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Molecular dynamics simulation investigation of hot nanometric cutting of single crystal silicon

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Abstract

In this study, molecular dynamics (MD) simulation is employed to investigate mechanisms occurring during nanometric cutting process of single crystal silicon on different crystallographic planes under a wide range of workpiece temperatures (300-1500 K) by comparing the results obtained from two types of interatomic potential functions i.e. an analytical bond order potential (ABOP) and a modified version of Tersoff potential. It was found that resultant force decreases up to 25% at workpiece temperature of 1173 K. A steep decrease of tool temperature at 1500 K was noticed on the (010) and (110) crystal planes when the modified Tersoff potential function was used, attributable to the decrease of the tool-chip contact length at 1500 K. Another point of interest was the decrease of magnitude of von Mises stresses on the cutting edge with the increase of the workpiece temperature for the different crystallographic planes.

MD simulation; Silicon; Temperature; Resultant force; Stresses; Hot nanometric cutting

1. Introduction

In order to fabricate scaled down single crystal silicon 3D components used in the optoelectronic and semiconductor industries, ultraprecision and nanometric cutting can be employed. However, single crystal silicon has poor machinability at room temperature due to its relatively low fracture toughness and high hardness. A common understanding about silicon is that high temperature reduces the yield strength and hardness, and improves the fracture toughness which in turn improves its plastic deformation.

The previous work on nanoscale cutting by MD simulation has primarily focused on demystifying the material removal mechanisms at room temperature [1]; very little work has been performed on examination of hot nanometric machining and nanoindentation [2-3]. Accordingly, the present study aims to investigate hot nanometric cutting of single crystal silicon on Si(010), Si(110) and Si(111) crystallographic orientations at various temperatures (300 K, 500 K, 750 K, 850 K, 1173 K and 1500 K) using MD simulation so as to obtain an unambiguous knowledge about this process.

2. Methodology

The three-dimensional MD model for nanometric cutting of silicon is illustrated in Fig. 1. Two potential energy functions, namely modified Tersoff and Analytical Bond Order Potential (ABOP) are employed to describe the interatomic interactions within single crystal silicon workpiece. To achieve precise simulation results, the corresponding equilibrium lattice constants at the mentioned temperatures were calculated for the potential energy functions employed in this study, as summarized in Table 1. In order to perform the simulations, a public-domain computer code, known as "large-scale atomic/molecular massively parallel simulator" (LAMMPS) was employed.

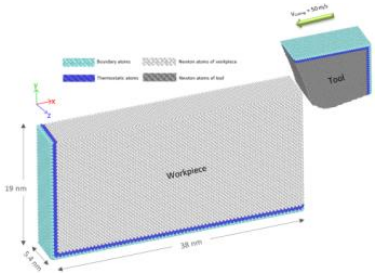


Figure 1. Schematic of the MD simulation model

Table 1. Calculated lattice constants using modified Tersoff and ABOP potential energy functions for single crystal silicon at different temperatures

Temperature (K)	Modified Tersoff lattice parameter (Å)	Modified Tersoff cohesive energy (eV)	ABOP lattice parameter (Å)	ABOP cohesive energy (eV)	Experimental lattice parameter (Å) [4]
300	5.436	-4.628	5.433	-4.627	5.431
500	5.439	-4.627	5.436	-4.626	5.434
750	5.443	-4.626	5.439	-4.625	5.439
850	5.444	-4.625	5.441	-4.624	-
1173	5.449	-4.623	5.446	-4.623	5.449
1500	5.454	-4.622	5.451	4.620	5.457

3. Results

Fig. 2 shows the variation of resultant force as a function of temperature and crystal orientation using ABOP potential. Clearly, large resultant force magnitudes corresponds to low workpiece temperatures, since the workpiece at a low temperature is more difficult to be deformed. At high temperatures, interatomic distances increase, leading to the decrease of the workpiece interatomic bonding energy. As a consequence, strength of single crystal silicon reduces. It is

found that resultant force decreases up to 25% at workpiece temperature of 1173 K. Also, it can be deduced that the (111)<$\bar{1}$10> crystal setup is the easy cutting combination of orientation and direction for cutting silicon which is in accord with the published experimental results [5].

