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Investigation of tool-workpiece interaction in nanoscale cutting: A Molecular Dynamics study

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Abstract

In the present day manufacturing, ultra precision surfaces are largely created through nano-regime machining processes like diamond turning where a few cluster of atoms on the substrate material are processed to generate the surface. The ultraprecise surfaces of copper (Cu) and silicon (Si) generated through the nanoscale cutting process are extensively used in electronics, semiconductor and optical industries. Since both the materials differ in their physical and mechanical properties and pose distinct interaction with tool, it is imperative to analyze the mechanism of material removal and tool-workpiece interaction. As the interaction takes place at nanoscale, it is very difficult to observe the phenomenon during the machining operation. Therefore, Molecular dynamics simulation is carried out to study the diamond tool and workpiece interaction in the nanoscale cutting of Cu and Si. Results show that material removal in Cu takes place through shear deformation by dislocation formation and motion while in case of Si, no shear deformation takes place; it is phase transformation of the material in cutting zone and subsequently the material is removed in the form of chips. Furthermore, radial distribution function reveals that graphitization of the diamond tool occurs during machining of Si whereas Cu doesn't affect the tool during the cutting operation.

Keywords: MDS, Diamond turning, Copper, Silicon, Nanoscale cutting.

1. INTRODUCTION

Ultraprecision nanoscale cutting of materials with diamond tool has enabled us to achieve nanometric finished surface with submicron accuracies of components. These ultraprecise components are finding applications in optics, aerospace, medical, micro-/nano-electromechanical systems (MEMS/NEMS), electronics & telecommunicationand micro-/nanorobotics. Single crystal copper (Cu) and silicon(Si) are two most popular materials in optics and semiconductor industries. Both the materials have different atomic arrangement, bonding and crystal structure and thus possess different properties. Therefore, in order to generate highly finished surfaces on these materials, various factors such as material removal mechanism, tool edge radius, uncut chip thickness, material properties, elastic-plastic deformation and subsurface damage play crucial role. Since nanoscale cutting involves a few number of atomic layers, there are experimental limitations to observe in-situ phenomena of structural changes, defects existence and dislocations formation and motions. Molecular dynamics simulation (MDS) allows the tracking of atomic trajectories and thus provide the valuable and deep insights into the various phenomenon occurring during nanoscale cutting. Various studies have been carried out on these materials by previous researchers.

Komanduri was one among the firsts who proposed MDS in nanoscale cutting of Cu and Si. Komanduri et al. suggested high hydrostatic stresses ahead of cutting zone in Si suppresses the crack generation [1]. Shi and Verma [2] compared the atomic scale machining of single and polycrystalline Cu and showed that nature of variation of tangential cutting forces and thrust forces is different in both the cases. Pei et al. [3] compared Morse pair potential and EAM potential for Cu and observed that tool forces can be precisely calculated with EAM potential. Further, they showed that machined surface integrity depends on the rake angle. Ye et al. [4] carried out MD simulation of nanoscale machining of Cu at two different speeds and observed the presence of dislocations at lower speed. Cai et al. [5] discussed the mechanism of material removal of Si with respect to tool edge radius and uncut chip thickness during nano-cutting with diamond tool. Through MDS, Goel et al. [6] showed effect of crystal orientation on the wear resistance of a diamond tool used for cutting Si. They suggested that cubic orientation is better than dodecahedral. The available literature discusses about the chip formation mechanism and parametric study, however, the subsurface damage and tool wear have received little attention for both ductile (Cu) as well as brittle material (Si).

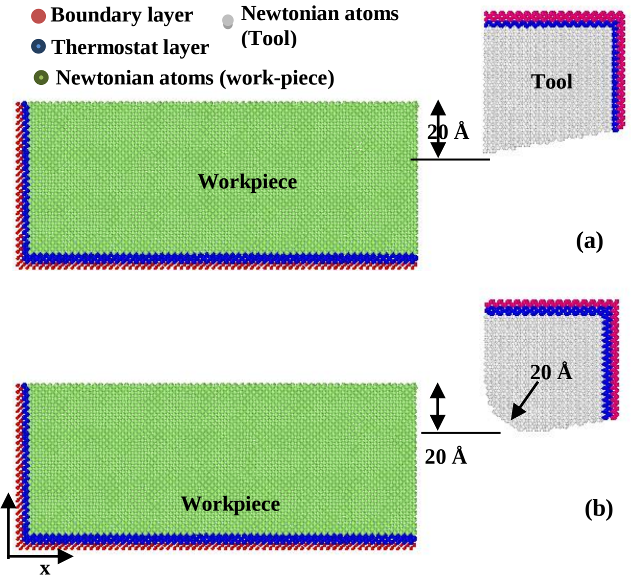

Fig. 1. MDS model for nanoscale cutting (of Cu and Si) with diamond tool having (a) Sharp edge (b) Round edge

