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Characterization of Atomic Surface Roughness in Nanometric Machining Molecular Dynamics (MD) Simulations

Characterization of Atomic Surface Roughness in Nanometric Machining Molecular Dynamics (MD) Simulations

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Abstract: The concept of atomic surface roughness is very important in the assessment of high performance nano surfaces. The molecular dynamics (MD) simulations were carried out, by using a diamond tool on copper workpiece, for nanomachining. The atomic surface roughness was evaluated after multi-pass runs and these were characterized for various conditions of machined thickness and machining velocity. It was observed that there was no systematic relationship between the depth of cut and the surface roughness. On the other hand, there is an overall increase in the surface roughness, with increase in the machining velocity, but this was with some fluctuations. The frictional forces during the nanomachining are high for low depth of cut and these decrease as depth of cut increases. The characterization of roughness could provide understanding of surface based properties.

Keywords: Atomic Surface Roughness, Nano Surfaces, Molecular Dynamics, Frictional Forces, Nanometric Machining, Multi-pass simulations.

1. INTRODUCTION

The atomic surface finish or roughness can be defined as the roughness limit of a surface. Its value has been demonstrated both in theory and in experiments to be non-zero [1], [2]. This parameter is very important in assessing the quality of high performance nano surfaces, and so its understanding is very crucial. The evaluation of the roughness limit of a surface is of great importance for ultra-precision machining and silicon fabrication. It is also significant in assessing the quality of performance of such surfaces, as this will influence the service life of the devices in which they are employed. Namba et al. [2] obtained equations for the evaluation of 2-D and 3-D atomic surface roughness on atomic topography. They presented estimated values of Root Mean Square (RMS) atomic surface roughness for pure metal crystals. The theoretical value of the atomic roughness of copper was assessed to be 0.032 nm. Shusterman et al. [3] worked on epitaxial films of Al and Cu grown on a substrate. The RMS roughness values of the films were evaluated by using the AFM. A value below 0.3 nm was achieved for Al films. The surface roughness of grown films of aluminium on copper substrate using the MD simulation was investigated by Hong et al [4].

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They found out that the average RMS values for the deposited films, ranged from 0.324 to 0.13 nm. For copper deposited on silicon substrate, the calculated RMS was in the range 0.079 to 0.15 nm [5].

The surface roughness of nano devices will invariably affect their quality and performance. Closely related to the performance of nano surfaces are the tribological properties. Rha et al [6] noted that tribological properties in microsystems would demand low friction, adhesion and wear. Also, Romero et al. [7] investigated the phenomenon of friction at the tool-chip interface in nanometric machining. They highlighted the relationship between adhesion and friction at the nanoscale. Also, they observed that friction decreased with increase in depth of cut. On another note, Timoshevski et al. [8] showed from first-principles theoretical calculations, that atomic surface roughness drastically reduces the electrical conductance of thin films.

It is evident that atomic surface roughness estimations can be obtained from theory, simulations and experiments. Atomistic simulations are frequently used and experimental studies are widely carried out with AFM [9]. In this study, multi-pass nanometric atomistic simulations were employed and the results provided the platform from which the atomic surface roughness was evaluated.

Multipass MD simulations were carried out to create nano surfaces by the nanomachining of copper workpiece with a

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diamond tool. The workpiece consists of 43240 atoms with FCC copper lattice, and has a dimension of 8.6 × 8.2 × 7.1 nm in the x, y and z directions respectively. It includes 3 kinds of atoms, namely; boundary atoms (green), Newtonian atoms (white) and thermostat atoms (red), Figures 1 and 2. The boundary atoms are kept fixed to reduce edge effects. The Newtonian atoms obey the Newton's equation of motion and are free to move. The thermostat atoms conduct the heat generated during the cutting process out of the cutting region. This is achieved by the velocity scaling of the thermostat atoms, (with the conversion between the kinetic energy (KE) and temperature via Eq. 1 [10, 11]);

