Molecular dynamics modeling of nanoscale machining of silicon

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Abstract

In this study, the brittle-ductile transition in nanometric machining of mono-crystalline silicon with precise tool specifications and parameter choices is accessed. Due to its brittle nature, silicon material requires a ductile-mode machining for improved surface quality. Molecular dynamics (MD) methods are thus applied to investigate the atomic scale reaction at the tool/workpiece surface to clearly expose the ductile transition response of this nanometric process. However, the need for experimental validations to determine the accuracy of these simulation models is essential. This research is particularly concerned with the application of the molecular dynamics simulation approach to the atomistic visualization of the plastic material flow at the tool/workpiece interface during orthogonal cutting. Simulated MD acting force and temperature outputs are evaluated to access the accuracy of the model. This evaluation substantiates the need for additional experimental validation of certain process conditions for verifiable MD results.

1. Introduction

Ultra-precision machining of monocrystalline silicon has become tremendously important in microelectronics, micromechanical and optical element manufacturing; and thus the mechanism of nanometric cutting of monocrystalline silicon has also been a focused research topic. Molecular Dynamics (MD) simulation is in so doing developed as an effective way for studying the material removal process at the nanometric scale [1, 2]. Due to the advance in technology, the semiconductor industry has also made considerable improvements to meet market demand. Silicon as an exemplary semiconductor is greatly used in today’s manufacturing. The applications of Monocrystalline silicon are seen in micro-electromechanical systems (MEMS) which require accuracy and high surface integrity [3]. Additional applications are also seen in the fabrication of high performance solar cells, semiconductor electronics and bio-medical imaging applications.

Currently, methods of preparation of silicon wafers are extremely costly and time consuming. The process for a finished piece involves grinding, lapping, polishing and back thinning. However, nanoscale ductile mode cutting of silicon wafer materials, which is fracture-free, requires no subsequent polishing, and tends to be a much better alternative approach for the technological advancements in semiconductor industry [4]. Ultra-precision single-point diamond machining (SPDM) is thus used in the fabrication of MEMS to meet its high requirements in surface accuracy.

Single point diamond turning (SPDT) as a reputable ultra-precision process was established by exploiting the “brittle-ductile transition” phenomenon which made brittle materials amenable to ultra-machining using diamond cutting tool [5]. SPDT is used to produce brittle optics with sub-micron nanometric accuracy. The literature shows that a vast amount of experimental work has been carried out in the field of nanometric machining. Many researchers using SPDT have attempted to fully explain the mechanism of nanoscale ductile mode when cutting silicon [4, 6]; however the nanoscale cutting dimension in SPDT forms a challenge in finding suitable approach. Furthermore, these procedures are time consuming and costly to run. Therefore, in an aim to broaden knowledge on these processes while minimizing experimental efforts,
a molecular dynamic approach has been introduced in the field of nanometric machining [7].

The objective of this study is to model the nanoscale cutting of monocrystalline silicon optics in ultra-high precision machining using Molecular dynamics simulations and substantiates the need for additional experimental validation of certain process conditions for verifiable MD results.

1.1. The MD method

Molecular dynamics as a computer simulation technique uses a time-based statistical mechanics method to study the interrelation of atoms for conditions prediction and analysis. Numerous researchers have used MD as a tool to access cutting condition of diamond machining of various materials with distinct mechanical properties [2]. Oluwajobi and Chen also have done extensive work on MD simulation of nanomachining of copper[8, 9]. In their studies they investigated various parameters in nanomachining such as minimum depth of cut, tool geometry and interatomic potential[2]. In addition, MD simulations results have also been successful in the past to address a number of problems concerning the nanometric cutting process of brittle materials such as silicon [3, 4, 7].

