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Influence of microstructure on the cutting behaviour of silicon

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ABSTRACT

We use molecular dynamics simulation to study the mechanisms of plasticity during cutting of monocrystalline and polycrystalline silicon. Three scenarios are considered: (i) cutting a single crystal silicon workpiece with a single crystal diamond tool, (ii) cutting a polysilicon workpiece with a single crystal diamond tool, and (iii) cutting a single crystal silicon workpiece with a polycrystalline diamond tool. A long-range analytical bond order potential is used in the simulations, providing a more accurate picture of the atomic-scale mechanisms of brittle fracture, ductile plasticity, and structural changes in silicon. The MD simulation results show a unique phenomenon of brittle cracking typically inclined at an angle of 45°–55° to the cut surface, leading to the formation of periodic arrays of nanogrooves in monocrystalline silicon, which is a new insight into previously published results. Furthermore, during cutting, silicon is found to undergo solid-state directional amorphisation without prior Si–I to Si-II (beta tin) transformation, which is in direct contrast to many previously published MD studies on this topic. Our simulations also predict that the propensity for amorphisation is significantly higher in single crystal silicon than in polysilicon, signifying that grain boundaries eases the material removal process.

1. Introduction

Silicon has been used extensively in both single crystal as well as in polycrystalline form for a wide range of microelectronic applications including solar cells and conducting gates for CMOS and MOSFET processing devices [1]. Recent technological trends have also led to the synthesis of nanospheres and nanowires of silicon, which would potentially provide an even broader range of applications. However, before this shapes into a reality, it is important to fully understand and characterize the mechanical response of silicon to be able to regulate its behaviour across several disparate engineering applications. Consequently, strenuous efforts are being made to continue Moore's Law (which says that the count of transistors on a silicon chip doubles every two years.) This will require production of ultra-thin silicon wafers. Moore's Law is not a fundamental law of nature, and sustaining this extraordinary rate of progress requires advances in our understanding and the ability to control the properties of materials. One of these properties is the ductile–brittle transition which limits the production of silicon wafers. Therefore, exploration and understanding of the mechanical properties and failure mechanisms of silicon and other nominal brittle materials have become an interesting research topic. In this regard, the existing research details several aspects of silicon, but this material is so versatile that many new phenomena are still being explored to bridge the missing gaps in our existing understanding. Across a number of those research studies, ductility in silicon by large has been attributed either to the occurrence of high pressure phase transformation (HPPT) [1], crystal twinning [2] or surface nucleation of dislocations [3,4]. It is understood that the nucleation of dislocations is more prevalent than HPPT in the presence of free surfaces, for examples in, nanoparticles of silicon [5] while no evidence of crystal twinning during contact loading of silicon has been reported in the literature other than the work of Mylvaganam et al. [2]. Reports of HPPT of silicon on the other hand have a richer history [6], and in the past, several phases of silicon were identified [7] by post-experimentation analysis, which are summarised in Table 1 along with the typical stress levels at which these phases persist.

A systematic representation of what happens to silicon during

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Abbreviations

ABOP	analytical bond order potential
BDT	brittle-ductile transition
CMOS	complementary metal-oxide-semiconductor
d	uncut chip thickness
DXA	dislocation extraction algorithm
Fx	tangential cutting force
Fy	thrust force
GB	grain boundary
HPPT	high pressure phase transformation
MOSFET	metal-oxide-semiconductor field-effect transistor
NVE	microcanonical ensemble
OVITO	open Visualization Tool
pbc	periodic boundary conditions
PC	polycrystalline
SC	single crystal
UNCD	ultra nanocrystalline diamond