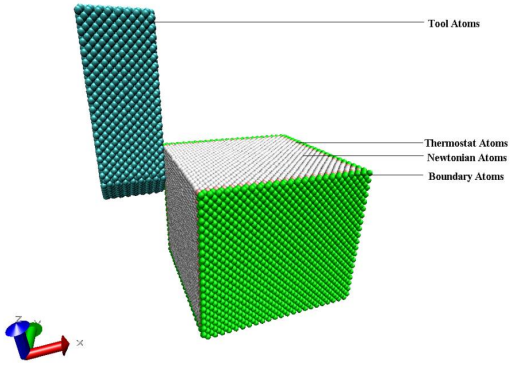


Figure 1: The Simulation Model

$$\sum_i \frac{1}{2} m_i v_i^2 = \frac{3}{2} N k_B T_i \qquad (1)$$

Where m_i is the mass of the ith atom, v_i is the resultant velocity of the ith atom, N is the number of the thermostat atoms, T_i is the temperature of the ith atom and k_B is the Boltzmann constant (1.3806504 x10^{-23} JK^{-1})

Whenever the temperature of the thermostat atoms exceeds the preset bulk temperature of 293K, their velocities are scaled by using Eq. 2 [12, 13];

$$v_{i,new} = v_i \sqrt{\frac{T_{desired}}{T_{current}}} \qquad (2)$$

Where $v_{i,new}$ is the newly scaled velocity of atom i, v_i is the velocity of atom i, $T_{current}$ is the current temperature that is calculated from the KE and the $T_{desired}$ is the desired temperature.

The tool consists of 10992 atoms with diamond lattice structure, and it is modelled as a deformable body.
The atomic interactions in the simulation are the following, namely;
Cu-Cu : interactions between copper atoms (workpiece)
Cu-C : interactions between copper atoms and diamond atoms (workpiece/tool interface)
C-C : interactions between the diamond atoms (tool)

The EAM potential was used for the Cu-Cu interactions [14][15][16] the LJ potential was used for the Cu-C interactions [15][16][17]. The C-C (tool atoms) interactions were modelled by using the Tersoff potential [15][16]. The other simulation parameters are as follows: the bulk temperature was 293 K, the cutting direction was [100] (x-direction), the cutting speed was 150 m/s, the feed was 1.5 nm, the rake angle was 0°, the clearance angle was less than 3° and the time step for the MD simulations was 0.3 femto second. The microcanonical (NVE) ensemble was applied in the simulation. The LAMMPS MD software [18] was used for the simulations and the VMD software [19] was used for the visualization of the results. A sharp pointed diamond tool with an edge radius of few atoms (0.6 nm) was used on the crystalline copper atoms workpiece. Figures 2 and 3 show the near perfect (atomically smooth) surface of the workpiece, and the surface atoms contributing to the surface roughness respectively. Figure 4(a) shows the machined grooves with consecutive passes (1 – 3) and Figure 4(b) shows the tool tip dimensions, with the upper part as variable, which depends on the depth of cut considered.
The MD simulations of the machined grooves, with the three passes are shown in Figure 5, for a depth of cut of 3 nm, which demonstrates the creation of a nano surface on the copper workpiece.

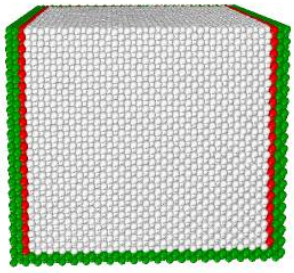


Figure 2: The Atomically Smooth Surface of the Workpiece [20][21]

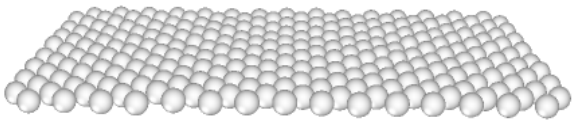


Figure 3: The Surface Atoms Contributing to the Surface Roughness [20][21]

