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Molecular Dynamics Simulation of Mechanical Polishing

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Abstract

Mechanical polishing, a nano-finishing process is extensively used for generating smooth surfaces on engineering materials. The mechanism of mechanical polishing is extremely complex due to its random nature of material removal at atomic scale. The need for a better understanding of the process at atomic scale is therefore necessary. Finite element method is not suitable for simulation of material removal at atomic scale. Hence, molecular dynamics simulation (MDS) was carried out to understand the complex behavior of material removal. This simulation work has been implemented on a few engineering materials like aluminium and silicon.

For polishing of silicon, TERSOFF pair-potential is selected. In case of aluminium, EAM pair-potential is selected. During this simulation work, material removal of rough asperities is discussed by abrasion with abrasive particles. The results of MDS work are analyzed and presented at atomic scale as follows;

1) Nanometric abrasion through adhesion de-bonding principle is a key phenomenon to generate nanometric material removal during mechanical polishing process.

2) Recoverable Phase transformation occurs during nanometric abrasion (deft of indentation =1-10nm) on aluminium which is soft and ductile materials.

3) Debris formation during finishing of brittle crystalline structures in form of non-crystalline or amorphous structures. This phenomenon is observed on silicon which is hard and brittle material.

Keywords: MDS, mechanical polishing, nano-finishing, TERSOFF, EAM.

1. INTRODUCTION

In the present era of manufacturing and challenging requirements with increasing demands for functional enhancement, ultra-precision lapping or polishing has played a critical role in the development of polishing technology for the functional elements of the precision machines including aerospace, nuclear, bio-medical, optical, etc. These functional elements or components should be produced to a completely smooth mirror like surface finish to efficiently work as functional materials.

Precision manufacturing has improved its capabilities upto few nanometers or few angstroms (at atomic scale) which is also called as nanofabrication technology. The nanofabrication technology needs to modify engineering surfaces for ultra-smooth and defect-free surfaces. Such requirements to modify engineering surfaces at atomic scale has approached extreme limit of the manufacturing technology. In general, a mechanism called as mechanical polishing (MP), has been conventionally used for lapping, grinding, honing etc. This process has capability for realizing the surface finish and planarization to the scale of few angstroms and few nanometers, respectively. The MP with extremely low material removal by controlling the process parameters, in order of atomic clusters, can generate surface finish of the order of few angstroms [1].

Furthermore, some advanced nanofinishing process such as, magnetic abrasive finishing (MAF), magnetorheological finishing (MRF), abrasive flow finishing (AFF), etc. [2] have capability to generate surface finish at nanometric scale in which material removal phenomenon belongs to the MP process by controlling abrasion or finishing force. The mechanical polishing process is being widely used in industries with less understanding about its science as the MP process comprises complex behavior of micro/nano-tribology at atomic scale of material removal. During the MP of crystalline materials, anisotropy effect on material removal rate (MRR) depends on the crystalline orientation of the surface being polished. However, the mechanism of this undesirable behavior is not investigated. In this direction, few interesting mechanisms have been investigated for evolving possible phenomena which are associated with the MP.

Thus, the MP is not only the geometrical downsizing of surface roughness, but the process also brings some novel phenomena from different domains of science and technology.

Interaction among nano-abrasive particles and work-surface varies at the microscopic scale. Hence, the conventional machining theory cannot be applied to investigate and accurately understand the science behind the mystery of the surface generation in the MP process. The interactions at molecular level for micro/nano-tribology are difficult to study experimentally. Moreover, experimental results are often not useful to reveal science of the process due to the complexity of the process dynamics.

Molecular dynamics (MD) simulation [3] is a theoretical method which offers high temporal and spatial resolution. The MD simulation is almost an ideal approach to investigate and analyze about a process at atomic scale [4-9], and therefore it has become a significant tool in this case. In the present paper, a large scale classical MD simulation method is employed to investigate the MP process and analyze the atomistic behavior.

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2. MOLECULAR DYNAMICS SIMULATION

MD simulations (MDS) are carried out with usage of the large-scale atomic/molecular massively parallel simulator (LAMMPS) [10]. Furthermore, software package OVITO [11] is applied for visualization and analysis of the simulation results.

