Molecular dynamics simulation investigation on the plastic flow behaviour of silicon during nanometric cutting

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Abstract

Molecular dynamics (MD) simulation was carried out to acquire an in-depth understanding of the flow behaviour of single crystal silicon during nanometric cutting on three principal crystallographic planes and at different cutting temperatures. The key findings were that (i) the substrate material underneath the cutting tool was observed for the first time to experience a rotational flow akin to fluids at all the tested temperatures up to 1200 K. (ii) The degree of flow in terms of vorticity was found higher on the (111) crystal plane signifying better machinability on this orientation in accord with the current pool of knowledge (iii) an increase in the machining temperature reduces the spring-back effect and thereby the elastic recovery and (iv) the cutting orientation and the cutting temperature showed significant dependence on the location and position of the stagnation region in the cutting zone of the substrate.

Keywords: Molecular dynamics; Material flow; Stagnation region; Nanometric cutting; Single crystal silicon

1. Introduction

An in-depth understanding of the plastic deformation mediated flow behaviour of single crystal silicon during its nanometric cutting is of significant relevance to adjudge surface quality of the machined substrate. Single crystal silicon is a brittle material at ambient temperature due to the *sp*^{3} bonding, relatively short bonding length and closely packed diamond cubic lattice structure, which makes it a difficult-to-machine material.

Despite an aggressive interest in studying nanometric cutting of silicon, there has been no theory till date suggesting material flow in different regions of the silicon substrate during its ductile-regime machining [1]. In this paper, an attempt was made to study the plastic deformation mediated flow behaviour of single crystal silicon during nanometric cutting processes at different machining temperatures. The research of this sort will help address an important research question which is at the pinnacle of nanotechnology i.e. what is the fate of silicon when it is acted upon by high deviatoric stresses and to what an extent it is sensitive to the temperature of the substrate? In order to understand these, this study adopts molecular dynamics (MD) simulation so as to shed some light on the flow behaviour of silicon and flow stagnation phenomenon during nanometric cutting which has not received due attention in the previously made research efforts in this direction.

2. MD simulation details

The MD simulations in this work were performed by using a public-domain computer code, “large-scale atomic/molecular massively parallel simulator” (LAMMPS) [2]. A schematic representation of the MD model has been shown in Fig. 1. The cutting was performed on the (010), (110) and (111) crystallographic planes and [100], [00$\bar{1}$], [$\bar{1}$10] directions of silicon, respectively, while cubic orientation was used for the diamond cutting tool. The machining temperatures used in this investigation were 300 K, 500 K, 750 K, 850 K, 1173 K and 1500 K. The methodology adopted to perform the simulation was similar to what has previously been used in numerous other contact loading simulation studies [3-10]. Since the point of interest was to study the flow behaviour of silicon at varying (high) cutting temperatures, a potential robust in predicting the melting point of silicon was required. Accordingly, a modified variant of the Tersoff interatomic potential function refined by Agrawal *et al.* [11], which is robust in predicting the melting point and thermal softening behaviour of silicon at elevated temperatures [3], was adopted in this study. In order to determine the atomic flow field in different regions of the substrate, the atomic displacement of each atom from its initial configuration was calculated and accordingly the displacement vectors were plotted.