Komanduri et al. conducted an MD simulation of nanometric cutting of single-crystal, defect-free, pure silicon using the Tersoff potential. In their study the effects of rake angle, width of cut, depth of cut and clearance angle on material removal and surface generation were investigated[10]. Goel et al. in their research investigated the atomistic aspects of ductile response of SiC during the nanometric cutting process. They discovered the presence of a sp’-sp’order-disorder transition which finally resulted in the graphitization of diamond[5]. Cai et al. [4] used MD to study the nanoscale ductile mode cutting of silicon. Their study observed the tool cutting edge and its effects on the shear stress in the workpiece material.

Various other researchers have also highlighted the conditions in the nanomachining of silicon using MD simulations based on; investigations of cutting forces[1, 4], depth of cut, temperature [5], shear stress [4] and other parameters. However, there is a lacks of adequate experimental validations in this area. Arafin et al. [11] discussed the effect of cutting edge radius in nanoscale ductile mode cutting of silicon wafer. The use of scanning electron microscope (SEM) images were employed to determine the subsurface roughness and findings were further analyzed based on Cai’s[4] MD study. However limited conclusive findings based on MD outcomes could be postulated. Aly et al. conducted their validation of nanometric machining for silicon using Finite Element Analysis (FEA) of force values. Their conclusion suggests several future perspectives to conclusively determine material behavior [7].

1.2. MD Simulation

A schematic diagram of the nanometric cutting simulation model is shown in figure 1. The simulation comprises of a single crystal diamond cutting tool with a nose radius of 0.714 nm. The workpiece is divided into three different atomic zones: Newton/movable atoms, thermostatic atoms and boundary atoms. The boundary atoms have no set force acting on them, remain fixed during simulation and therefore avoid unexpected movement of the workpiece during cutting. These atoms aid in maintaining lattice symmetry and reduce boundary effects during simulation. The thermostats layer is set to a temperature of 293K which assists to dissipate high heat generated from cutting away from the cutting zone.

Following made contact from the three-dimensional tool, the motion of the Newtonian and thermostats atoms, act according to Newton’s second law of motion
which can be computed from their interatomic forces. For a set of N particles or atoms,

\[ F_i = m_i a_i \]  

(1)

Where \( m_i \) is the mass of atom \( i \), \( a_i = \frac{d^2 r_i}{dt^2} \), the acceleration of the atom \( i \) and \( F_i \) is the force acting on atom \( i \).

In this study thermostat atoms were slightly increased to three Angstrom to observe high heat dissipation and its effects at the atomic conditions.

### 1.3. Simulation conditions

In this study, the simulated model specimen contains 16,972 monocristalline silicon atoms, and 2,944 arranged in the diamond cubic crystal structure. Boundary conditions were fixed and initial conditions for temperature and integration constants were set. Selected potential energy functions were then applied to simulate atomic reactions.

### 1.4. Potential energy function

Force potentials encompass the force fields interactions amidst the various atoms in a simulation. It accounts for the stability of the atomic environment and in turn defines the reliability and accuracy of the MD simulation [6]. Three different force interactions exist amidst various atoms:

- Amidst the workpiece atoms
- Between the workpiece and the cutting tool
- Within the cutting tool [1]

The interactions possess different potential forces acting on the atoms during cutting process. In this study, Tersoff potential and the Morse potentials were used on the workpiece. The diamond tool is however classified as a single rigid body and thus no forces were integrated amidst its atoms.

#### Tersoff potential

The Tersoff potential function is used to describe the interatomic relations between the silicon atoms from the workpiece. The concept of the potential is based on the concept of bond order. In this potential, the strength of a bond found between two atoms is not constant, but depends on the local environment. The potential energy thus is in the form of [8]:

\[ E = \sum_i E_i = \sum_i \frac{1}{2} \sum_{i \neq j} V_{ij} \]  

(2)

\[ V_{ij} = f_c(r_{ij}) \left( a_{ij} f_B(r_{ij}) + b_{ij} f_A(r_{ij}) \right) \]

(3)

where

\[ f_c(r) = \begin{cases} \frac{1}{2} - \frac{1}{2} \sin \left( \frac{\pi (r - R)}{D} \right), & R - D < r < R + D \\ 0, & r > R + D \end{cases} \]

(4)

\[ b_{ij} = (1 + \beta n^\alpha)^{-1/2n} \]

(5)

Where \( E, E_i \) are the energies of interacting atoms, \( V_{ij} \) is the pair potential, \( R \) and \( D \) are cut-off parameters [8]. Also \( b_{ij} \) is a function of the cut-off radius.