MDS was carried out to study the effect of various finishing parameters, as shown in Table1.

Table 1: Parameters for the MD simulation to investigate various attributes of the MP.

S.N.	Parameters	Value/description
1	Workpiece materials	Aluminium (Al) and Silicon (Si)
2	Abrasive particles	Iron (Fe) for 'Al-workpiece' and Silicon (Si) for 'Si-workpiece'.
3	Inter-atomic Potentials	Embedded atom model (EAM) for Al-Al, Al-Fe & Fe-Fe [12]. TERSOFF for Si-Si [13].
4	Boundaries	Shrink along indentation direction, and periodic boundary condition along other directions.
5	Group of atoms	Fixed layers of atoms (bottom and top) are set to rigid. Remaining atoms are allowed to move as per Newtonian atoms.
6	Statistical Ensembles	Constant number of atoms, energy, constant and volume ensemble (NVE) is also known as the microcanonical ensemble.
7	Time step	1fs.

The MD simulation model consists of workpiece with asperity and abrasive particle with rigid platform as shown in Fig.1.

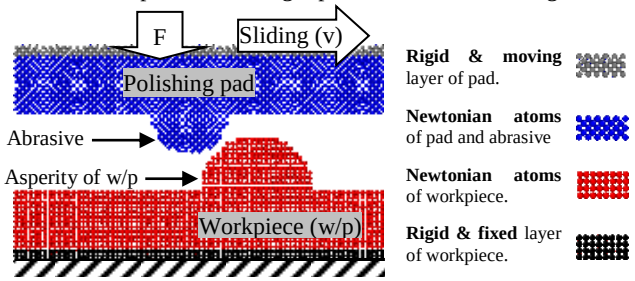


Fig.1. MD model in which types of atoms are labeled on right-side. Here, 'F' represents holding force, and polishing or sliding velocity is indicated by 'v'.

3. ANALYSIS PROCEDURE

The simulated results are analyzed using OVITO software to extract information, and their procedure is discussed as follows.

3.1 Common neighbor analysis

Structure analysis of any material is a critical parameter to characterize lattice structure towards segregation of numerous structures or phases within a given engineering material. Common neighbor analysis (CNA) is an efficient algorithm technique, which has capability to analyze the local structural changes in the simulated results.

Two atoms can be stated as bonded form in a known structure (like FCC, BCC, HCP, DC, etc.) provided their separation (or interatomic distance) has been maintained within a specified cutoff distance (r_c). CNA is also being used to filter the atoms in crystalline systems according to its relevance with phases and defects.

4. RESULTS AND DISCUSSIONS

The MD simulation is carried out for following two materials. Aluminium w/p material is used to investigate mechanism of MP in soft or ductile material. And Si-w/p is selected to study behavior of MP in brittle and hard materials.

1) MP on aluminium by using iron nano-particles.
2) MP on silicon with silicon nano-particles.

After this simulation, the output data are investigated for different analyses such as lattice structure, material removal and temperature variation during MP.

4.1. MP of aluminium with iron particle

4.1.1. Lattice structure

Lattice structure of the MD simulated results are analyzed by CNA technique and presented in Fig. 2(a-f).

