

The Effect of Interatomic Potential Function on Nanometric Machining of Single Crystal Silicon

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1. Introduction

Nowadays, silicon is widely used for producing ultra-precision components. Nanometric machining is an advanced process for fabrication of such highly accurate optical elements. With this method, ductile mode machining of brittle materials, such as silicon, is feasible. Due to the fact that experimental tests have some limitations, Molecular Dynamics (MD) simulation has been turned to a promising method for investigating in this area. The proper definition of the interaction between particles, which is defined by the potential function, is a key factor in a reliable MD investigation. In this paper, the effect of Tersoff, Stillinger-Weber, and Morse potential function on MD simulation results of nanometric machining process is examined. To this end, other machining parameters such as workpiece dimensions and tool geometry are considered constant in all simulations. The evolution of atom structure, workpiece temperature, machining forces, and energies are the outputs that are studied.

2. MD Simulation Method

The workpiece used in this research is a monocrystalline silicon with a diamond cubic crystal structure and an initial temperature of 293 K (Fig. 1). Three different zones are defined in the workpiece: Newtonian, thermostat, and fixed. Due to the high wear resistance in the diamond tool during the machining process, the tool is considered as a rigid body. Besides, all of the system was subjected to 2 steps of minimization and 1 step of equilibration for perfect locating of atoms. MD simulations were conducted by LAMMPS software. OVITO software was used for visualization.

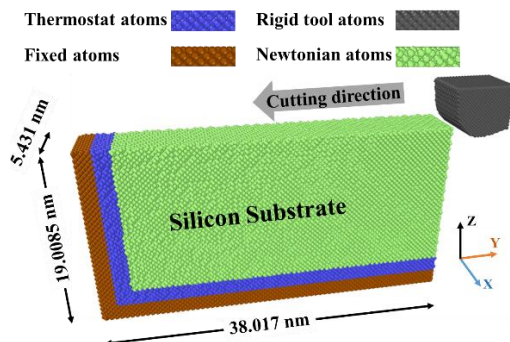


Fig. 1. Schematic of the MD Simulation model (workpiece and tool).

3. Results and Discussion

The effect of potential function on chip formation

Due to the features of Tersoff potential function in describing the elastic properties, tool advancement leads to distortion in the surface particles (Fig. 2.a&b). However, the application of the Morse potential function in the description of the tool-workpiece interactions (Fig. 2.a) results in segmented chips and brittle mode machining. It is due to the elimination of the many-body interatomic term between the workpiece and tool particles. As demonstrated in Fig. 2.c, using Stillinger-Weber potential function causes less atomic distortions and better surface roughness. The reason is providing higher yield stress in this potential function.

The effect of potential function on temperature evolution

The workpiece temperature evolution in all situations are always incremental (Fig. 3). This can be explained by the presence of friction, increasing the kinetic energy as well as entering the machining-induced heat into the workpiece. Nevertheless, it is seen that the potential function which describes the interaction between tool and workpiece has a greater effect on the temperature changes.

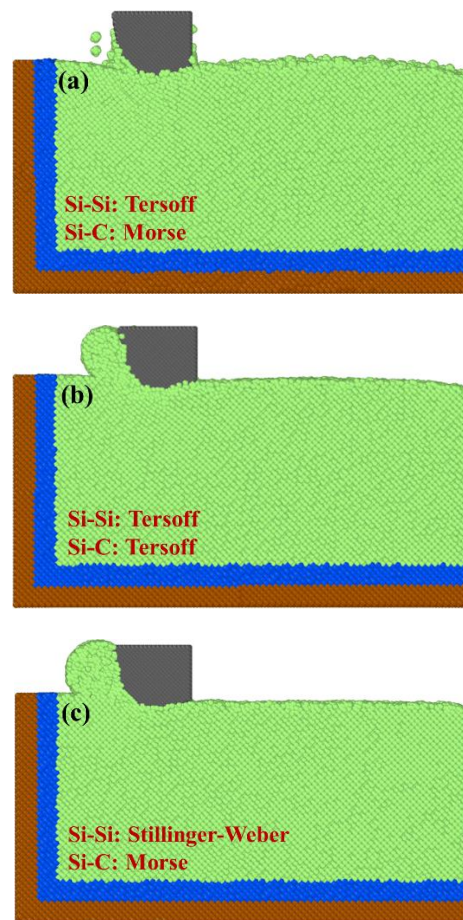


Fig. 2. The effect of potential function on the evolution of atom structure after 30nm tool advancement