In the present study, MDS is employed to perform the comparative study of tool and workpiece interaction in the nanoscale cutting of Cu and Si. The effect of tool edge radius on the material removal mechanism, subsurface deformation is

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investigated on both the materials. Furthermore, the effect of workpiece materials on the tool is also studied in terms of tool edge deterioration and diamond phase change.

2. SIMULATION METHODOLOGY

2.1. Cutting simulation geometry and conditions

Fig. 1 shows the MD model of tool and workpiece employed for both Cu and Si. The dimension of the workpiece used is 200 Å x70 Å x 80Åand tool comprises two configurations: one is sharp and the other is a cylindrical configuration of edge radius 2 nm. Both the tool and workpiece are composed of three layers viz. Newtonian layer, thermostat layer and boundary layer. Thermostat and Newtonian layer together forms a mobile layer in which positions and velocities of atoms are calculated and updated based on Newton's second law of motion. Boundary layer atoms support the mobile layer atoms and also eliminate the boundary effects. Thermostat atoms are kept at constant temperature (293 K) by updating the atoms velocities to the desired temperature which assist in dissipation of the heat generated during cutting. Periodic boundary condition (PBC) is applied to the z-direction in order to reduce the size effects and realize the bulk material conditions.
The computational parameters used in the MD simulation are presented in Table 1.

Table 1

Computational parameters used in MDS of nanoscale cutting.

Workpiece material	Single crystal Cu & Si
Cutting plane and direction	(010)and[$\bar{1}00$]
Dimensions	200 Å x70 Å x 80Å
Tool (Deformable)	Single crystal diamond
Cutting edge radius (R)	0 and 20 Å
Uncut chip thickness (a)	20Å
Cutting velocity	1 Å/ps
Equilibration Temperature	293 K
Time step	0.001 ps

2.2. Choice of Potential Energy function:

MDS provides accurate results only if the appropriate interatomic potential function is adopted. Cu is a metallic material and possesses face centered cubic (FCC) lattice structure. Interaction between the copper atoms is precisely expressed by Embedded Atom Method (EAM) potential[7]. The total potential energy of an atomic system based on EAM potential is expressed by the following equation:

$$U_{tot} = \frac{1}{2}\sum_{j\neq i} V(r_{ij}) + \sum_{i} F_i(\rho_i) \qquad (1)$$

Where V represents a pair potential and is a function of the distance r_{ij} between atom i and surrounding atom j. F_i denotes an embedding energy that represents the energy to place an atom iin a host electron density (ρ_i) at the site of that atom i, induced by all other atoms in the system and expressed as:

$$\rho_i = \sum_{j\neq i} \phi_j(r_{ij}) \qquad r_{ij} < r_c \qquad (2)$$

Si and diamond (sp3 bonded Carbon) has diamond cubic structure in which atoms are bonded together with covalent bonds. A 3-body potential based on ABOP formalism base on was used to describe the Si-Si, C-C and Si-C interaction [8]. Total energy using ABOP function is a sum over each bond energies:

$$E = \sum_{i>j} f_c(r_{ij}) \left[V_R(r_{ij}) - \frac{b_{ij} + b_{ji}}{2} V_A(r_{ij}) \right] \quad (3)$$

Where E is the cohesive energy which is the sum of individual bond energies which has following pairwise repulsive and attractive contributions.

The interaction between tool and workpiece is well approximated through a Morse pair potential function. Morse potential function is expressed by Eq. 4.

$$\begin{aligned} V(r_{ij}) = D[&\exp(-2\alpha(r_{ij} - r_o)) - \\ &2\exp(-\alpha(r_{ij} - r_o))] \end{aligned} \qquad (4)$$

Where, D, α, r_{ij}, r_0 and are the binding energy, elastic modulus, arbitrary distance between i and j atoms and equilibrium atomic spacing, whose values are listed in Table 2.