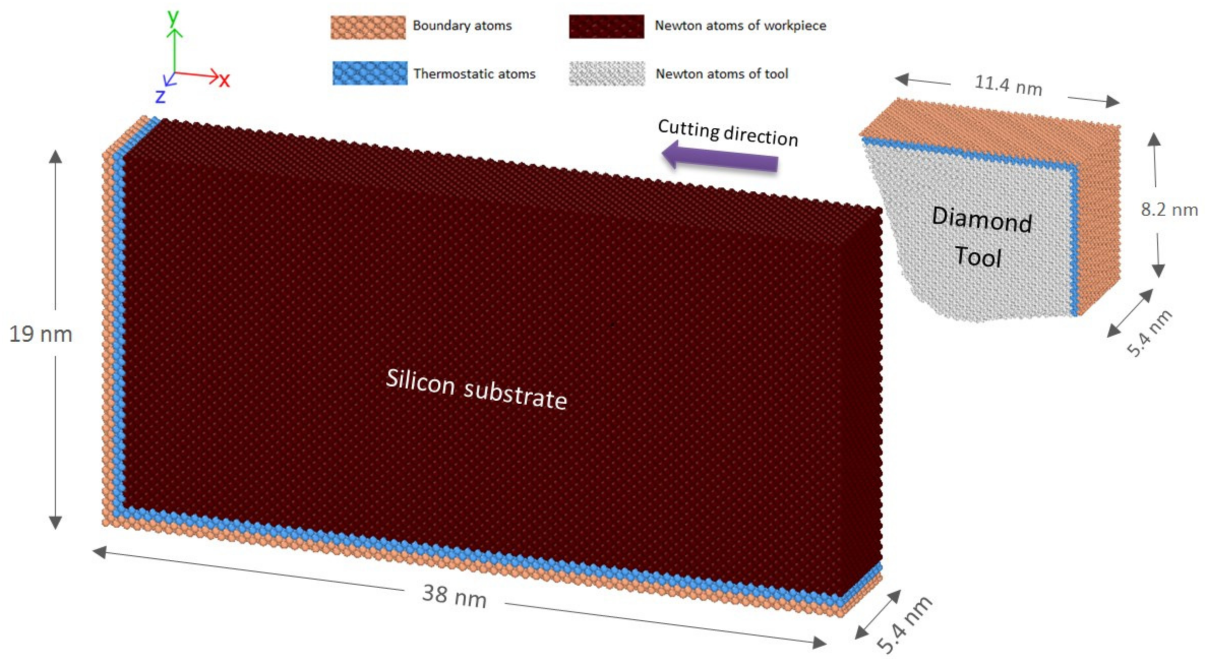


Fig. 1. Schematic representation of the MD simulation model for nanometric cutting

3. Results and discussion

In order to explore the atomic flow field within the substrate, the substrate was divided into five distinct regions, as shown in Fig. 2, and these were cut region, region underneath the tool flank face, region between the flank face and the tool tip, region ahead and beneath the tool tip and uncut region. This division was adopted for the ease of illustration. The stagnation region is the region where the shearing action (leading to chip formation) separates from the compressive action underneath the cutting edge of the tool (eventually leading to spring-back effect) resulting in the appearance of two stagnation angles (θ_s) shown in Fig. 2, and this can be calculated from:

$$\theta_{s1,2} = cos^{-1}(1 - \frac{h_{1,2}}{r}) \quad (1)$$

where $h_{1,2}$ stands respectively for the upper and lower bounds of stagnation region, and r for the tool tip radius.

A snapshot from the MD simulation after 20 nm of steady state cutting is presented in Fig. 3 depicting the displacement vector of silicon atoms in the *XY* plane while machining at 300 K on the (010), (110) and the (111) crystal planes. Following conventional crystallographic convention, this paper uses ( ) and [ ] notations to represent crystallographic plane orientations (direction of plane normal) and crystallographic directions, such as cutting and slip, respectively. From Fig. 3, one can observe a rotational flow of atoms underneath the cutting tool akin to fluid flow and a distinct distribution of atomic flow field in different regions of the substrate.