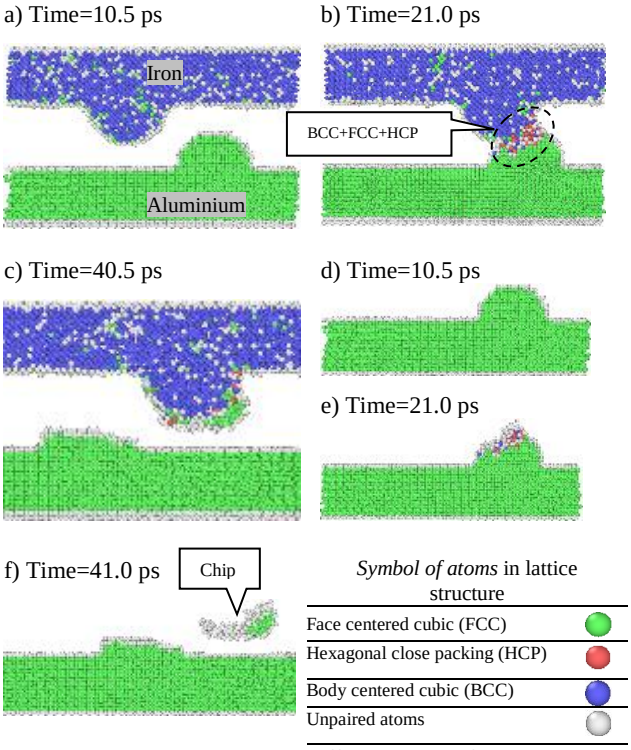
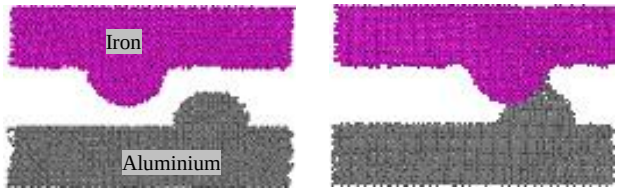


Fig.2. Structural variation with different levels of polishing time. (a-c) Structures in polishing region including abrasive and workpiece (w/p). (d-f) Structure of Al-workpiece only, during the MP.

Fig.2a shows lattice structure of workpiece and abrasive before polishing process. During the mechanical polishing, material gets deformed, and it alters the parent lattice structure as shown in Fig.2b. This figure indicates that the workpiece and abrasive particle makes perfect metallic bonds as interface of them are mixture of FCC, BCC and HCP lattices (indicated in Fig.2b). In this process, atoms of the workpiece change their lattice structures from FCC to a mixture of FCC, BCC and HCP as shown in Fig.2 (b & e). Moreover, removed chip from the workpiece during the polishing process recovers its own lattice structure as shown in Fig.2f. This structure recovery also happens with the workpiece material.

4.1.2. Material removal

a) Time=10.5 ps b) Time=21.0 ps



c) Time=40.5ps d) Percentage of Material removed.

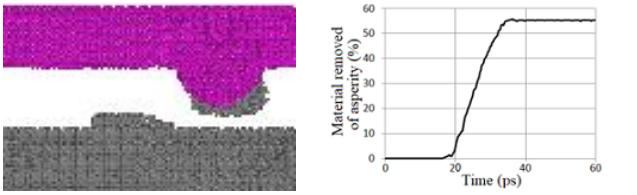


Fig.3. (a-c) Material removal from aluminium at different polishing times. (d) Plot of 'total amount of removed material from asperity of the w/p' with respect to the polishing time in single stroke of polishing.

Fig.3 (a-c) shows the material removal during polishing of aluminium workpiece. It is observed that the abrasive particle deformation during MP is insignificant. However, the workpiece material is getting deformed and sheared off as shown in Fig.3 (b-c). Fig.3c shows that the chip removed from the workpiece is adhered on the abrasive particle, and this is how the asperity height reduces towards generation of smooth surface during the mechanical polishing process. Percentage of material removal is computed by counting number of atoms within defined region of workpiece by using count command. Fig.3d shows percentage of material removal in single stroke of polishing, in which 55% of the asperity's atoms have been removed. Hence, during mechanical polishing of ductile material like aluminium has tendency for higher material removal. The material removal depends of overlapping length of asperity and abrasive, hence the material removal before and after abrasion becomes zero and constant.

4.1.3. Temperature of polishing zone

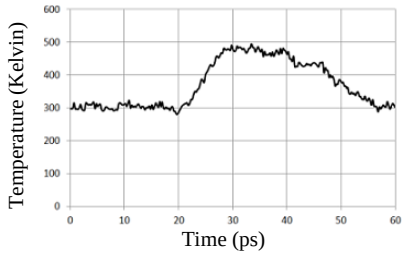


Fig.4. Variation in average temperature of the asperity of the workpiece with varying polishing time.