The term \( \xi_{ij} \) (equation 4) defines the effective coordination number of atom \( i \), i.e. the number of nearest neighbors, taken into account the relative distance of two neighbors \( r_{ij} \) and the angle between the atomic bonds (equation 5). This angle \( \theta \) within function \( g(\theta) \) has a minimum for \( h = \cos(\theta) \), in which the parameter \( q \) determines how sharp the dependence on angle is, and \( p \) expresses the strength of the angular effect.

\[ \xi_{ij} = \sum_k (x_{il} x_{jk} f_c(r_{lk}) g(\theta_{ijk}) e^{[\alpha_2^2/r_{ij}^2 - \alpha_1^2/r_{jk}^2]} \]

(6)

\[ f_B(r) \] & \( f_A(r) \) in equation 3, are the repulsive and attractive forces between atoms \( i \) and \( j \) can be represented as (equation 6) [7]:

\[ f_B(r) = A e^{-\lambda_1 r}, f_A(r) = -B e^{-\lambda_2 r}. \]

The Tersoff potential models the total energy of the system as a sum of pair like interactions. Based on its suitability for covalently bonded materials such as silicon germanium and diamond it was selected for this study [2].

Some of the computational parameters used in the MD model are listed in Table 1.

| Tersoff potential parameters for silicon | Values |
|-----------------------------------------|--------|
| \( A \) (eV) | 1.8308×10^{8} |
| \( \beta \) (eV) | 4.7118×10^{2} |
| \( \alpha (\text{nm}^{-1}) \) | 24.799 |
| \( \mu (\text{nm}^{-1}) \) | 17.322 |
| \( n \) | 7.8734×10^{-1} |
| \( c \) | 1.0039×10^{5} |
| \( d \) | 1.6217×10{1} |
| \( h \) | 5.9825×10^{-1} |
| \( R \) (nm) | 0.27 |
| \( \delta \) (nm) | 0.3 |
Morse Potential

Morse potential is a pairwise potential energy function for bonded interactions. Many researchers have supplied different constants for the Morse potential for different materials [1, 9]. From figure 2, the potential trails a reaction curve of energy to distance between atoms, yielding a repulsive force down the curve in the short range, attractive force along the rising curve in the medium range and a decay which stabilize in the long range of atomic force energy.

\[
\varphi (r_{ij}) = D \exp \left[ -2\alpha (r_{ij} - r_0) \right] - 2 \exp \left[ -\alpha (r_{ij} - r_0) \right] \]

(5)

Where \( \varphi (r_{ij}) \) is a pair-potential function, and \( D, \alpha \) and \( r_0 \) correspond to the cohesion energy, the elastic modulus and the atomic distance at equilibrium, respectively. The Morse potential was selected due to its suitability for cubic metals. This potential can adequately be used to model the interaction between an atom and a surface [2]. The values of the chosen parameters are:

\[
D = 0.435 eV, \quad \alpha = 46.487 \text{nm}^{-1}, \quad r_0 = 0.19475 \text{nm}.
\]

In this simulation the interaction between the atoms of the workpiece and the tools are attained from the Morse potentials.

2. Simulation Analysis

2.1. Analysis setup

In this study, a three-dimensional MD simulation model was employed. Figure 3 shows a schematic of the output of the MD simulation system. The diamond tool with a nose radius of 0.714 nm, cutting speed of 35 m/s and a depth of cut 1.086 nm were used to cut the silicon workpiece. The dimension of the control volume of the silicon specimen was made sufficiently large to eliminate the boundary effects. Some parametric values used in the MD simulation are shown in Table 2.