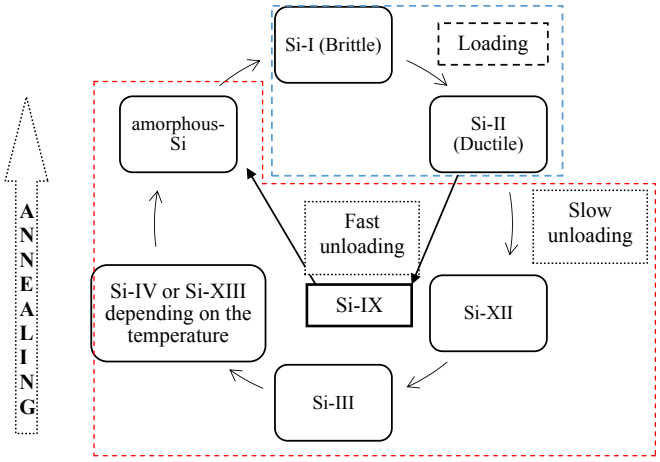

Fig. 1. High pressure phase transformation of silicon during its contact loading [1] – Blue line signifies high pressure phase transformation of silicon to cause metallisation while the red line signifies back transformation after HPPT to an atmospheric phase depending on the rate of release of load. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.).

contact loading (nanoindentation, nanoimpact, loading in a diamond anvil cell and nanometric cutting) is shown in Fig. 1. Literature suggest that a critical magnitude of stress leads to metallization of silicon (Si–I transforms to metastable Si-II phase), and it is this process which facilitates a brittle–ductile transition [8,9] in silicon during contact loading [10]. Thus, our current understanding is that HPPT facilitates a brittle–ductile transition, which in turn enables its ductile-regime machining as revealed in experiments [11]. Subsequently, the kinetics of structural transformation in silicon depends on the rate at which the pressure or load is released. As shown in Fig. 1, upon release of load, the metastable phase of Si-II transforms to amorphous silicon, although, different phases other than Si–I and Si-II appear depending on the release rate. The transformation from high pressure metallic phase (Si-II) to an atmospheric phase (a-Si) is usually accompanied by a volume expansion of ~10%, contributing to the elastic recovery of the cut surface.

Molecular dynamics (MD) simulation has played a key role in developing our understanding of such processes, and an overview of insights gained from atomic-scale modelling of diamond machining of silicon has recently been given by the authors [1]. Typically, three-body potentials of the Tersoff [12,13] or the analytical bond order potential (ABOP) [14] 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. Pastewka et al. [15] recently developed an improved screened cutoff scheme, which extends the range of these potentials to overcome the described limitations. 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.

In addition to the quality of the employed interatomic potential used in an MD simulation study, an analysis of the mechanism of deformation and a precise identification of phases are crucial. Following experimental reports, many atomistic simulation studies of nanoindentation and other surface nano-modification processes have described a Si–I to Si-II phase transition to occur at pressures starting at 12 GPa [16–18]. However, the evidence presented by these simulation-based reports for the presence of the Si-II crystalline phase remains only suggestive. Typically, a change in the radial distribution function computed from the atomic positions and the appearance of some highly coordinated atoms are presented as indications that a phase transformation has taken place. However, it must be noted that these analysis tools cannot give conclusive proof of the presence of an ordered crystalline phase, especially if it comprises only a relatively small group of atoms. In particular, the direct amorphisation of the cubic diamond phase of silicon cannot be excluded, as it would manifest itself in a very

Table 1
Various high-pressure phases of silicon [7].

Phase of silicon	Lattice structure	Stress (GPa)
Pristine Si-I (brittle)	Diamond cubic	0 to 12.5
Si-II (metallic)	Body centred tetragonal (Beta-Sn)	8.8 to16
Si-III or bc8	Body centred cubic (BCC)	0 to 2.1 (ambient)
Si-IV	Hexagonal diamond (Lonsdaleite)	Martensitic transformation from Si–I
Si–V	Primitive Hexagonal	14 to 35
Si-VI	Unidentified	34 to 40
Si-VII	Hexagonal close packed	40 to 78.3
Si-VIII	Tetragonal (30 atoms/unit cell)	0 to 14.8
Si-IX	Tetragonal (12 atoms/unit cell)	0 to 12 (Upon rapid decompression from Si-II
Si-X	Face centred cubic (FCC)	78.3 to 230
Si-XI (Isma)	Body centred orthorhombic	13 to 15
Si-XII (R8)	Trigonal (8 atoms/unit cell)	2 to 12