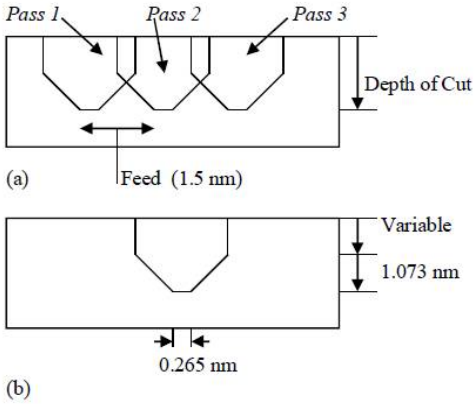
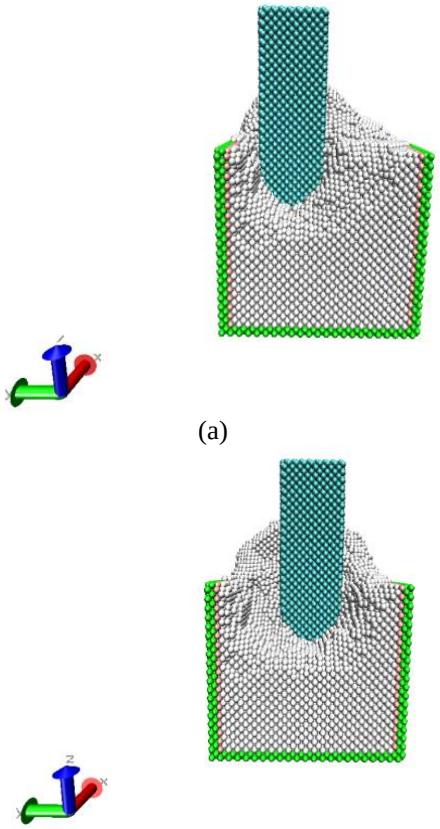
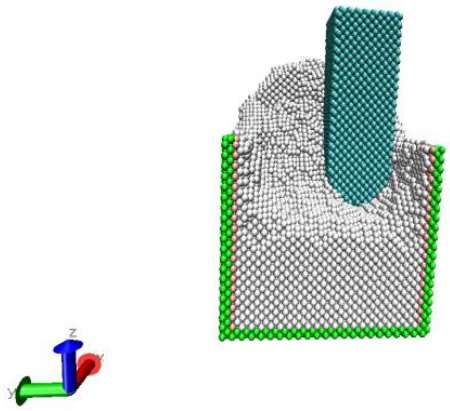


Figure 4: Cross Section of the Machined Grooves with Passes 1-3 (direction of cut is perpendicular to the paper face) [20][21]



(a)

(b)



(c)

Figure 5: MD Simulation of Multipass Nanometric Machining (a) pass 1 (b) pass 2 (c) pass 3 [21][22]

2.1. The algorithm for the evaluation of atomic surface roughness

The theory of the 3-D atomic surface roughness has been presented by [1],[2], and it is given by Eq. 3,

$$S_a = \frac{2}{\pi^2} r \tag{3}$$

where S_a is the arithmetic deviation of the surface, r is the radius of the surface atoms.
This shows that the surface roughness is proportional to the radius of the surface atoms theoretically.

The actual implementation of the surface roughness is based on Eq. 4.

$$S_a = \frac{1}{MN} \sum_{j=1}^{N} \sum_{i=1}^{M} z(x, y) \tag{4}$$

where M,N are the numbers of atoms in the x, y respectively and z is the height of the measured point in the co-ordinates x and y.

The following are steps [20] to take to evaluate the surface roughness from the simulation results;

- Read the input file of the simulated results
- Extract the surface atoms that contribute to the surface roughness evaluation
  To extract the surface atoms:
  - Carry out coordination analysis to determine the number of nearest neighbours of each atom
  - Then the area of interest on the surface, for the evaluation of the surface roughness is selected
- Obtain the (x,y,z) data of the surface atoms
- Transform the (x,y,z) data to a grid data

- The grid data is then fed into a suitable surface analysis software to obtain the surface roughness

The above algorithm was implemented by using the following techniques/software. The OVITO visualization software [23] was used to select and to extract the surface atoms. Then the (x,y,z) data of the surface atoms was transformed into a grid data by using the Matlab. The grid data was used as input to Surfstand, a 3D surface roughness standard software [24] for the evaluation of the surface roughness.

4. RESULTS AND DISCUSSIONS

The simulation results for the depth of cut range (0.5-3.0nm) are shown in Table 1. The variation of the surface roughness, Sa with the depth of cut is shown in Table 3 and Figure 6. The Sa increases initially up to 1.5nm depth of cut, that is, during ploughing, then it decreases with the initiation of cutting phenomenon [25], before showing another upturn. Otherwise, there seems to be no systematic relationship between depth of cut and the surface roughness. The tool geometry is constant and the variation of the depth of cut should not generally affect the surface roughness, except that the area of contact between the tool and the workpiece will increase with increase in the depth of cut. The increase in contact area may increase the tool-chip frictional force and the cutting zone temperature, which may in turn affect the surface roughness [26]. For the different depth of cut, different layers of atoms were removed. For the depth of cut of 0.5 nm, up to 3 layers of atoms were removed; for the depth of cut of 1.0nm, up to 5 layers of atoms were removed. Similarly, for 1.5nm, 2.0nm, 2.5nm and 3.0nm depths of cut, up to 8 layers of atoms, 10 layers of atoms, 13 layers of atoms and 16 layers of atoms were removed respectively. In all, only the surface atoms contributing to the surface roughness were taken into account.

