

## The ultra-precision cutting Titanium alloy (Ti-6Al-4V): Effects on its microstructure and surface mechanical properties

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### Abstract

During practical ultra-precision cutting, the titanium alloy specimens suffer a combination of various deformations, has great influence on machining precision and properties. Here we report, the microstructure changes and surface mechanical properties evolutions were studied using two-dimensional climb assisted discrete dislocation dynamic technology. The plastic deformation is modeled through the motion of edge dislocations in an elastic matrix with dislocation nucleation, lock, interaction with obstacle and grain boundary, annihilation incorporated a series of constitutive equations. It was found that the micro-structure was obviously refined due to the variation of cutting force, which can be described as following: the formation and development of dislocation lines in initial grain, the formation of dense dislocation walls, the transformation of dislocation lines and walls into subgrain boundaries. In addition, the variation of surface microstructure results in higher flow strength and hardening rate due to the accumulation of geometrically necessary dislocations. The numerical result is helpful to reveal the effects of these microstructural factors on the surface generation mechanism in ultra-precision machining.

Keyword: ultra-precision cutting; dislocation dynamic; mesoscale; grain refinement; grain size effect

### 1. Introduction

Titanium alloy is widely used in aviation, spaceflight, energy, medical fields due to its high strength and lightweight properties [1-2]. Ultraprecision manufacture (UPM) technology is one of the most important methods to produce high quality alloy components with surface precision and roughness in the nanometer range [3-4]. A better understanding of the mechanism during UPM cutting, dynamics characteristics and factors affecting surface quality become important for improvement of the developed manufacturing process. In addition to aluminum alloys, equiaxed nanostructures were reported in various materials, including AISI stainless steel, iron, inconel 718 and titanium [5-6]. While most of the studies on microstructure changes induced by machining were focus on the machined chips, there are few publications regarding the machined surface, which is more important than the chips in most cases [7].

As a process different to conventional cutting machining, high energy continuous impact can lead to the dynamic recovery and dynamic recrystallization, meanwhile, the thermal mechanical coupling results in grain sliding, lattice distortion, twins, it eventually causes changes in the effects of surface generation mechanism in ultraprecision machining. During practical ultra-precision machining titanium alloy, we found that micro-structure changes promote the uncertainty of surface-topography and affect surface mechanical properties. A significant account of researches have contributed to explore the optimum cutting conditions and assessing their ultimate capability to provide precision and integrity at machined surface, but only limited attempts were made on the full comprehension and predictive assessment of the micro-

structure generation. To solve that, a multi-scale model is introduced to research dislocation evolution during micro-cutting process. It is helpful to choice reasonable micro-cutting method to obtain the high-performance and high-properties titanium alloy surface.

### 2. Multiscale methodology and micro-cutting model

The mesoscale simulation methods such as dislocation dynamics (DD) can provide new insights into aspects of material behaviour heretofore not explained using continuum approaches. In particular, unlike fully discrete methods, such as molecular dynamic (MD), DD methods offer better scalability to larger and more complex problem at the micrometer and sub-micrometer length scale. In present study, we developed a multi-scale simulation framework by coupling the DD code into a finite-element package via python scripting. In this algorithm, the dislocation processes of generation, kinetics, junction, immobilization, recovery, and annihilation are calculated by DD simulation, and a finite element method (FEM) solver was used for the solution of applied stress of dislocation during micro-cutting process. In the presence of a large number of dislocations, the Peach-Koehler force on dislocation  $l$  as

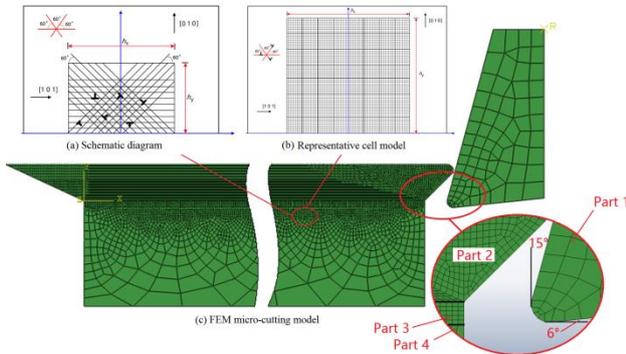
$$f_g^{(l)} = \left( \sigma_{ij}^{app} + \sum_{J \neq I} \sigma_{ij}^{(J)} \right) b_j^{(l)} m_i \quad (1a)$$

$$f_c^{(l)} = - \left( \sigma_{ij}^{app} + \sum_{J \neq I} \sigma_{ij}^{(J)} \right) b_j^{(l)} s_i \quad (1b)$$

where  $f_g^{(l)}$  is the dislocation slip force,  $f_c^{(l)}$  is the dislocation climb force,  $b_j^{(l)}$  is Burger's vector of dislocation  $l$  with unit normal  $m_i$  and a unit vector  $s_i$  in the slip direction. The  $\sigma_{ij}^{app}$  is the applied shear stress and  $\sigma_{ij}^{(J)}$  denotes the internal resolved shear stress field induced by dislocation  $J$ . The nucleation event

and close encounter among dislocations must be described by such material special rules.