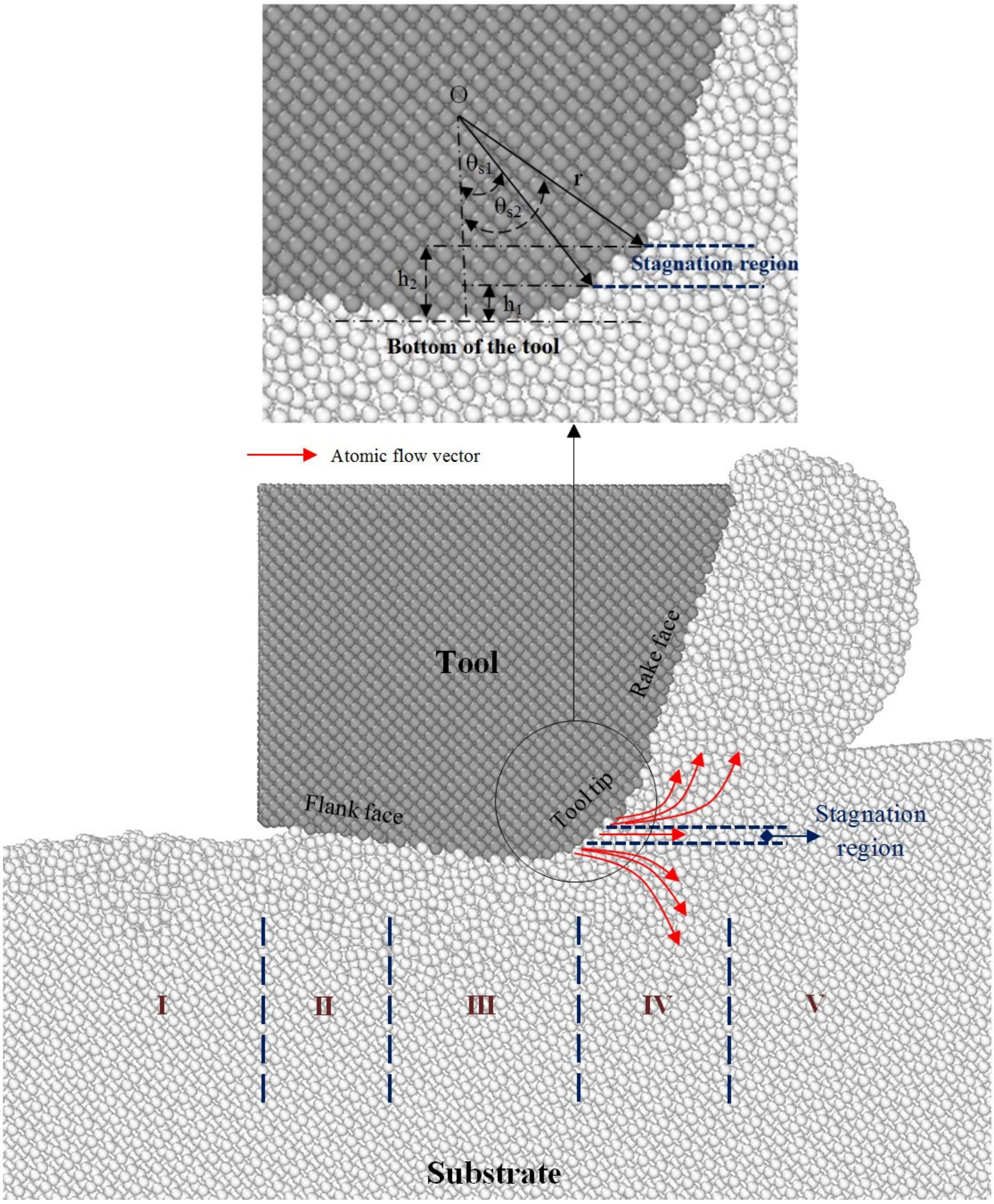


Fig. 2. Five regions in the substrate: I- Cut region, II- Underneath the flank face, III- Between the flank face and tool tip IV- Ahead and beneath the tool tip, V- Uncut region. Red arrows are flow vectors around the stagnation region. In the detailed snapshot, $\theta_{s1,2}$ and $h_{1,2}$ represent the limiting bounds of the stagnation angles respectively in the stagnation region.

In a nanometric cutting process, there exists a so called stagnation/neutral region around the tool tip (as shown in Fig. 2) whereby the atomic flow separates into two opposite directions. The atoms above the stagnation region are separated from the substrate, and flow upward on the rake face of the cutting tool forming the cutting chips whereas atoms below the stagnation region are compressed downward by the tool tip, eventually resulting in the observed spring back effect.

