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Self-healing of cracks during ductile regime machining of silicon: Insights from molecular dynamics simulation

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Abstract

During nanoindentation and ductile-regime machining of silicon, a phenomenon known as “self-healing” takes place in that the microcracks, microfractures, and small spallings generated during the machining are filled by the plastically flowing ductile phase of silicon. However, this phenomenon has not been observed in simulation studies. In this work, using a long-range potential function, molecular dynamics simulation was used to provide an improved explanation of this mechanism. A unique phenomenon of brittle cracking was discovered, typically inclined at an angle of 45° to 55° to the cut surface, leading to the formation of periodic arrays of nanogrooves being filled by plastically flowing silicon during cutting. This observation is supported by the direct imaging. The simulated X-ray diffraction analysis proves that in contrast to experiments, Si-I to Si-II (beta tin) transformation during ductile-regime cutting is highly unlikely and solid-state amorphisation of silicon caused solely by the machining stress rather than the cutting temperature is the key to its brittle-ductile transition observed during the MD simulations.

Silicon; Diamond machining; MD simulation; ductile-regime cutting; high pressure phase transformation

1. Introduction

The process of ductile-regime machining of silicon is well documented [1]. The experimental characterisation of machined surfaces shows that the ductile behaviour is based on the phase transformation (diamond-structured cubic silicon transforms into the denser metallic β -tin structure at room temperature) induced by contact stresses. The machining stress is directly proportional to the thrust force and inversely proportional to the projected contact area at cutting edge. Thus, the smaller the area, i.e., the sharper the cutting tool or the smaller cutting edge radius, the cutting action is more favourable. It is also postulated that the release of the pressure upon the movement of the cutting tool past the machining surface results in amorphisation. Studies have revealed that complete ductile-regime machining of brittle materials like silicon is hardly achieved by a careful selection of the cutting parameters only and crack formation in the machined surface is inevitable [2] as evident from figure 1(a).

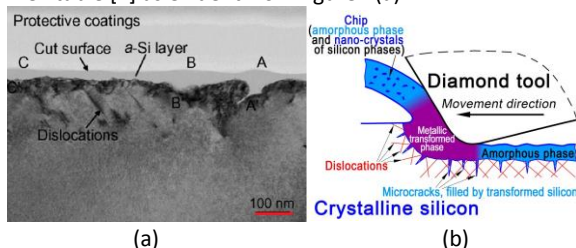


Figure 1. (a) TEM micrograph of the near-surface region after the ductile cutting of silicon. Microcracks are filled by the flowing phase of silicon especially at point A, B and C and (b) schematic representation of ductile-regime machining [2].

Based on this, a schematic representation to reflect on our current understanding has been postulated which is depicted in

figure 1(b). The verification of this hypothesis using state-of-the-art simulation methods such as molecular dynamics (MD) became the motivation behind this work.

2. MD Simulation methodology

As with the other works, the methodology adopted in this work is generic and has been discussed and described in details elsewhere [2-3]. The key difference in this study, in comparison with the previously performed simulations was the use of a long-range potential function. As highlighted in the review by the authors [1], three-body potentials of the Tersoff or the analytical bond order potential (ABOP) type have been used in the past to model the interaction between Si and C atoms. These potentials are short ranged and yield ductile instead of brittle behavior for covalent materials such as silicon or diamond. This shortcoming of the potentials used in the past raises questions about previously performed MD studies of nanometric cutting processes. An improved screened cutoff scheme, which extends the range of these potentials to overcome the described limitations was used in order to overcome these shortcomings [3]. These new, screened potential formulations, which will be used in this simulation study, correctly describe the brittle materials response and improved description of amorphous phases.

2.1. Simulation inputs

A wealth of literature suggests that a very sharp tool should promote brittle-regime machining and for this reason, a sharp cutting edge was deliberately used in this study to probe brittle-regime dominated machining. Further details of the MD simulation model are shown in Table 1 for the purpose of reproducibility.

Table 1 Process variables and details of the MD simulation model

Silicon workpiece dimensions	49.39 nm × 24.7 nm × 8.165 nm , width of cut(w) = 8.165 nm
Uncut chip thickness (d)	3.08 nm => (w/d ratio is 2.65)
Workpiece cut surface and cutting direction	(0 1 0) and <100>
Cutting tool (rake and clearance angle)	(-25° and 10° respectively) and extremely sharp edge (deformable)
Velocity of the tool	250 m/s = 0.25 nm/ps

3. Results and discussions

Simulation results revealed a periodic brittle cracking identifiable from the appearance of equidistant nanogrooves on the machined surface (figure 2a). In experiments, such nanogrooves have been observed from the TEM images of diamond turned silicon specimens (figure 2b). A characteristic quality of these nanogrooves (on the (010) orientation) is that they are oriented at an angle of between 45° and 55° to the direction of cutting. The physical origin of this observation can be seen from the fact that the cleavage face of the (010) oriented silicon substrate was oriented at an angle 45° to the machined surface. The grooves are then filled by the plastically flowing phase of silicon as the cutting progresses. This provides direct evidence that microcracking due to brittle fracture occurring on the machined silicon surface is healed by a plastically flowing phase. The question arises, what is the microstructure of this flowing phase? The local coordination number shown in figure 2c shows a change to 6.