The commercial software Abaqus with its explicit approach was employed to capture the applied stress of dislocations in each increment step, fully coupled thermo–mechanical analysis was carried out for a time step of 1ns. The resultant solution of unit increment was then imported to the DD framework constantly which treats plastic deformation as the evolution of a large number of dislocations. Because of the directly calculation of long-range interactions between dislocations has brought the extremely computation burden, the area of DD simulation is focus on a representative cell in surface severe plastic deformation area, as Fig. 1.

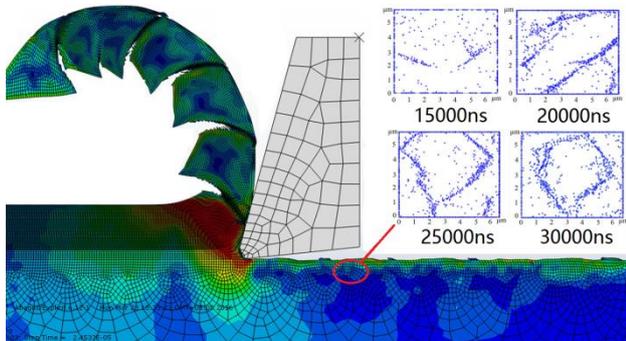


**Figure 1** A multiscale simulation methodology

A two-dimensional representative cell model was built to perform the dislocation evolution mechanism in local area of workpiece surface as above figure. The edge dislocation moves in three dislocation slip system, and the relative in-plane angles among slip systems are  $60^\circ$ .

### 3. Results and discussion

During micro-manufacturing process, the workpiece surface has suffered the coupling between high stress impact and thermal impact, which caused dislocations nucleation, obstacle, slip, climb and annihilate. Fig. 2 shows the FEM-DD observations in the surface plastic deformation subjected to complex cutting force, in which three typical deformation-induced micro-structure features are identified: dislocation lines, dense dislocation walls, and subgrain boundaries.



**Figure 2** Micro-structure evolution of surface grain

In the micro-cutting process, the interaction of tool and workpiece results in the variation of residual stresses, which can affect the dislocation motion and micro-structure evolution. A mass of dislocations are generated from the F-R sources when the cutting stress may meet or surpass the theoretical strength threshold of the material under the high strain rate conditions. During the initial stage of micro-cutting, the matrix materials is difficult to timeliness response for the tool energy impulse so that the mushrooming of dislocation density. According to fig.2, the dislocations pattern forms the matrix

walls at 15000ns, which has present irregular arrangement. The result accords the dislocation theory, which means the dislocations get an equilibrium distribution. When the simulation time increases to 20000ns, it is easy to obtain that original grain forms the dislocation walls. At the same time, large number of dislocations has been pinned-up at obstacle and grain boundary because the impenetrability of grain boundary and impurity particle. With further increasing cutting stress, development of these dislocation configurations gradually results in subdivision of original grains by forming individual dislocation cells primarily separated by dislocation lines and dislocation walls. Finally, at 30000ns, the continuous dynamic recrystallization processes result in a progressive accumulation of boundary disorientation, and finally lead to a gradual transition of boundaries character until the formation of high angle grain boundaries. The stress-strain relation can be solved by Tylor law and Orowan equation as following

$$\tau_{f1} = \tau_0 + \alpha G b \rho^{-1/2} \quad (2)$$

$$\dot{\gamma}_p = \Phi b \rho \frac{d\bar{l}}{dt} + \Phi b \bar{l} \frac{d\rho}{dt} \quad (3)$$

The results showed that the hardening is more pronounced in small domain. The linear work hardening observed when dislocations are active and in particular the increasing work hardening rate with decreasing grain size is responsible for the observed with Hall-Petch relation. But the simulation results show that with the introduction of dislocation sources, the surface hardening rate is constant at initial stage. The reason is that new mobiles dislocations are constantly being produced to control the change mechanism of surface strength. The grain refinement in workpiece surface has increased materials strength and anti-deformability ability with inhibiting the dislocations movement.

### 4. Conclusions

In this study, the surface dislocation motion evolution mechanism in ultra-precision machining process has been studied by developing multiscale simulation framework. A special focus was given to the evolution of plastic behavior and mechanics response under micro-manufacturing process. The micro-structure of surface appears grain refinement: the development of dislocation lines in original, the formation of dense dislocation walls, transformation of dislocation walls into subgrain boundaries, and evolution of the continuous dynamic recrystallization in subgrain boundaries to refined grain boundaries. At the same time, grain refinement can improve surface strength and anti-deformability ability by inhibiting dislocations movement. The present study obtains the generation mechanism of surface microstructure and surface properties.

### Acknowledge

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