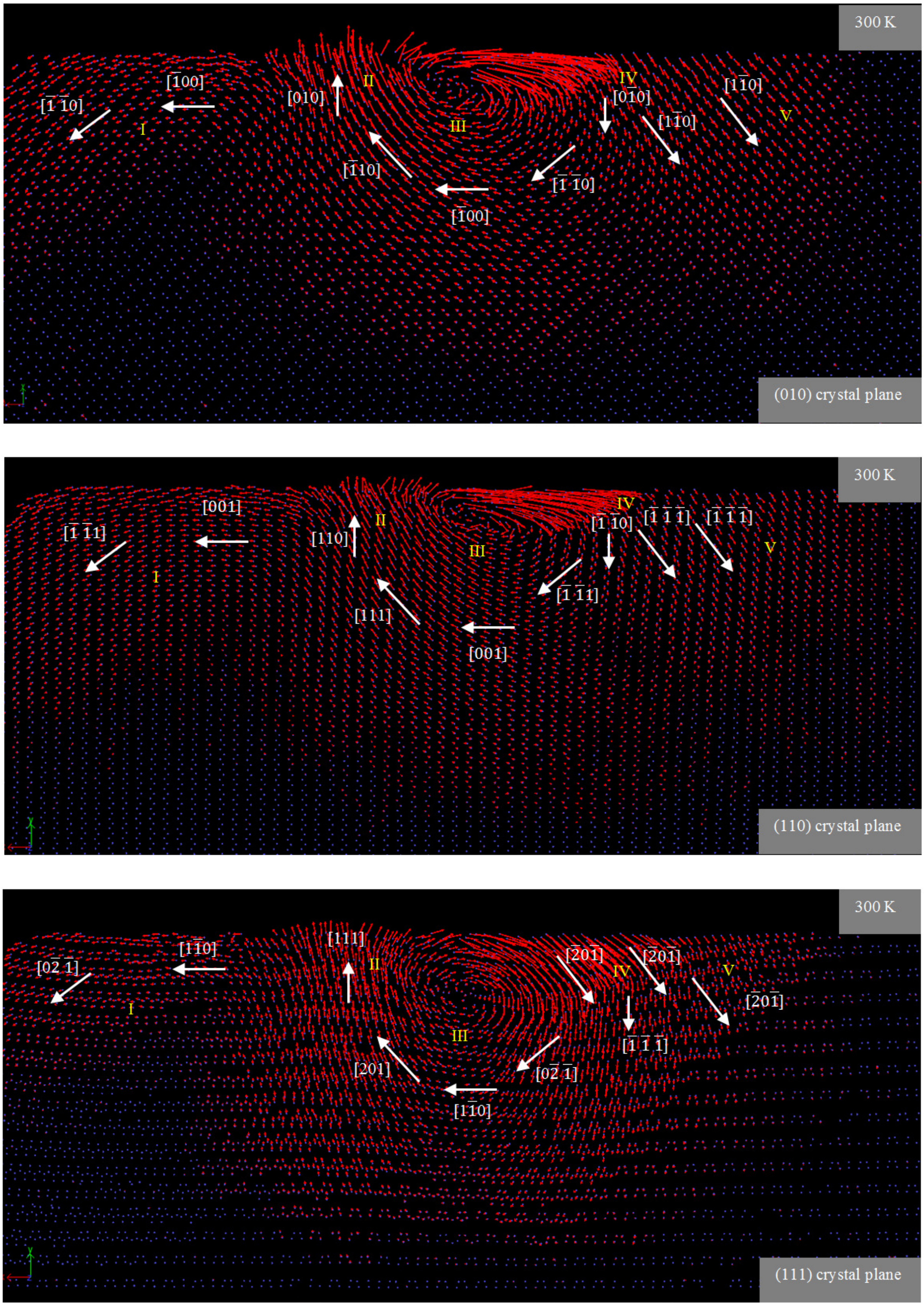

300 K
I
II
III
IV
V
(010) crystal plane
300 K
I
II
III
IV
V
(110) crystal plane
300 K
I
II
III
IV
V
(111) crystal plane

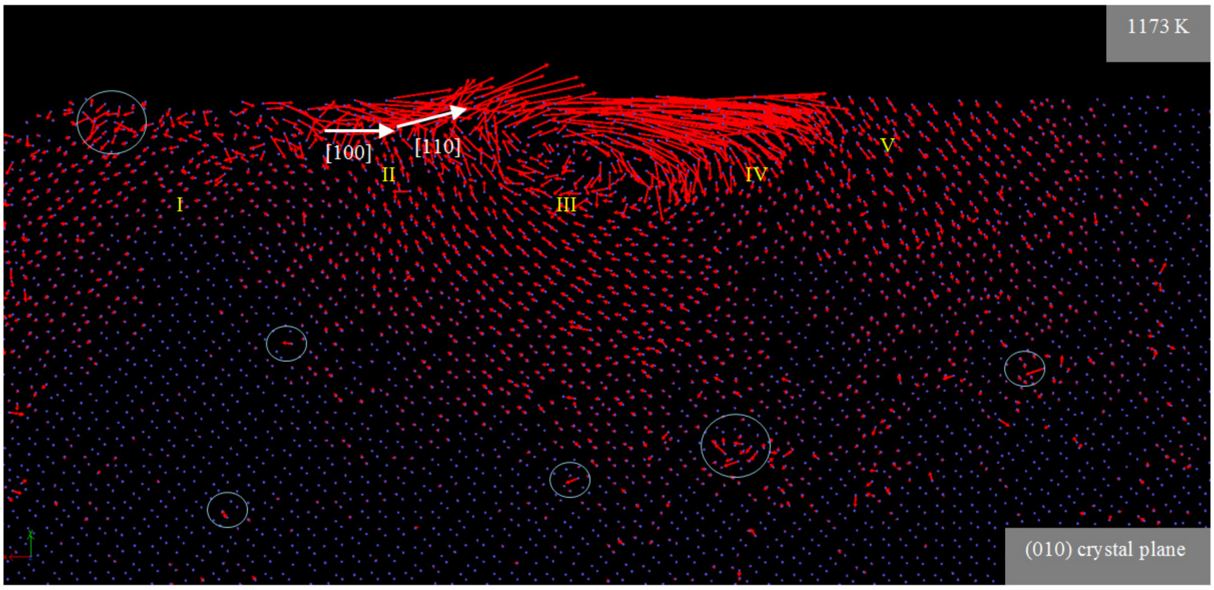
Fig. 3. Snapshots of atomic flow field in the *XY* plane while cutting silicon on the different crystal orientations at 300 K. The red arrows indicate displacement vectors of atoms and their lengths demonstrate the relative magnitude of displacement. The atoms of the cutting tool are deliberately kept hidden so the position of the cutting tool with regard to the five regions in the substrate can be traced from Fig. 2.