Fig. 3 illustrates the temperature evolution in the diamond tool while cutting single crystal silicon on the (010) crystal surface at different temperatures obtained by the modified Tersoff potential function. It should be noted here that the same trend was observed for the other two crystallographic orientations and hence only one result is presented here for brevity. As seen in Fig. 4, less heat is generated when the hot nanometric cutting was performed on the (111) crystal plane in comparison to the other two orientations, which is in agreement with the results obtained for resultant forces.

A remarkable finding from Figs. 3-4 presented here is that a steep decrease of tool temperature at 1500 K is noticed on the (010) and (110) crystal planes when modified Tersoff potential function was used. This behaviour can be attributed to the decrease of the tool-chip contact length at 1500 K, as illustrated in Fig. 5. Less heat is transferred to the rake face of the tool from chip when the tool-chip contact area decreases, causing a lower tool temperature. However, this behaviour was not observed while using ABOP function due to overestimated melting temperature of silicon by this potential function (~2490 K).

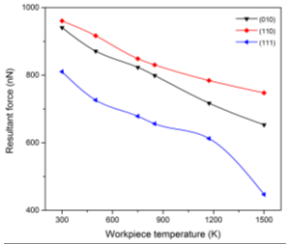


Figure 2. Resultant force as a function of temperature and crystal orientation using ABOP potential

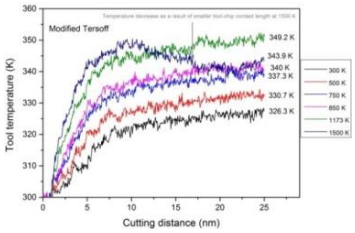


Figure 3. Evolution of the average temperature over 15-25 nm cutting distance while cutting on the (010) crystal plane obtained by modified Tersoff potential function

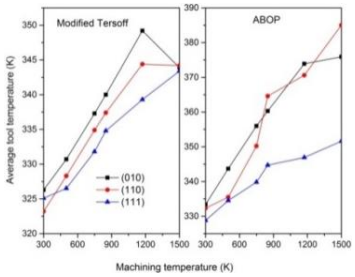
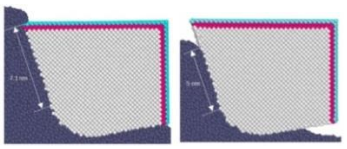


Figure 4. Average tool temperature as a function of machining temperature and crystal orientation

Fig. 6 illustrates the evolution of von Mises stress on the cutting edge of the diamond tool. Overall, the magnitude of von Mises stresses on the cutting edge decreases with the increase of the workpiece temperature for the different crystallographic planes. The von Mises stress acting on the cutting edge during nanometric cutting of silicon at low and high temperatures is in the range of 18-26 GPa, implying that diamond-graphite transformation is improbable.



(a) 1173 K (b) 1500 K

Figure 5. Tool-chip contact length at 20 nm cutting distance obtained by modified Tersoff potential. Smaller tool-chip contact length is observed on the (010) and the (110) crystal planes at 1500 K.

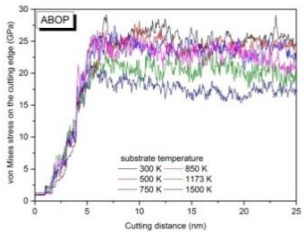


Figure 6. Evolution of von Mises stress on the cutting edge of the tool while cutting silicon on the (110) crystal plane

4. Summary

Using MD simulation, it was revealed that resultant forces and in turn energy required to cut the silicon is decreased in nanometric cutting at high temperatures. Moreover, the role of interatomic potential function in predicting material flow behaviour of silicon at high temperature was manifested. For instance, less heat was found to be generated when the hot nanometric cutting was performed on the (111) crystal plane in comparison to the other two orientations, which was in agreement with the results obtained for resultant forces. Further analysis showed that the value of von Mises stresses on the cutting edge decreases with the increase of the workpiece temperature and diamond-graphite transformation was found to be improbable.

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