The results for the cutting speed/velocity range (40-220m/s) are shown in Table 2. A depth of cut of 2.0nm was used for all the cutting velocity. The variation of the surface roughness, Sa with velocity is shown in Table 4 and Figure 7. The Sa increases and then decreases with increase in velocity, but it demonstrates an average/overall increase with increase in machining speed. This is similar to certain results in conventional machining [27], where surface roughness increases and decreases for certain velocity ranges. A previous article also showed that the surface roughness was high, at high cutting speeds (180 m/s), and the roughness was smoother for lower cutting speeds (1.8-18m/s) [28]. In conventional machining, the increase in cutting speed should reduce the surface roughness, but in nanoscale machining, size effects may affect this relationship.

The simulations show two peaks and three valleys for all the depth of cut and the cutting velocity range. These waviness displayed by the surface atoms contributing to the roughness, are due to the overlap caused by the consecutive passes, the tool geometry and the choice of the interatomic potentials used in the simulations.

The force ratio F_x (tangential force)/F_z (normal force), which is a measure of the friction between the tool and the interacting workpiece atoms for depth of cut (0.5-3.0nm) are shown in Table 5. For the depth of cut of 0.5nm, the normal force is low in comparison with the cutting force/tangential force. Actually, at this machined thickness, ploughing, and not actual cutting, occurs. This is visible for passes 1 and 2, but for pass 3, there is a slight variation, which is unclear. But, as soon as cutting initiates at around 1.5nm [25], the value of the normal force increases and subsequently, the force ratio stabilizes for higher depth of cut (Figure 8). Invariably, frictional forces are high for low depth of cut and decreases as the depth of cut increases, which could indicate that adhesion is more pronounced at this low depth of cut [7].

Other process parameters could influence the surface roughness, like the tool nose radius, flank angle, the tool geometry et cetera. From theory, increasing the tool nose radius should cause a decrease in surface roughness. A variation of this was observed in ultraprecision machining, where the arithmetic roughness decreases with increasing nose radius at a small radius, and it increases at large radius [29].

CONCLUSION

There is a noticeable variation of atomic surface roughness, Sa with machined thickness and machining velocity, in the evaluation of conducted molecular dynamics simulations. The estimated Sa from the study, is in the range of around 0.2- 0.35nm. The Sa increases initially up to 1.5nm depth of cut, then it decreases before showing another upturn. It seems there is no logical relationship between the depth of cut and the surface roughness. Furthermore, Sa increases and decreases for a certain range, as velocity increases. In conventional machining, the Sa should improve as the velocity increases. However, on the nanoscale, the parameters are very sensitive to small variations. This variation may either be due to size effects of the simulation model or some other factors. Also, the importance of adhesion is highlighted in the investigation of friction between the tool atoms and interacting workpiece atoms, as friction is shown to decrease with increase in the depth of cut. The importance of this study of atomic surface roughness and its clearer understanding can be useful in atomically flat silicon, where it has been showed to decrease transistor noise and subsequently enhance reliability and device performance [6].