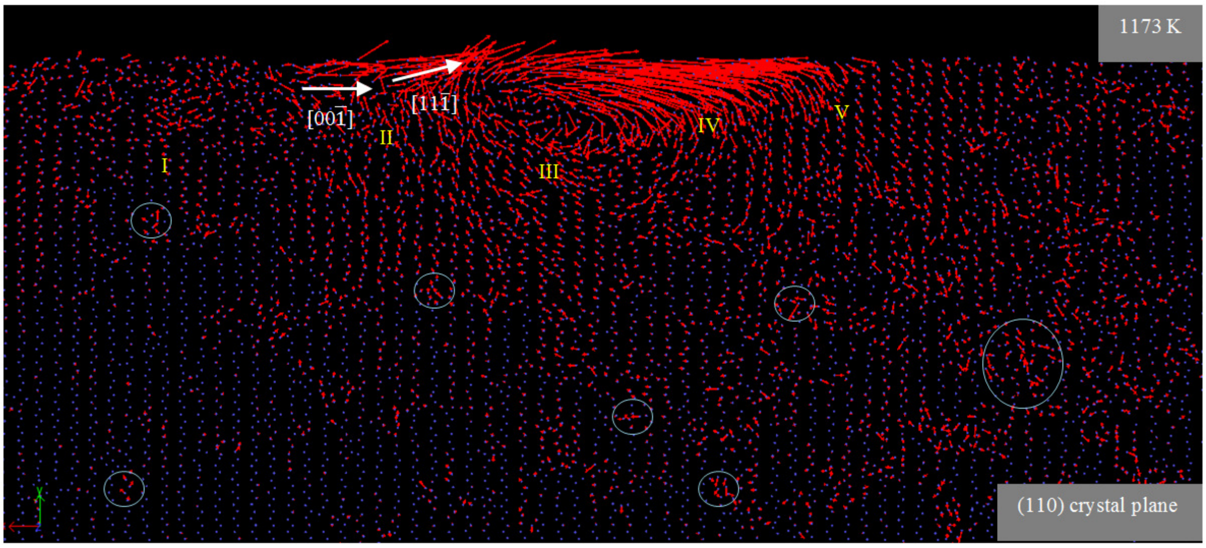
Although shown explicitly in Fig.3, by and large, the five manifold distribution of the atomic flow field for the three crystal planes was found identical and hence only the (110) orientation has been used here for illustration purposes. The chip formation process during nanometric cutting of single crystal silicon involves extrusion of the material [12] and in this study it was observed that on the (110) surface it proceeds in $[00\bar{1}]$ and $[11\bar{1}]$ directions. As the cutting tool goes past region *I*, the highly compressed atoms in this region tend to restore their equilibrium positions in order to relieve the residual stresses. At macroscopic scale, this is recognized as material recovery or spring back effect. Consequently, few distinct backward and transverse movements along the [001] and $[\bar{1}\bar{1}1]$ directions were observed in the region *I*. As the substrate temperature increases, the magnitude of atomic displacement decreases in both the aforementioned directions, as shown in Fig. 4. In region *II* (underneath the flank face), the upward motion of the atoms along the [110] direction results in elastic recovery on the flank face. As the substrate temperature increases, the movement of the atoms in this region was observed to change from the [110] to $[11\bar{1}]$ and $[00\bar{1}]$ directions, indicating reduced spring back underneath the flank face. One plausible reason for this phenomenon could be the fact that an increase of the substrate temperature results in an increase in the amplitude of atomic vibration signifying increased number of phonons which in turn contributes to additional atomic displacements. The atomic displacements within the substrate result in an increase in the interatomic distances and a decrease in the restoring forces due to thermal expansion, leading to the generation of elastic strain in the cohesive bond and corresponding lowering the energy required to break the atomic bonds. Consequently, thermal softening enhances the plasticity of the silicon substrate.

The highly strained atoms in region *III* (between the tool flank face and tool tip) under the wake of the cutting tool experience flow (site of vorticity), which comprises movement of the atoms in the $[\bar{1}\bar{1}1]$, $[001]$, $[111]$ and $[110]$ directions. The initiation of the material flow, $[\bar{1}\bar{1}0]$, occurs underneath the lowest part of the tool tip. The centre of the flow region can be perceived as a stagnant point of the atomic flow where the theoretical displacement of the material approaches zero. Interestingly, except for 1500 K, the vortex flow of the atoms in region *III* was a consistent observation at all the simulated temperatures. From a visual perspective, the flow was seemingly a laminar flow whereas at higher temperatures, such as at 1173 K and 1500 K, the flow of the material was seemingly turbulent. The flow characterisation of plastically deformed material is a newly identified area of research from this paper and we shall expand on this later.