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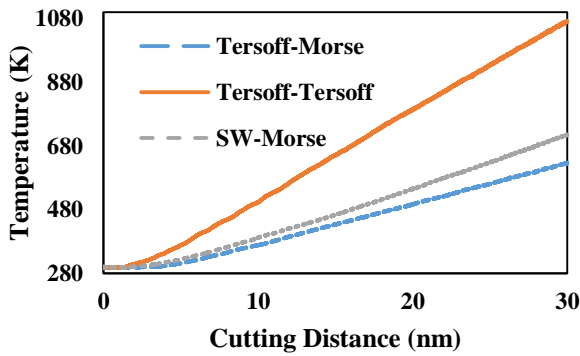


Fig. 3. The effect of potential function on temperature evolution

The effect of potential function on machining energy

As the tool moves forward on the specimen surface, the total system energy is increases (Fig. 4). It occurs because the external forces which enter into the workpiece. The interaction between workpiece particles plays a pivotal role in determining the total energy of the system.

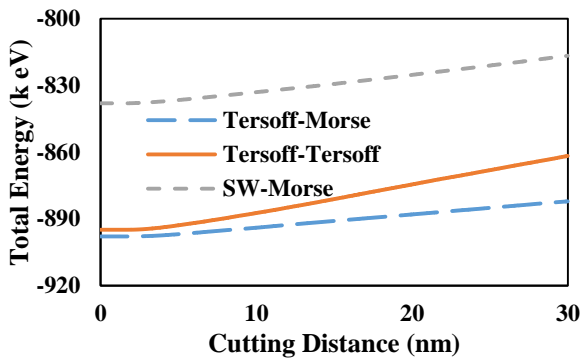


Fig. 4. Variation of total energy by tool advancement in different potential functions

The effect of potential function on subsurface damages

The examination of subsurface damages (SSD) using common neighbor analysis (CNA) demonstrates the presence of an amorphous layer on the machined surface due to the high contact pressure between the tool and the machined Si surface. Moreover, a large number of dislocations and vacancies can be found in using Tersoff-Morse combination of interactions. They stem

from long-range terms in Tersoff potential function which shows its effect in the underneath particles. Changing the tool-workpiece interaction to Tersoff results in the reduction of the dislocations as well as their concentration beneath the tool. The source of these dislocations is the hydrostatic pressure under the cutting tool. In the case of Stringer-Weber and Morse combination, a few hexagonal phase transformation can be observed on the machined surface.

4. Conclusion

The main achievements of this paper are as follow:

- Using the pairwise Morse potential function in defining tool-workpiece interactions leads to brittle mode machining and subsequently, segmented chips.
- Stillinger-Weber potential function provides the best surface roughness and the least edge distortion in nanometric machining of a silicon workpiece. Besides, using the Tersoff potential function for defining the interaction between the atoms of the tool and the workpiece increases the average machining force by 32.1%. It also causes a 26% increase in machining forces fluctuations in comparison to Morse potential function.
- The interaction between tool and workpiece atoms plays a crucial role in machining forces, kinetic energy, and workpiece temperature. In contrast, the interaction of workpiece particles has more influence on the potential and total energy of the system.
- On average, around 98% of the system's total energy consists of potential energy. Therefore, the potential function used to define the interaction of the workpiece particles will have a higher effect on this value.
- The use of Tersoff potential function for defining the interactions of silicon particles as well as the diamond tool, provides the closest result in terms of deformation mechanism and nanoscale material removal behavior.