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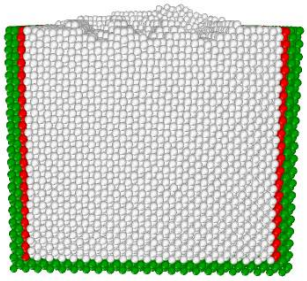
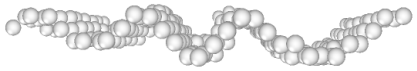
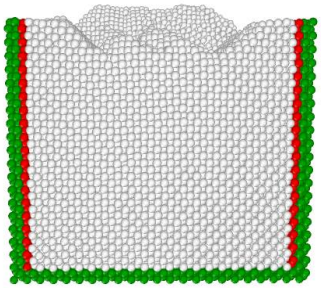
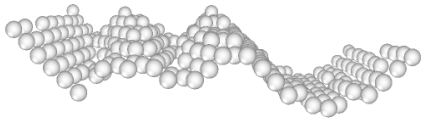
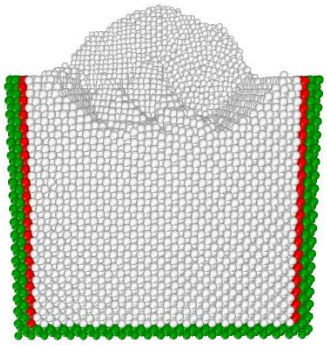
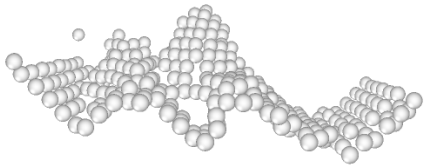
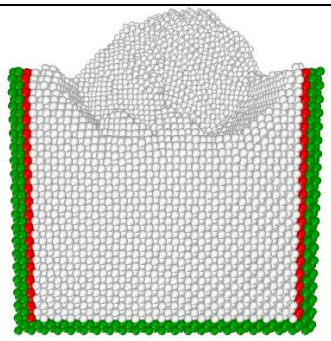
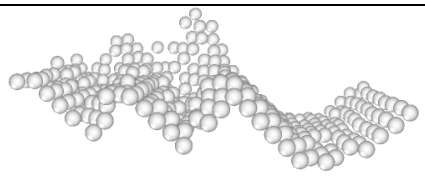
Table 1: Surface Roughness Results for the Depth of Cut (0.5-3.0nm)

Depth of Cut (nm)	Simulation Results	Surface Atoms Contributing to Sa	Layers of Atoms Removed	Sa (nm)
0.5			Up to 3	0.189
1.0			Up to 5	0.273
1.5			Up to 8	0.345
2.0			Up to 10	0.276