Table 2

Morse potential parameters for Cu and C [9]

Element	D (eV)	α ($Å^{-1}$)	r_0 (Å)
Cu-C	0.1	1.7	2.2

2.3 MD procedure

After the tool and workpiece were created, initial velocities to the atoms were assigned at 293 K according to Maxwell-Boltzmann distribution and the combined system was equilibrated at the same temperature under the micro canonical ensemble (NVE) for sufficient time. Once the equilibration period is over, velocity scaling is removed from all the atoms and applied only to thermostat atoms of the tool and work-piece to dissipate the heat generated during cutting. Cutting velocity is applied to the tool in the negative x direction and the system is allowed to follow NVE dynamics. In the NVE ensemble, the atoms in the Newtonian and thermostat layers are allowed to follow classical Newton's second law of motion. For each atom in a system of N atoms, force acting upon it due to other atoms is expressed as

$$F_i = m_i a_i = -\nabla V \qquad (5)$$

m_i is the atom mass, a_i is its acceleration and V is the potential energy. The equations of motion are integrated with the help of velocity- Verlet algorithm with a time step of 1 fs and atoms positions and velocities are updated each time step. Large-scale atomic/molecular massively parallel simulator (LAMMPS) [10][11], a molecular dynamics program from the Sandia National Laboratories, was employed to conduct the MD simulation and OVITO [12], a 3D visualization software, was used for the visualization and analysis of atomistic data obtained from the LAMMPS.

3 RESULTS AND DISCUSSION

3.1 Material removal mechanism

Since both Cu and Si have different lattice structure and bonding, they differ in their behavior when cutting action is performed. Also sharp and round configuration of tool affects the deformation zone. Sharp tool edge in Cu enables the material removal by shear slip ahead of tool. The shear slip is assisted by the coherent twin boundary which manifests itself as HCP structure shown by red colored layer in Fig. 2(a).For round edge, shear deformation zone instead of single shear plane takes place ahead of cutting edge.

When the tool comes in contact with workpiece, rake part of the tool compresses the workpiece axially and shear slip occurs whereas round cutting edge compresses the material ahead of it and squeeze it to flow through either side of the tool. Therefore, initially chip removal takes place by shear slip and extrusion due to high pressure ahead of cutting edge. During stable cutting period, both the deformation mechanisms merge into one and material removal takes place through shear zone as shown in Fig. 2 (b).

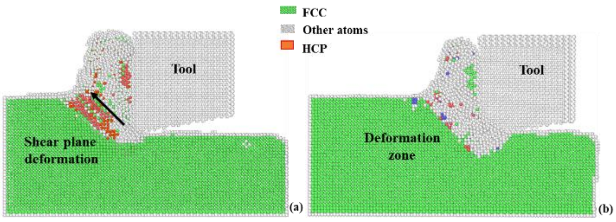

Fig. 2. Material removal mechanism during nanoscale cuttingof Cu (a) Sharp edge (b) Round edge

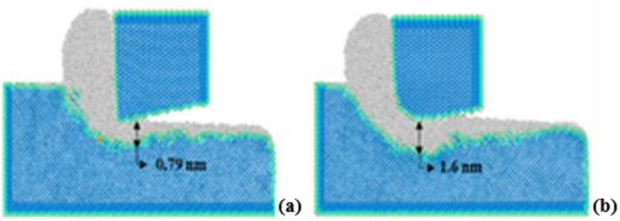

Fig. 3. Material removal and subsurface damage during nanoscale cutting of Si with (a) Sharp edge (b) Round edge tool.

In case of Si being a brittle material, shear slip does not occur and the material in a narrow zone ahead of cutting tool is compressed and the covalent bonds are crushed which in turn changes the atomic arrangement in the narrow deformation zone and transforms the diamond cubic structure to amorphous phase due to high hydrostatic pressure as shown in Fig. 3 (a). The distorted phase possesses low bonding energy and thus is easy to remove by the cutting action of the tool. The amorphous phase exists upto few atomic layers beneath the tool which manifests itself as a subsurface damage. Similar behavior is shown by round cutting edge in Fig. 3(b), however, higher material deformation takes place underneath the tool.

3.2. Subsurface damage

As depicted form Fig. 3 and 4, the subsurface quality is impaired in both the materials by cutting action with highly sharp and round edged tools. In case of Cu, it happens through the dislocation loops gliding into bulk materials while for Si, it takes place through amorphous layer of atoms. Since sharp edge tool poses higher cutting action and less thrust is posed, the dislocations are mostly oriented to move in front of tool as shown in Fig. 4(a). However, round cutting edge has sufficient amount of thrust action on the material which constrains the dislocations to move into bulk of the material and leads to higher subsurface deformation as shown in Fig. 4(b). Si presents the similar behavior, the only difference is here subsurface damage occurs by the presence of amorphous layer of atoms. Fig. 3 (a) & (b) shows that the round cutting edge causes twice the damage than that caused by sharp edge tool. The subsurface damage may change the subsurface properties and distortion in electrical properties of both the materials.