In region *IV*, the tool tip pushes the atoms downward and along the $[\bar{1}\bar{1}\bar{1}]$ direction. It is well acknowledged that slip in a diamond cubic lattice structures occurs preferentially in the <110> family of directions on the {111} family of planes. Atoms in region *V* move downward along the $[\bar{1}\bar{1}\bar{1}]$ direction, which is consistent with the slip system of silicon on the (111) plane. Slip in single crystal silicon is normally expected to take place on broadly spaced shuffle planes, yet micro-compression experiments at high temperatures showed that slip in silicon occurs by the movement of dislocations on more closely spaced glide planes [13]. Fig. 5 demonstrate that when the nanometric cutting was performed at 1500 K, the substrate atoms move along the $[00\bar{1}]$ and $[\bar{1}\bar{1}\bar{1}]$ directions plausibly due to weaker van der Waals interactions between atoms. Additionally it can also be seen that the turbulence in the substrate atoms scales linearly with the increase in the machining temperature.

Another key finding from Fig. 3 is that when the nanometric cutting was performed on the (111) orientation, the position of the centre of rotational flow in region *III* was observed to be located lower than those on the other crystal planes, and thereby contributing to a more influential flow of the atoms in the substrate which facilitates the material removal process during nanometric cutting. The observed phenomenon can be considered as a confirmation for the fact that the [$\bar{1}$10] is the easy cutting direction on the (111) plane of silicon [3, 14]. In addition, by comparing the distorted atoms highlighted by grey circles in Fig. 4, one can deduce that when hot nanometric cutting is performed on the (110) crystal plane, the number of displaced atoms will be higher than those on other crystal planes.





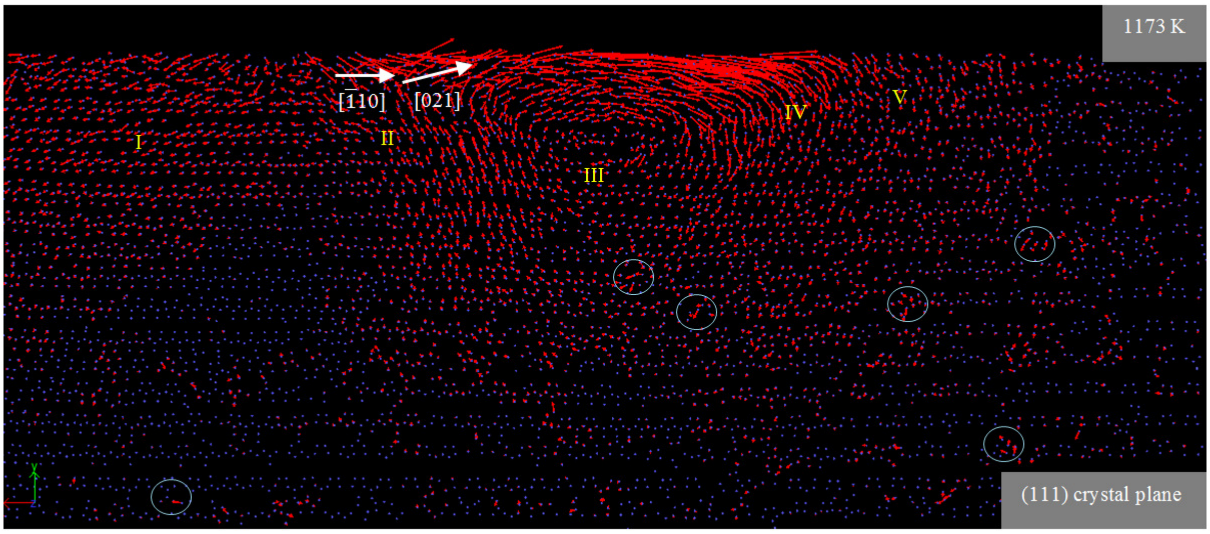


Fig. 4. Snapshots of atomic flow field while cutting silicon on the different crystal planes at 1173 K. At high temperatures, the upward movement of atoms is eliminated, leading to decrease of the spring back on the flank face. More distorted atoms are highlighted by grey circles.