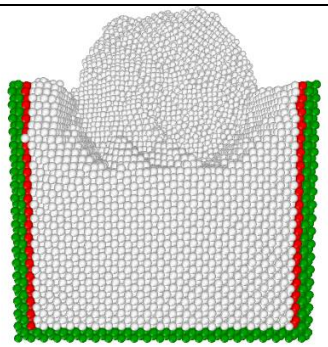
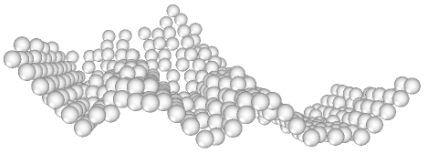
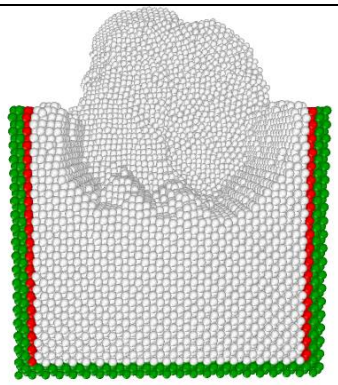
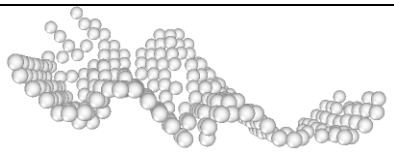
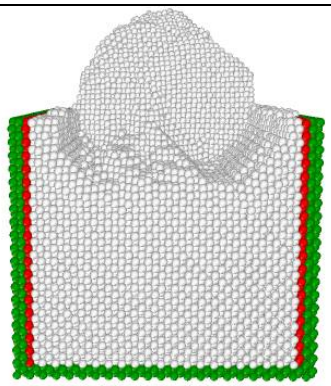
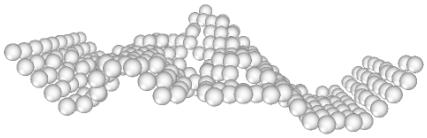
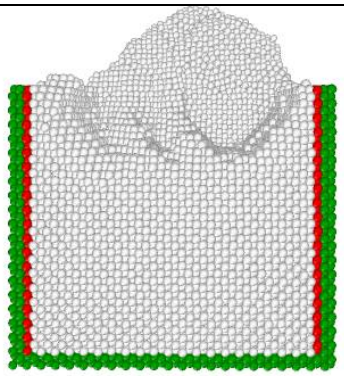
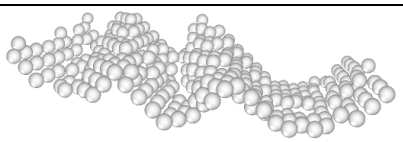
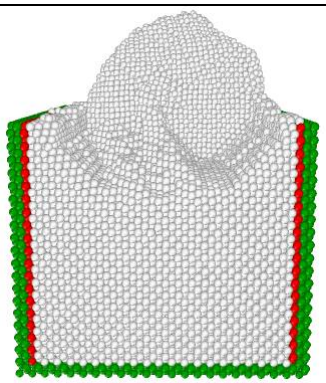
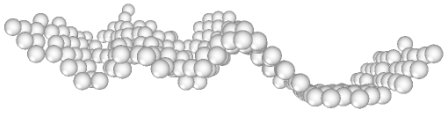
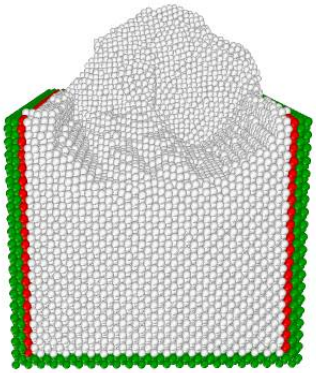
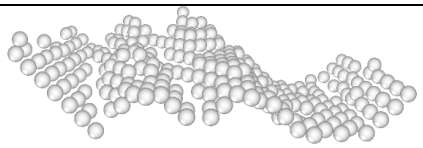
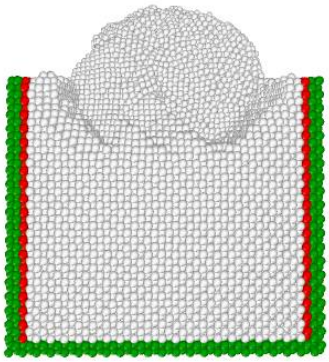
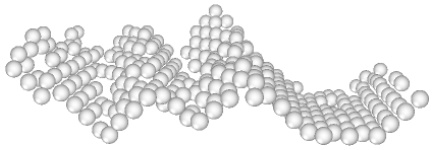
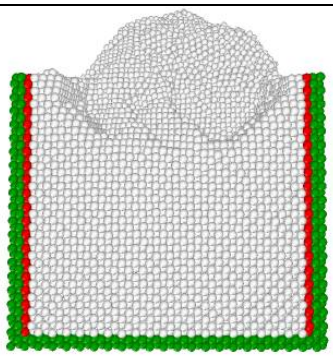
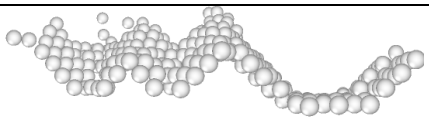
2.5			Up to 13	0.251
3.0			Up to 16	0.323

Table 2: Surface Roughness Results for the Velocity (40-220m/s) (Depth of Cut – 2.0nm)

Velocity (m/s)	**Simulation Results**	**Surface Atoms Contributing to Sa**	**Sa (nm)**
40			0.260
60			0.294

80			0.268
100			0.300
120			0.270
140			0.322

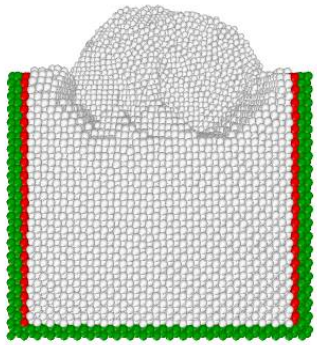
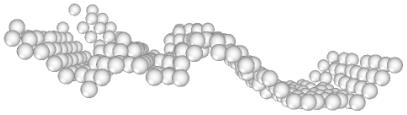
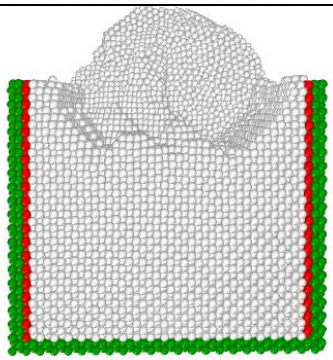
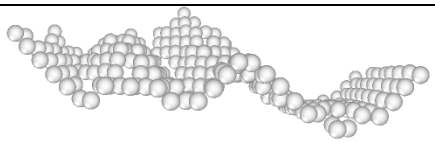
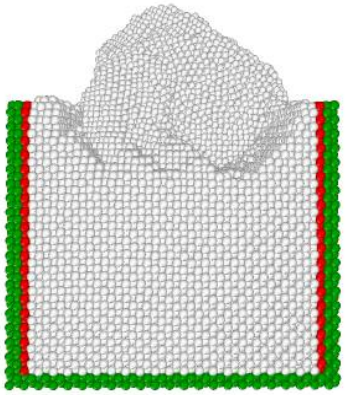
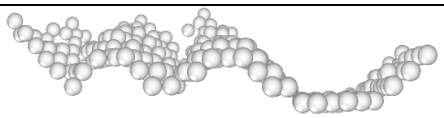
160			0.265
180			0.316
200			0.293

