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Dislocation-mediated plasticity in silicon during nanometric cutting: A molecular dynamics simulation study

Saeed Zare Chavoshi [a], Shuozhi Xu [b], Xichun Luo [a,*]

[a] Centre for Precision Manufacturing, Department of Design, Manufacture and Engineering Management, University of Strathclyde, Glasgow G1 1XJ, UK
[b] GWW School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0405, USA

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ABSTRACT

The nucleation and propagation of dislocations and its consequence on the defect structure in silicon during nanometric cutting are not well known, although the amorphization and high pressure phase transformation studies on silicon have remained at the epicentre of research across various disparate disciplines for over a decade. This paper proposes a new mechanism of crystal plasticity identified by a fully automated dislocation extraction algorithm in molecular dynamics simulations of nanometric cutting of silicon for different cutting planes/directions at a wide range of temperatures (300–1500 K). Alongside amorphization of silicon, our simulations revealed nanoscale stochastic nucleation of dislocations and stacking faults, which serve as mediators of microscopic plasticity during various contact loading operations and manufacturing processes of silicon. Of interest is that, irrespective of the cutting temperature, the stacking faults, which were not formed for either the (010)[100] or (111)[$\bar{1}$10] crystal setups, were generated with three atomic layers in the (110)[00$\bar{1}$] cutting.

1. Introduction

Silicon, a diamond cubic lattice structured material, exhibits strong and directional sp^3 bonding and has two sets of {111} slip planes, the shuffle and the glide sets. Recent molecular dynamics (MD) simulation studies of high-power, pulsed, laser-driven shock compression of silicon revealed that partial dislocations and stacking faults can be emitted from the surface under pressures that are slightly higher than 10 GPa [1,2]. Likewise, in MD simulations of strained silicon nanowires of different lengths, the yield was exhibited by dislocation nucleation [3,4]. Nevertheless, previous studies in nanometric cutting of silicon showed that the ductility and plasticity of silicon are direct consequences of amorphization rather than dislocation nucleation and migration [5,6].

A key question thus is whether the nucleation and migration of dislocations and other crystal defects assist in crystal plasticity of silicon during nanometric cutting at room and high temperatures. Previous MD studies failed to answer this question primarily due to the application of an improper interatomic potential function, i.e. Tersoff [7], to describe the dislocation cores [8]. Accordingly, the present study aims to gain an in-depth understanding of the plasticity mechanisms of silicon during nanometric cutting at different temperatures, using the Stillinger-Weber (SW) potential function [9] with the aid of the dislocation extraction algorithm (DXA) [10]. The DXA has a proven ability to identify dislocations in diamond structure such as Si [5] and Ge [11]; its algorithm is based on a discrete Burgers circuit integral over the elastic displacement field and is not limited to specific lattices or dislocation types [10]. The virtual X-ray diffraction (XRD) [12] analysis is also carried out to quantify the structural changes of silicon.

2. Computational method

The three-dimensional MD model of nanometric cutting is illustrated in Fig. 1, with the details of simulation model and process parameters summarized in Table 1. The simulation methodology is the same as in our previous work [13–15], i.e. the region of atoms in the tool and the substrate were divided into three zones namely, boundary atom zone, thermostatic atom zone and Newtonian atom zone. The boundary atoms were held rigid to reduce the boundary effects and to maintain the symmetry of the lattice. The Newtonian region followed the Newtonian dynamics (NVE ensemble) while the thermostat zone was updated according to the Berendsen thermostat to emulate the effect of heat carriers like chips and lubricants. The periodic boundary conditions (PBCs) were imposed along the z direction of the simulation domain to reduce the effects of simulation scale. The MD simulations were conducted using LAMMPS [16] with an "Open Visualization Tool"

* Corresponding author.
E-mail address: xichun.luo@strath.ac.uk (X. Luo).

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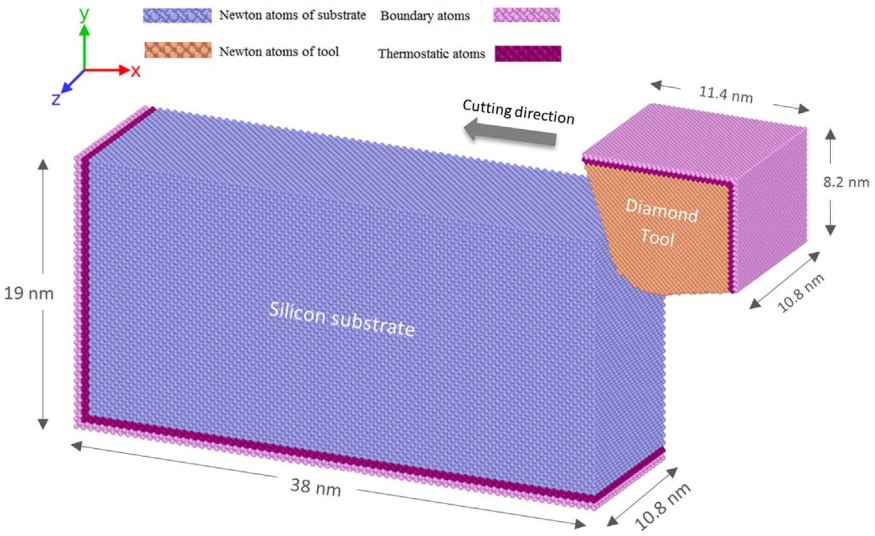