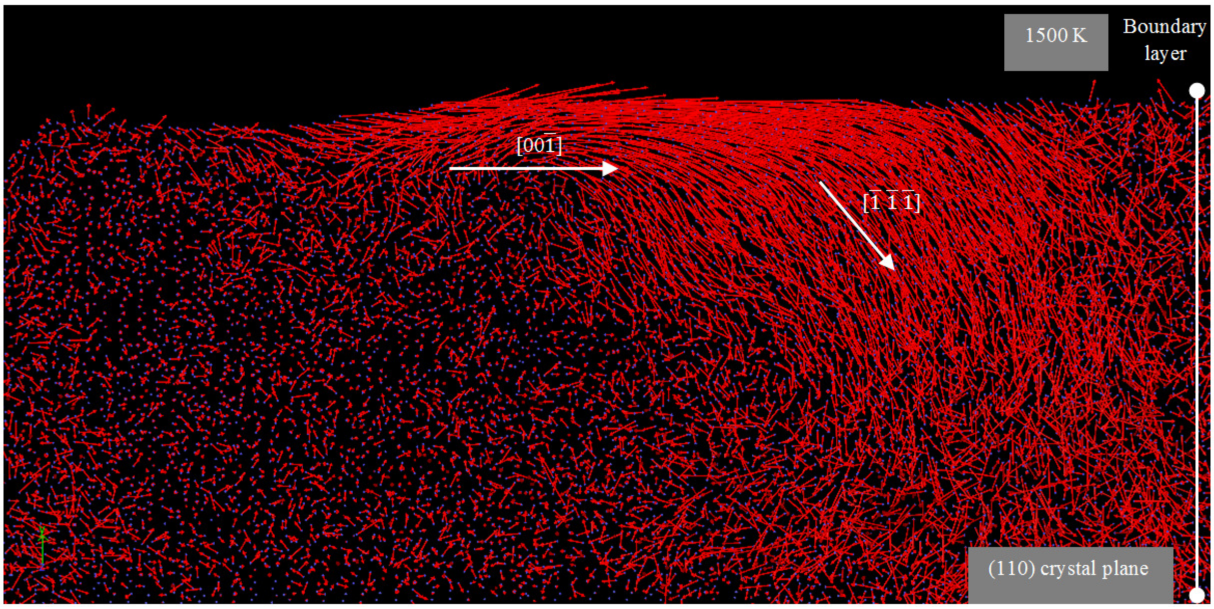


Fig. 5. Snapshot of atomic flow field while cutting silicon on the (110) crystal plane at 1500 K. Substrate atoms move along the cutting and slip system directions owing to the very weak interaction between atoms and viscous flow of the material. Chaotic behaviour of the atoms can be observed as well.

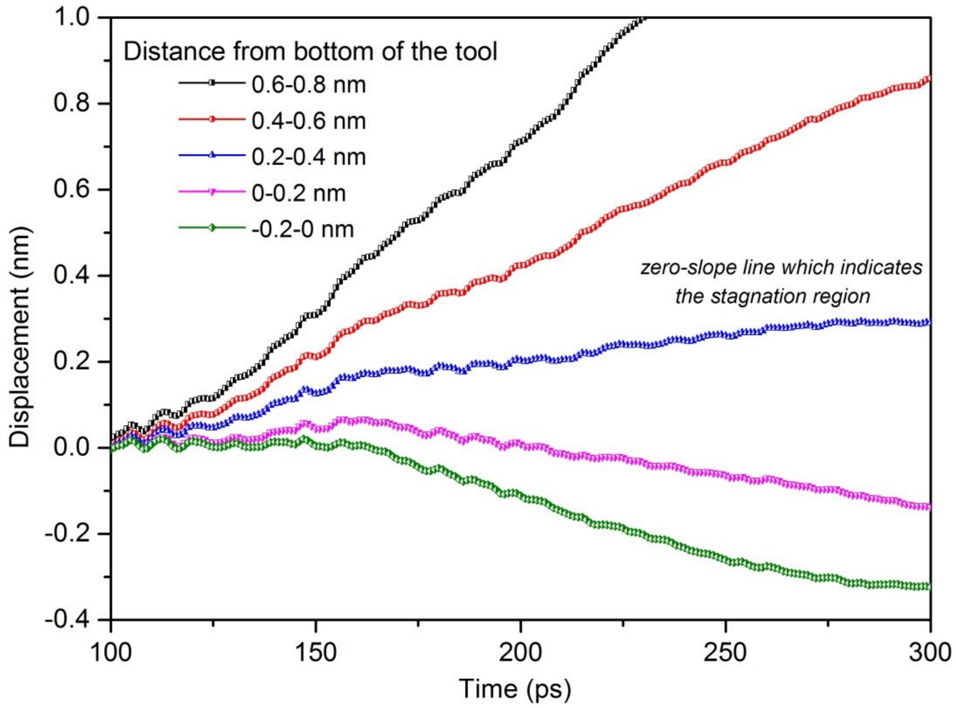


Fig. 6. Displacement of different layers in *y* direction

In order to locate the stagnation region during the nanometric cutting process, the average displacement of substrate atoms in the *y* direction in different layers were plotted. Fig. 6 shows the quantified displacements of various layers within the substrate while cutting silicon on the (110) crystal plane at 300 K. In Fig. 6, the slope alteration from positive (+) to negative (-) indicates the stagnation region. Thus, the region in the space of 0.2 nm to 0.4 nm (from the bottom of the tool) was identified as the stagnation region for the simulated cutting configuration for the cutting at 300 K on the (110) orientation. Table 1 summarizes the position of stagnation region and corresponding angles while cutting silicon on the different crystal planes and at various temperatures. This table highlights strong dependence of the orientation and temperature on the stagnation region.