Table 3: Surface Roughness Results for the Depth of Cut – (0.5-3.0nm)

Depth of Cut (nm)	Sa (nm)
0.5	0.189
1.0	0.273
1.5	0.345
2.0	0.276
2.5	0.251
3.0	0.323

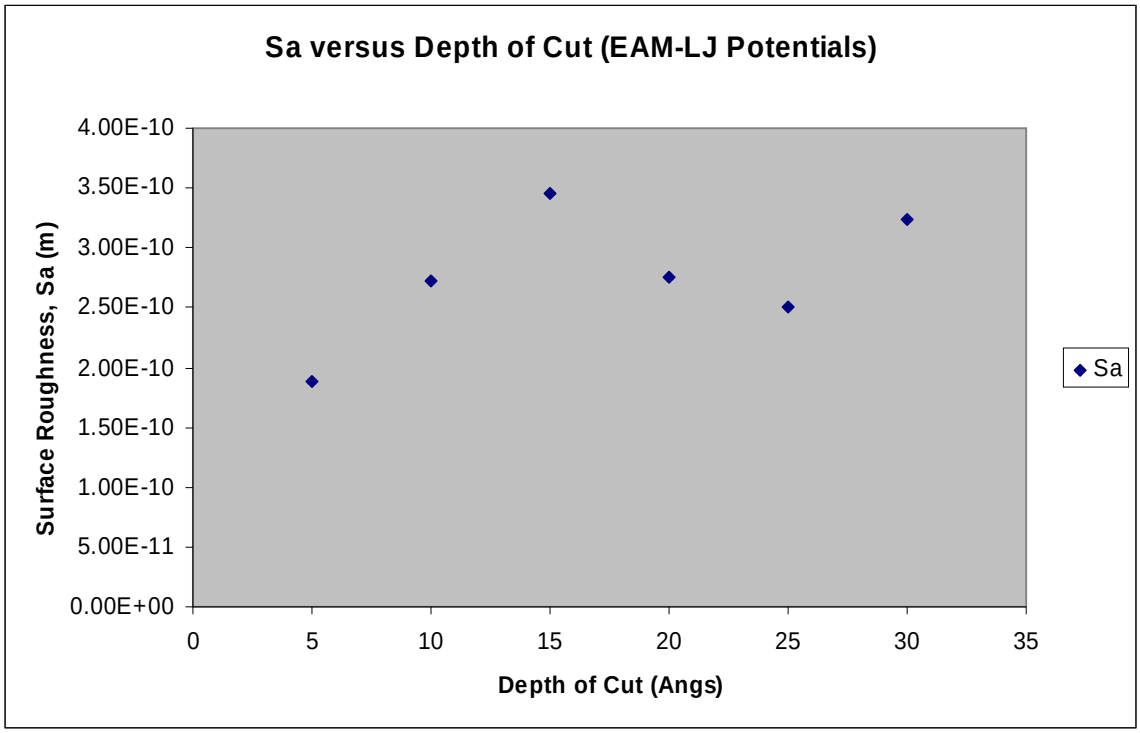


Figure 6: Variation of Sa with Depth of Cut

Table 4: Surface Roughness Results for the Velocity – (40-220m/s)

Velocity (m/s)	Sa (nm)
40	0.260
60	0.294
80	0.268
100	0.300
120	0.270
140	0.322
160	0.265
180	0.316
200	0.293
220	0.344

