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Comparison of subsurface damages on mono-crystalline silicon between traditional nanoscale machining and laser-assisted nanoscale machining via molecular dynamics simulation

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ABSTRACT

Molecular dynamics is employed to compare nanoscale traditional machining (TM) with laser-assisted machining (LAM). LAM is that the workpiece is locally heated by an intense laser beam prior to material removal. We have a comprehensive comparison between LAM and TM in terms of atomic trajectories, phase transformation, radial distribution function, chips, temperature distribution, number of atoms in different temperature, grinding temperature, grinding force, friction coefficient and atomic potential energy. It can be found that there is a decrease of atoms with five and six nearest neighbors, and LAM generates more chips than that in the TM. It indicates that LAM reduces the subsurface damage of workpiece, gets a better-qualified ground surface and improves the material removal rate. Moreover, laser energy makes the materials fully softened before being removed, the number of atoms with temperature above 500 K is increased, and the average temperature of workpiece higher and faster to reach the equilibrium in LAM. It means that LAM has an absolute advantage in machining materials and greatly reduces the material resistance. Not only the tangential force (F_x) and the normal force (F_y) but also friction coefficients become smaller as laser heating reduces the strength and hardness of the material in LAM. These results show that LAM is a promising technique since it can get a better-qualified workpiece surface with larger material removal rates, less grinding force and lower friction coefficient.

1. Introduction

Nanoscale machining processes plays an essential role in the modern manufacturing industry [1]. With the development of micro-electro-mechanical systems (MEMS) and nano-electro-mechanical systems (NEMS), nanoscale machining technology is more significant in our scientific and technological progress [2–4].Nanoscale materials due to their superior strength, strong hardness and good wear resistance have become a frontier subject of academic research [5–6]. However, the material radius involved in the nanoscale machining process are very small, generally only a few nanometrics or even less length scale, which makes it extremely difficult to get data through the experiment. Therefore, the molecular dynamics (MD) simulation can meet the requirements as a kind of atomic scale simulation [7–8].Precision laser equipment has been widely used as a machine tool to modify engineering materials surfaces. It can improve the heat treatment process and the surface quality of the workpiece through rapid precision heating [9–15]. Conventional grinding and diamond machining are the most widely applied machining methods for the high hardness and brittleness of ceramic materials. However, the conventional machining methods yield high tool wear and low material removal rates. Laser-assisted machining (LAM) has been suggested to machine ceramic materials for achieving higher material removal rate and improve tool wear in recent years. This is because LAM uses a strong laser beam as the heat source to heat the material and make it soften before removing the materials with a tool. Thus, it changes the deformation behavior of the material from brittle to ductile. In comparison with the general laser machining, the grinding tool used to remove the material in the LAM can eliminate the threat of a thermal damage layer and generate the required surface finish and dimensional tolerances [9]. Purdue University scholars ROZZI etc. [10–11] have studied laser-assisted cutting of Si_3N_4, ZrO_2 etc. ceramic materials and analyzed workpiece surface temperature, cutting force and tool wear. Laser-assisted machining Al_2O_3 ceramic materials which are difficult to cut have been studied by CHANG etc. In contrast to conventional machining, when machining high hardness ceramic materials, LAM can produce a much better qualified workpiece surface quality with less cutting force, larger material removal rates and moderate tool wear [12–15].

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In the past few years, many studies have used MD simulation to analyze the nanoscale machining. Furthermore, MD simulation have been applied to study the nanometric machining of many materials, including Si [16,17], Cu [18], Au [19], Ge [20]. The previous works have studied materials removal mechanisms, tool wear, energy consumption, crack formation and propagation, and dislocation nucleation and emission. Little work has been done on study the mechanism of material removal and subsurface damage in nanoscale laser-assisted machining, which provides much motivation for our present work. The main objective of our work was to study the influence of moving laser heating on the properties of materials, especially for the material grinding performance. However, the stringent conditions used for LAM, i.e., the thermal spot size of < 50 nm and laser-induced heating rate of $\sim 10^{11}$–10^{12} K/s, causing great technical limitations to current experimental methods that cannot get accurate answers [21–24].

In this work, we will perform two large-scale MD simulations of nanoscale LAM and TM of silicon using the Tersoff potential and Morse potential. The behavior of silicon atoms is monitored during the LAM and TM process. We have compared the LAM and TM from the atomic phase transformation, the temperature distribution, the grinding force, the friction coefficient and the atomic potential energy of the workpiece. To this end, our work will consist of the following several key parts. In Section 2, the detail of the two simulation models, method, potential energy function and visualization techniques to use will be described. In Section 3, it includes the results of comparison in the atomic trajectories, phase transformation, radial distribution function, chips, temperature distribution, number of atoms in different temperature, grinding temperature, grinding force, friction coefficient and atomic potential energy. Finally, in Section 4 we summarize the results.