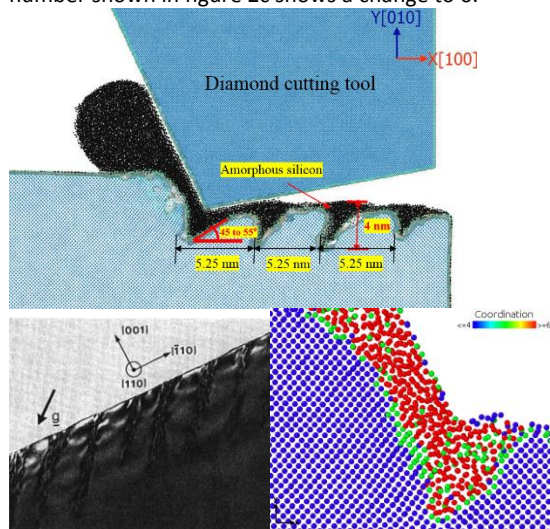


Figure 2. (a) Formation of nanogrooves on the machined sub-surface (b) Experimental image obtained from the diamond turned specimen on the (010) orientation showing periodic array of sub-surface damages inclined at an angle of 55° spaced at 190 nm and (c) Atomic coordination numbers in the cutting zone of SC silicon (tool not shown). [3].

A wealth of literature [1-3] suggests that the coordination number of 6 represents the formation of β -Sn phase (Si-II) silicon, typically at a pressure of about 12 GPa which is approximately the stress level also seen during these simulations. However, the value of coordination number of β -Sn silicon cannot be perfectly 6 because there is always a difference of 5.6% between the subsequent nearest neighbour atoms and secondly, Mizushima et al. [4] used stability analysis and direct MD simulation to show that at least 64 GPa is the minimum pressure required to cause a direction Si-I to Si-II phase transition in an ideal diamond cubic defect free silicon lattice such as the one which is typically modelled. Their ab-initio calculations and classical MD simulation results

demonstrate that the activation energy at the critical pressure needed to transform diamond cubic silicon to β -Sn structure Si is 0.3 eV/atom, which is achieved typically at a pressure of about 64 GPa at 300 K. The process of Si-I to Si-II transformation is known to be an outcome of tetragonal shear instability of the silicon lattice structure. The materials used in experiment carry various types of lattice defects, and these defects lower the magnitude of the stress (~12 GPa) required to cause Si-I to Si-II transformation and hence direct amorphisation during MD simulations is more likely than Si-I to Si-II transformation. Another view of looking at the process of nanometric cutting in contrast to nanoindentation and hydrostatic compression is that it is a deviatoric stress dominating process which results in combined bond stretching and distortion. This bond configuration state does not guarantee a state of tetragonal shear and hence direct amorphisation is more likely during the MD simulations rather than Si-I to Si-II transformation.

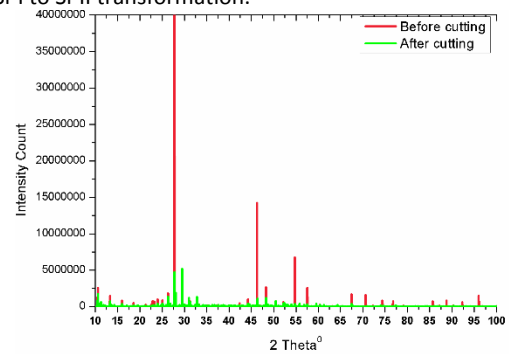


Figure 3. Simulated XRD spectra of silicon before and after cutting. Red peaks signifies crystalline silicon before cutting while scattered green peaks signifies solid state amorphisation of silicon after cutting.

The simulated XRD spectra shown in figure 3 compares the state of the microstructure before and after the cutting. Several distinct peaks at 27.775°, 46.225° and 54.775° corresponds to the standard XRD peaks in crystalline silicon. During cutting, several scattered peaks were observed to appear which are emotive of the presence of amorphous silicon rather than the Si-II silicon proving the direct amorphisation. In addition to amorphisation of silicon, occasionally, some partial dislocations with Burgers vector $\frac{1}{4}\langle 111 \rangle$ and perfect dislocations with Burgers vector $\frac{1}{2}\langle 110 \rangle$ in the silicon substrate's machined sub-surface were also observed from the simulations.

4. Conclusions

A new insight of the formation of periodic nanogrooves oriented at an angle of 45° to 55° in the sub-surface of silicon during its ductile-regime machining is being reported. The nanogrooves appearing in the form of microcracks, microfractures, and small spillings generated during the machining heals due to the filling of the amorphous silicon. Furthermore, direct amorphisation from the pristine crystalline phase, in contrast to Si-I to Si-II transition is identified as the root cause of plasticity in silicon during the MD simulations. This contradicts the established experimental understanding that Si-I phase first transforms to the β -Sn phase (Si-II) typically at a pressure of about 12 GPa.

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