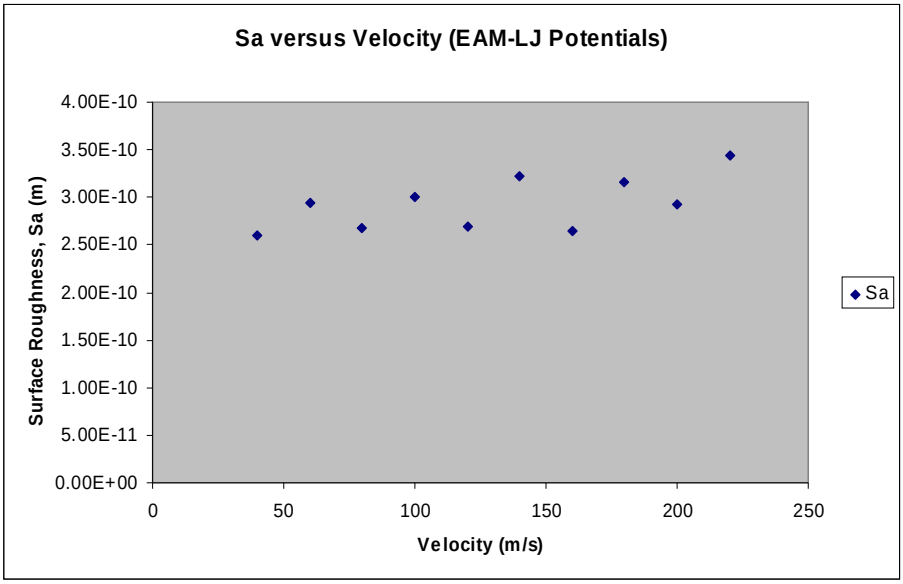


Figure 7: Variation of Sa with Velocity

Table 5: Variation of F_x/F_z Depth of Cut

Depth of Cut (nm)	F_x/F_z Pass 1	F_x/F_z Pass 2	F_x/F_z Pass 3
0.5	8.80451	7.327466	3.972255
1.0	2.499458	1.850369	4.287728
1.5	1.766585	1.318857	2.692763
2.0	1.624994	1.143788	1.938106
2.5	1.783232	1.331824	2.240153
3.0	1.822619	1.217562	2.377118

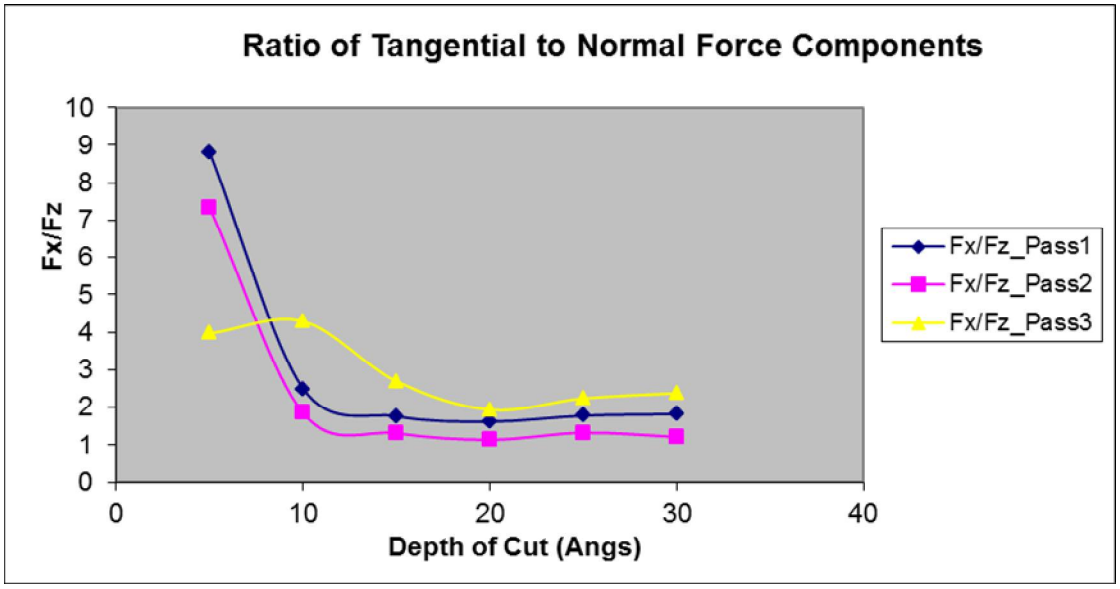


Figure 8: The Variation of F_x/F_z with Depth of Cut