In general, when cutting was performed on the (111) plane, the stagnation region (irrespective of the cutting temperature) was observed to locate at an upper position than for the (010) and (110) orientations. This signifies that ploughing due to compression is relatively higher on the (111) plane and thus the extent of deformed surface and sub-surface leading to higher spring-back is more pronounced on this orientation. Also, at high temperatures, the stagnation region was observed to shift downwards than what was observed at room temperature.

Analytical and experimental approaches have shown a clear correlation between stagnation angle and friction angle especially during cutting of soft materials [15]. Therefore, it is instructive at this point to examine the relation between stagnation angle and friction angle in single crystal silicon. The friction angle (β) for a rounded edge tool was estimated through equation (2), which uses the effective rake angle in place of nominal rake angle.

$$\beta = \alpha_{ef} + tan^{-1}(\frac{F_c}{F_t}) \qquad (2)$$

$$\alpha_{ef} = sin^{-1}(1 - \frac{d}{r})$$

where α_{ef} is the effective rake angle, F_c is the tangential cutting force, F_t is the thrust force and d is the uncut chip thickness. The values of friction angle have been listed in Table 1.

While cutting silicon on the (111) and (010) at lower machining temperatures *viz.* 300 K to 850 K, the magnitude of stagnation and friction angle were observed to be closely related. However, an inconsistency was observed as soon as the machining conditions were changed i.e. on the (110) crystal plane, an average difference of 15° to 25° was observed between the two angles. A noteworthy finding is that the discrepancy between stagnation and friction angle increases with the increase of the substrate temperature for the different crystallographic planes.

Table I: Stagnation region, stagnation angle and friction angle in nanometric cutting of single crystal silicon at various temperatures

Substrate Temperature (K)	Crystal orientation	Position of Stagnation region from bottom of the tool ($h_{1,2}$) (nm)	Stagnation angles ($\theta_{s1,2}$) (degree)	Friction angle (β) (degree)

300	(010)	0.5-0.7	31-36.9	39.3
	(110)	0.2-0.4	19.5-27.7	38.6
	(111)	0.7-0.9	36.9-42	38.3
500	(010)	0.5-0.7	31-36.9	38.7
	(110)	0.2-0.4	19.5-27.7	38.9
	(111)	0.8-1	39.9-44.4	40.6
750	(010)	0.3-0.5	23.9-31	38.2
	(110)	0.2-0.4	19.5-27.7	36.3
	(111)	0.5-0.7	31-36.9	37.1
850	(010)	0.4-0.6	27.7-34	36.7
	(110)	0.1-0.3	13.7-23.9	38.2
	(111)	0.8-1	39.9-44.4	42.8
1173	(010)	0.2-0.4	19.5-27.7	35.9
	(110)	0.1-0.3	13.7-23.9	37.7
	(111)	0.4-0.6	27.7-34	43.2
1500	(010)	0.2-0.4	19.5-27.7	50.6
	(110)	0.2-0.4	19.5-27.7	45.7
	(111)	0.3-0.5	23.9-31	53.1

4. Conclusions

In summary, this work for the first time elucidated flow behaviour of solid silicon in the machining zone during nanometric cutting akin to fluids using a parameter called as atomic displacement vector. MD simulations were performed using a modified variant of Tersoff function to reveal that a vortex flow brings higher machinability on the (111) orientation in comparison to the other two orientations. It was recognized that the stagnation region during cutting of silicon is highly dependent on the crystal orientation and the machining temperature. Furthermore, it was observed that the degree of turbulence in the machining zone scales linearly with an increase in the machining temperature. At higher temperatures, elastic recovery is negated by the turbulence, and movement of atoms along the cutting direction was more pronounced. Lastly, the analysis showed that the values of the stagnation and friction angle were identical when the cutting was performed on the (111) and (010) crystal planes and at low temperatures.

Acknowledgment

The authors gratefully acknowledge the financial support from the EPSRC (EP/K018345/1) and Royal Society-NSFC international exchange programme (IE141422) for this study. The authors also acknowledge the use of the EPSRC (EP/K000586/1) funded ARCHIE-WeSt High Performance Computer at the University of Strathclyde.

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