![Fig. 3. MD simulation of nanometric cutting of silicon](image)

Table 2. Parametric values used in MD simulation

| Configuration                  | Value                  |
|-------------------------------|------------------------|
| 3D                            | 14×11×12 dimension     |
| Lattice constant \((r_0)\)    | 5.43 Å (0.543 nm)      |
| Diamond lattice \((r_1)\)     | 3.57 Å (0.357 nm)      |
| WP dimensions                 | 14 \(r_0\) × 11 \(r_0\)× 12 \(r_0\) |
| Crystal orientation \([001]\) |                        |
| Depth of cut                  | 1.086 nm               |
| Width of cut                  | 1.428 nm               |
| Cutting Speed                 | 35 m/s                 |
| Temperature                   | 293K                   |
| Time steps                    | 0.2 fs (2 x 10^{-15})  |

Figure 3 shows the change effect on the 3 dimensional model of monocrystalline silicon. The model consists of a 14×11×12 dimension based on a lattice constant of 5.43 angstrom for silicon. A machined area with a depth of cut of 1.086 nm and a width of cut of 1.428 nm was machined. The simulation was performed on a crystal orientation \([001]\) in the cutting direction, over a 100,000 steps at 0.2 fs per step.
3. Results and discussion

3.1. General appearance

The MD cutting process of monocrystalline silicon displayed an initial atomic break in the lattice depicted by a clear scattering of atoms. However, this is followed by a tightly bonded atomic observation of atoms during cutting (as seen in Figure 3).

3.2. Thermodynamic information analysis

Observations of the temperature, cutting force ($f_x, f_y$ and $f_z$) as well as the potential energy is analyzed in this study. An initial unstable temperature of force signal is observed in Figure 4 (a & b). This observation could propose the initial atomic shatter reaction of atoms which could have resulted from tool entry which later stabilizes with prolonged cutting.

For the Tersoff-Morse potential utilized, the temperatures and cutting force stabilized after 4400 steps. This cutting action is further detected by the wide increase in the potential energy found on the atoms as stabilization occurs (Figure 5).

Various conclusions could be attributed to this stabilization at the atomic level. Some of which are:
- High thermal conductivity of monocrystalline silicon
- Choice of potential energy function
- And scale of nanomachining simulation

However, these analyses require additional information to sufficiently determine appropriate the simulation choices. Simulation outcomes could both relate to potential energy function, simulation design or scale of design. The high thermal conductivity of the silicon piece could be the result of the influence of the increased thickness of the thermostats layer atoms found within the workpiece.

Furthermore, the phenomenon of ploughing was very faintly observed with a pile-up of two layers of atoms from the external Van der Wall (VDW) simulation drawing method (figure 3). However, using a CPK lattice in figure 6, a cushion bed of atoms is formed from the displacement of atoms within the workpiece in the compressive stress zone. This alternate drawing method shows a more robust internal ploughing phenomenon.

Fig. 5. Simulation of total/potential energy

Fig. 6. MD simulation showing atomic movement within the silicon workpiece
Silicon (monocrystalline) has a high thermal conductivity of 148 k [W m\(^{-1}\)K\(^{-1}\)]. This was reflected in the temperatures marked with an initial rise at tool entry which later stabilized during cutting operation (Figure 4b).

4. Conclusion

Despite the capacity of MD to investigate atomistic reaction at the tool/workpiece surface, however, the shortfall of the simulation dimension is portrayed by the fact that MD simulations only observes a nano-portion of the cutting effect which does not proportionally apply to an experimental larger scale nanomachining process. Adequate validation of MD simulation using a combination of in-process monitoring sensing techniques to its thermodynamic outputs is essential to certify MD simulations. Various sensing techniques provide different information for validation at atomic level during simulation.

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