2. Molecular dynamics simulation and methodology

2.1. Simulation method

In the current study, a three-dimensional MD model is employed to describe the mechanical of laser assisted grinding and traditional grinding. In order to understand the process of LAM and traditional grinding, the diamond tools are created by the perfect diamond atomic lattice, which is a spherical shape with radius 5 nm, and periodic boundary is applied to the z direction, as shown in Fig. 1.Fig. 1(a) shows the physical model of Model-A, the model consists of two parts, monocrystalline silicon workpiece and diamond tool. The dimension of the workpiece is 25.521 nm × 9.231 nm × 17.376 nm, including 208,672 silicon atoms. The dimensions of the workpiece must be large enough to eliminate the boundary effect and size effect. The grinding is conducted along the [1 0 0] direction on the (0 1 0) surface of the silicon workpiece, in which the three orientations of the workpiece are in x-[1 0 0], y-[0 0 1], z-[0 1 0]. The silicon workpiece consists of three types of atoms: boundary atoms, Newtonian atoms and thermostat atoms. Boundary atoms are fixed to eliminate the rigid body motion of workpiece. The motions of thermostat atoms and Newtonian atoms obey the classical Newton second law. Fig. 1(b–d) shows the physical model of Model B, The model consists of three parts, monocrystalline silicon workpiece, diamond tool and laser beam. The dimensions of both workpiece and diamond tool in this model are the same as those of Model A.

Velocity-Verlet algorithm is used to solve the Newton's equations of motion for these two models (Model A and Model B) with a time step of 1 fs. The initial temperature of workpiece in both models is selected as 300 K under the microcanonical ensemble (NVE). In order to ensure proper thermal transport during MD simulation, the temperature of thermostatic atoms is maintained at 300 K using the velocity rescaling method.The system reached equilibrium after the initial relaxation, a stable structure of workpiece is obtained, after which diamond tool are applied along the [1 0 0] direction on the (0 1 0) surface of silicon at a constant grinding speed of 100 m/s in Model A, laser-assisted machining began to carry on in Model B. Laser spot radius is 4 nm, as shown in Fig. 1(c) the laser beam moving at v = 100 m/s is initially centrally located at coordinate (40 Å 92.31 Å, 86.88 Å) of the simulation cell and is irradiating onto the machined surface along z = 86.88 Å for duration of 205 ps before it is turned off. The laser heating on the silicon workpiece is performed by adding non-translational Kinetic energy (fix ehex method in LAMMPS) into silicon atoms in laser spot region in a way such that the aggregate momentum of the atoms can be conserved [25]. For simplicity, in this study, we mainly study the effect of heat on the workpiece material softening. Hence, the motion of the electrons during LAM can be ignored [26]. In our simulation, the laser pulse intensity $P(r_{laser})$ is assumed to follow the Gaussian distribution (see Fig. 1(c)) and is expressed as

$$P(\mathrm{r}_{laser}) = \frac{2p_0}{\pi r_h^2}\exp\left(-\frac{2r_{laser}^2}{r_h^2}\right) \quad (1)$$

where r_{laser} is the radial distance, P_0 is the total laser power, r_b is laser spot radius [25,27]. All the MD simulations are carried out using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software [28,29], Ovito are utilized to visual MD date and generate MD snapshots [30]. More parameter values are shown in Table 1.

2.2. Selection of potential energy function

For such an atomic simulation, a suitable and reliable potential function is a prerequisite for obtaining accurate results. Three atomic interactions are adopted in our simulation. Which are the interaction between silicon atoms (Si-Si) in the workpiece, interaction between carbon atoms (C—C) in the tool, and interaction between workpiece and tool atoms (Si—C).

According to many previous works [31–41], Tersoff potential is adopted to describe the interaction between workpiece atoms in our simulation (Si—Si). However, Tersoff potential are short ranged and yield ductile instead of brittle behavior for covalent materials such as diamond or silicon. Pastewka et al. [42] developed an improved screened cutoff scheme, which extends the range of Tersoff potential to overcome the described limitations. This new Tersoff potential will be used to dictate the interaction in workpiece atoms (Si—Si) and between diamond atoms and workpiece atoms (C—Si), which can improved description of amorphous phases and correctly describe the brittle materials response.

Since the diamond material has high thermal conductivity, heat transfers can quickly take place from diamond tool to outer, and between tool and silicon workpiece. To analyze the temperature distribution of silicon workpiece, the interaction between diamond atoms (C—C) needs to be considered, although the diamond tool is considered as a rigid body in many studies [14,35,43]. Hence, Tersoff potential is used to describe the interaction between diamond atoms in our simulation [42].

3. Results and discussion

In order to save computational cost, the grinding speed is selected as 100 m/s in current MD simulations, though this grinding speed is higher than the real velocity. According to the previous works [44–46], at a relatively higher processing speed, the main characteristics of the atomic rearrangements for MD simulation finished could be revealed.

3.1. Analysis of phase transformation in the workpiece

Fig. 2(a and b) shows the cross-sectional views of the workpiece with different coordination numbers (CN) at grinding distance 20 nm. It is observed that a large area of phase transformation appears beneath the tool, a large number of atoms appear around the diamond tool with five and six coordination atoms, many of them are stacked in the groove