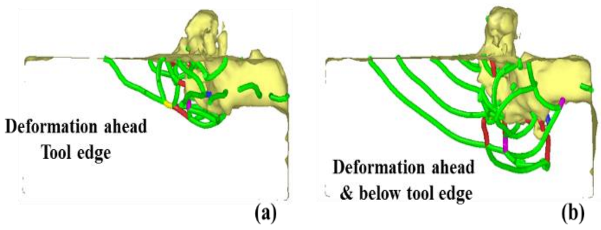

Fig. 4. Subsurface deformation (Dislocation generation) during nanoscale cutting of Cuwith (a) Sharp edge (b) Round edge tool.

3.3. Tool wear Mechanism

As the tool geometry influences the workpiece material deformation and chip formation, work material also affects the tool during cutting operation. Tool wear is a serious concern which affects the surface quality. The mechanism of wear is different for different materials. Since Cu is a soft material, it poses low cutting resistance on the tool edge. The tool wear in Cu for nanoscale cutting distance is insignificant as the tool atoms are not affected by the lower stresses. However, in case of Si, sharp edge is subjected to very high stresses. Highly concentrated stresses on the sharp tool edge enable removal of C atoms from the diamond tool which eventually get dissolved with the workpiece material on its surface. In other words, chipping at the tool edge takes place.

Since Si atoms on the surface are energized due to deformation, they readily form Carbides as shown in Fig. 5. The formation of SiC leads to hard particles on Si surface which subsequently may abrade the tool in subsequent machining passes in actual practice. Round edge does not show the physical removal of C atoms from diamond tool. Therefore, RDF is carried out to notice any phase transformation during nanoscale cutting of Si with round edge tool. At 0 ps, there is only one peak corresponding to the bond length of diamond, however, another peak arises at 1.42 Å after 200 ps of cutting time. It corresponds to the bond length in sp2 C structure. This shows the occurrence of graphitization in diamond tool.

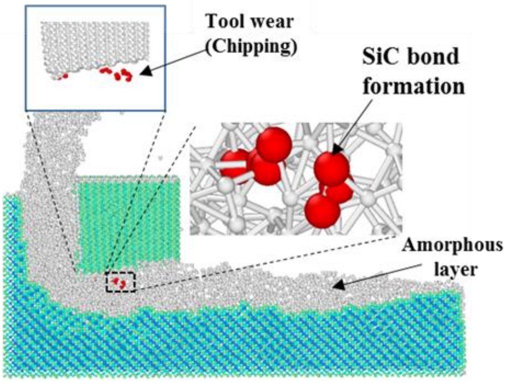

Fig. 5. Tool wear mechanism during nanoscale cutting of Si with Sharp edge tool.

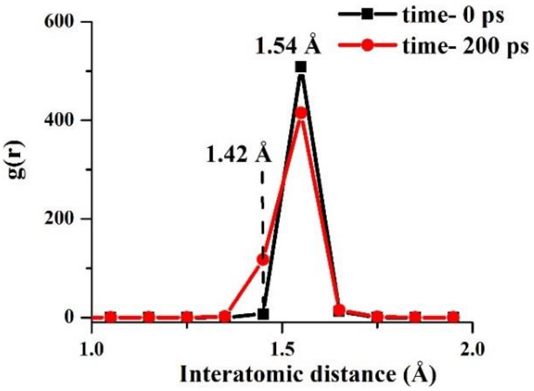

Fig. 6. Radial distribution function of diamond tool with round edge at initial and 200 ps time step.

4. CONCLUSIONS

1. Material removal mechanism depends on both the tool edge configuration and material properties. In Cu, it occurs by shear deformation while in case of Si, it takes place through structural transformation due to high pressure.
2. Tool edge affects the subsurface damage. The sharp edge cause damage ahead of tool edge while round cutting edge extends the damage under the tool in normal direction in bulk material.
3. The work material decides the nature of subsurface damage. Dislocations generation and evolution cause the subsurface deformation in Cu while amorphous layer manifests as a subsurface damage in case of Si.
4. Wear mechanism in Si is different for both tool edge configurations. Wear is insignificant in case of Cu while in Si, it is substantial. Tool wear occurs by chipping for sharp tool edge and graphitization for round edge. The wear out atoms are then diffused in Si and contaminates the surface by forming SiC.

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