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Effects of Fluid on Heat Distribution during Nanometric Cutting of Silicon

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Abstract. To understand the effect of fluid on thermal behaviour of material removing in nanoscale, molecular dynamics (MD) simulation method is performed to model the heat distribution by considering the effects of fluid during nanometric cutting of monocrystalline silicon. Most of earlier atomic simulations were focused on material removing mechanism and carried out in vacuum without considering the effect of fluid or atmosphere, nevertheless taking fluid into account represents a more completely thermal equilibrium and heat convection. In this work, a fluid containing model was used by considering fluids like coolants and concentrating on its impact during machining.

Keywords: Molecular dynamics, Nanometric cutting, Heat distribution, Phase transformation.

1 Introduction

In the rapid development of modern technologies and manufacturing of nanoscale device, monocrystalline silicon is a widely used material in micro-electro-mechanical systems (MEMS) and nano-electro-mechanical systems (NEMS). Understanding the basic action of how material removing in nanoscale is a critical issue of producing well-formed components. The material removing, actually, is the removing of surface atoms and subsurface atoms, at such a small governing length scale, traditional continuum representation of the problem is become questionable. Though computational simulation, atomic-scale material removing process can be observed and analyzed directly. Since 1990s, molecular dynamics (MD) has been used to study cutting mechanism in atomic scale. Some typical work has been done by many researchers [1-3]. The previous work provides significant insight into workpiece-tool interactions phenomena and mechanical aspects. Little research has been down in studying the influence of environmental conditions such as atmosphere or fluid, these environmental factors, however, have significant effect on the performance of system during nanometric cutting process and hard to measure by experiment.

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2 Simulation methodology

The MD model of nanometric cutting is shown in Fig. 1, in which workpiece and tool are composed with mono-crystalline silicon and diamond, respectively. The atomic model has the size of 48 nm × 27 nm × 5 nm. Both workpiece and tool are divided into fix atoms, thermostat atoms and Newton atoms, to represent a more reality machining model. A reflection wall is used in the outer surface of water atoms to maintain the density and pressure of water unchanged. The temperature of thermostat atoms is stabilized at 300K during machining. Newton layer atoms are marked as grids in order to ease tracking of lattice deformation. The top surface of workpiece is (100) plane and the X direction is in the [100] orientation. The cutting speed is set as 100 m/s for saving simulation time and the corresponding cutting depth is 1.5 nm. The initial velocity of silicon and carbon atoms were assigned based on Maxwell distribution, Velocity-Verlet algorithm was applied to the time integration method, and the integration time step size was set as 0.5 fs, the time interval was a relatively small value compared to the oscillation frequency between carbon and silicon.

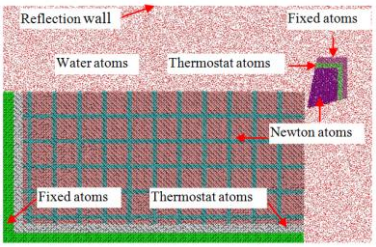

Fig. 1. The initial MD simulation model for nanometric cutting.

Initially, workpiece and tool were relaxed in a NPT assemble with the pressure controlled in 0.1 Mpa and the temperature fixed at 300 K for 30 ps, after adding the TIP3P water into system, sampling was carried out in a NVT assemble for 10 ns and the density of water was kept at 1.0 g/cm3. Distinct empirical potentials appropriate in simulation the C-C, Si-Si, Si-C and O-O bonding was employed, respectively. Tersoff potential is found to be suitable for describing the interactions between atoms with covalent bond .

3 Results

The temperature of fluid is controlled at 300 K after adding into the simulation model and acted as coolant. Furthermore, fluid provides a way to achieve heat equilibrium during machining. Fig. 2 (a) and Fig. 2 (b) show the heat distribution between with and without water, respectively. The various temperature ranges are coded by different colours to distinguish the temperature ranges of system during machining. In both cases, it can be found that the heat distribution topology is unanimous and roughly presents a concentric shape, a steep temperature gradient can be observed in tool and the highest temperature lies in chip.

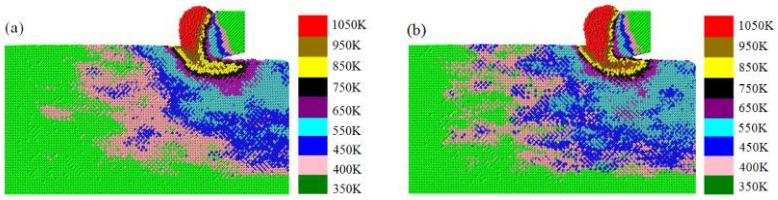

Fig.2. The cross-sectional views of heat distribution at cutting distance of 10.5 nm.

When machining at vacuum condition (Fig.2 (b)), most of heat is taken away by chips, but the relative small chip size and lack of energy conversion raised the system temperature ultimately. The thermostat atoms (next to fixed layer) are so far away that they can not affect the temperature of Newton atoms significantly. After adding water into the simulation cell, more heat can be "absorbed" by fluid. A significative phenomenon is that there are about two layers atoms in the surface of tool rake face, which has a much lower temperature than in chips, the temperature of some tool atoms even lower than 350 K. Compared with silicon, diamond has a much higher heat conductivity and could transform heat faster, which result in a steep temperature gradient is appeared in diamond tool. Additionally, the temperature gradient is much distinctness in the fluid containing model.

The high temperature region in shear zone means a build up of large stress in a local region. Most of heat is generated by friction and excursion between tool and workpiece atoms, the atoms in shear zone with high temperature moves along the rake face of tool forward, bonds are broken and bond energy released due to the plastic deformation in workpiece material, almost all the chemistry and kinetic energy are transformed into heat energy, the system temperature raised gradually with the increase of cutting length. In nanoscale, the flow stress of material is reduced due to rising of temperature, which indicates the decrease of workpiece material strength. The atoms vibrated more frequently and the distance between neighbour atoms increased with the raise of temperature, which inevitable result in weakening the bonding force between atoms. Surface and inner atoms have more energy at a high temperature and move easily when external force are imposed on the tool, that is why workpiece could be deformed under a relative low cutting force as the temperature rising. Large numbers of grain boundary provide a short cut for heat energy to diffuse from the shear zone to the inner of workpiece and promote the deformation of workpiece material.

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