Fig. 1. Schematic diagram of the MD simulation model of nanometric cutting. Different cutting planes (y plane) and cutting directions (x direction) are tested at a wide range of temperatures.

Table 1
Details of the MD simulation model and the cutting parameters used in the study.

Substrate/tool material	Single crystalline silicon/diamond
Substrate dimensions	$38 \times 19 \times 10.8$ nm^3
Cutting edge radius (tip radius)	3.5 nm
Uncut chip thickness (cutting depth in 2D)	3 nm
Cutting plane (y plane) and cutting direction (x direction)	Case 1: (010)[100] Case 2: (110)[00$\bar{1}$] Case 3: (111)[$\bar{1}$10]
Rake and clearance angle of the cutting tool	$-25°$ and $10°$
Substrate temperature	300 K, 750 K, 850 K, 1173 K, 1273 K, 1500 K
Cutting speed	50 m/s
Time step	1 fs
Potential energy function	SW [9]

(OVITO) [17] and DXA [10] to visualise and analyse the atomic trajectories.

The SW potential function [9], which incorporates a linear combination of two- and three-body terms, was employed to describe the interactions between silicon atoms (Si-Si) in the substrate whereas an analytical bond order potential (ABOP) formalism [18] was adopted to dictate the interactions between diamond atoms (C-C) in the cutting tool as well as those between substrate and tool atoms (Si-C). The SW potential provides a better approximation of the maximum restoring force, the theoretical shear strength, and the strain associated with the critical stress for both shuffle and glide sets planes than the Tersoff [7] and Environment-Dependent Interatomic Potential [19] potentials. Moreover, the SW potential leads to smooth stacking fault energy (SFE) variations, in agreement with *ab-initio* simulations [8,20,21]. Some caveats of the SW potential include an underestimation of the unstable/stable SFE for the shuffle set-plane and an overestimation of them for the glide set-plane. As a result, it is expected that for the glide set-plane, using the SW potential, (1) both the leading and trailing partials are more difficult to nucleate and (2) the stacking fault width is smaller, compared with *ab-initio* simulations. The opposite is true for the shuffle set-plane. Nevertheless, in the motion of dislocations, the unstable SFE is less important than the rebound force of the lattice subject to large deformations, which is accurately given by the SW potential [8]. The SW potential also accurately reproduces the melting temperature of silicon which, however, comes as a price that the cohesive energy is rescaled; by consequence, the elastic constants are also rescaled, leading to some inconsistencies in reproducing relevant mechanical properties of silicon with those of experiments, as indicated in Appendix A. Taking into account the restricted transferability of empirical potentials, the SW potential is a good choice for exploring dislocation-mediated plasticity of silicon at room and elevated temperatures during nanometric cutting.

In order to obtain accurate simulation results, we first calculated the cohesive energies and corresponding equilibrium lattice constants of silicon at various temperatures using the SW potential energy function, as shown in Table 2; these lattice constants are subsequently utilized to build the geometry of the substrate. In all cases, the tool was equilibrated at 300 K; hence the lattice constant of 3.568 Å calculated using the ABOP function at 300 K was used for the carbon atoms. Note that the cohesive energy was time-averaged over 1 ns under NPT ensemble.

3. Results and discussion

Nanometric cutting involves plastic deformation of materials at high strain rates. The slip systems with the largest resolved shear stress along the Burgers vector are activated on the threshold of plasticity. Dislocation glide in silicon occurs in two widely and narrowly spaced {111} dense planes, shuffle and glide sets, respectively [8]. However, at high temperatures slip can also take place in the {110} and {100} planes [24].

Table 2
Calculated equilibrium lattice constants and cohesive energies of silicon at different temperatures using SW potential energy function. The cohesive energy calculated here is slightly lower than the experimental value of -4.62 ± 0.08 eV [22], which potentially results in smaller elastic constants. We assume that such effects are small in the context of this work, which focuses on the plastic response of silicon.

Temperature (K)	lattice constant (Å)	cohesive energy (eV)	Experimental lattice constant (Å) [23]
300	5.4348	−4.3355	5.431
750	5.4405	−4.3338	5.439
850	5.4423	−4.3326	–
1173	5.4458	−4.332	~ 5.449
1273	5.4473	−4.3312	~ 5.452
1500	5.4502	−4.3308	~ 5.457