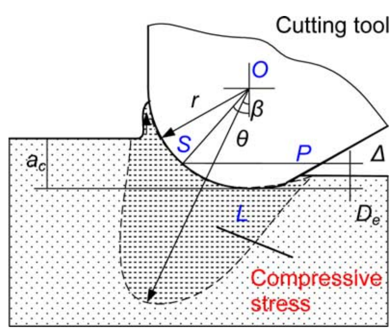

Fig. 2. Schematic illustration of nanometric cutting model at ratio of undeformed chip thickness to cutting edge radius greater than the threshold.

Monocrystalline silicon has a brittle nature at ambient temperature. However, its amorphous modification exhibits a plastic flow under low loads so that possible phase transformation events in machining operation are of great significance in producing damage-free components by machining [32]. The amorphous transformation is governed by the octahedral shear stress, τ_{oct}, with its threshold $\tau_{oct}=4.6$ GPa in $<100>$ direction and 7.6 GPa in $<110>$ direction [32]. The amorphous phase appeared during loading will disappear when the unloading takes place at a small indentation load, because in this case a re-crystallization from the amorphous to the original diamond structure will occur during unloading. Only when the compressive stress in loading, σ_0, reaches a critical value of 8 GPa, such that a second phase transformation from amorphous silicon to β-silicon takes place, an amorphous phase will remain after unloading [32]. For amorphous silicon, the silicon atoms are not arranged in an ordered structure, differently from crystalline silicon. The loss of structure order results in defects such as dangling bonds and distorted Si–Si bonds as shown in Fig. 3. Hence, the phase transformation significantly reduces the threshold stress of dislocation. Unfortunately, very little is known about the mechanical properties of amorphous silicon.

Because of the cutting edge radius effect, the effective rake angle of the cutting tool can be derived with the following equation

$$\gamma_e = -\frac{\pi}{2} + \frac{1}{2}\cos^{-1}\left(1 - \frac{a_c}{r}\right) \quad (1)$$

where γ_e is the effective rake angle as shown in Fig. 4(a). Assuming that the chip formation was by shearing, according to the plasticity mechanics theory, the shearing angle, ϕ would be $(\pi/4-\eta+\gamma_e)$, where η is the friction angle between the cutting tool and the work material. The friction coefficient between diamond and silicon is as low as 0.05 [34] so that the friction angle is about 2°52′. Taking the cutting edge radius of 5 nm and the undeformed chip thickness of 1 nm for instance, the shearing angle is about −29°26′. This is a contradiction with the actual cutting

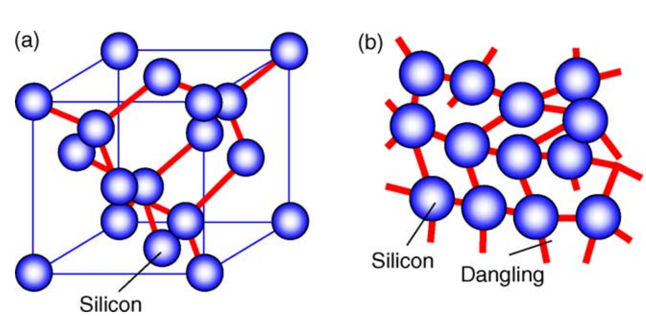

Fig. 3. Micro structure of silicon. (a) Monocrystalline silicon; (b) amorphous silicon.