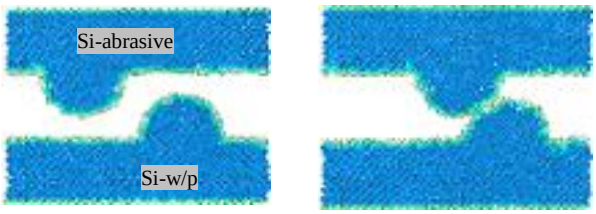
Average temperature near the polishing zone has been computed and plotted as shown in Fig.4. Average temperature of the polishing zone goes upto 500 K which is less than melting temperature of aluminium. At this temperature, FCC is only stable lattice structure for aluminum workpiece. Hence, phase recovery occurs after MP as discussed in section4.1.1.

4.2. MP of silicon with silicon particle

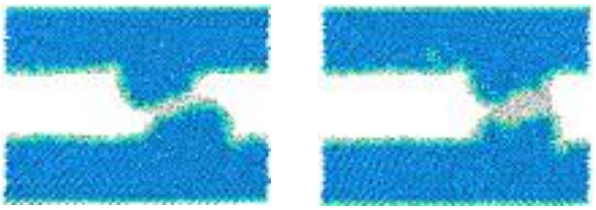
4.2.1. Lattice structure

Fig.5 (a-e) shows lattice structure of silicon during the mechanical polishing process. When abrasive particle approaches in case of crystalline structure of silicon (diamond cubic) workpiece, the interface between them gets phase alteration in the form of non-crystalline or amorphous phase as shown in Fig.5(c-d). During this process, it is also observed that the abrasive and workpiece are getting deformed near the interface as shown in Fig5(c-d). Fig.5e shows the debris or chip formation in the form of amorphous phase (non-crystalline structured lattice). Moreover, the polished surface also shows amorphous phase of the order of few atomic layers as shown in Fig.5e. This amorphous phase remains permanently, which does not vanish after polishing.

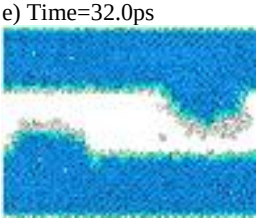
a) Time=2.5 ps b) Time=8.5ps



c) Time=12.0ps d) Time=15.5ps



e) Time=32.0ps



Symbol of atoms in lattice structure

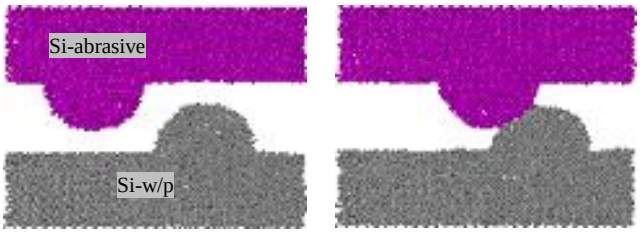
Diamond Cubic (DC)	
DC (1st neighbor)	
DC (2nd neighbor)	
Amorphous phase	

Fig.5. Structural variation with different levels of polishing time. (a-e) Structures in polishing region which include abrasive as well as w/p during the mechanical polishing of silicon.

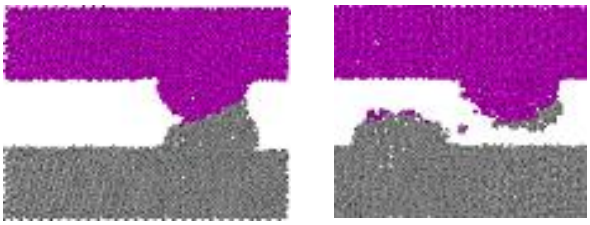
4.2.2. Material removal

Fig.6 (a-d) shows atomic configuration during mechanical polishing of silicon. It is observed that the material of the debris or chip is a combination of workpiece as well as abrasive particles. The chip removed from this process is also getting attached or adhered with the abrasive particle as shown in Fig.6d.

a) Time=2.5 ps b) Time=8.5 ps



c) Time=15.5 ps d) Time=32.0 ps



e)

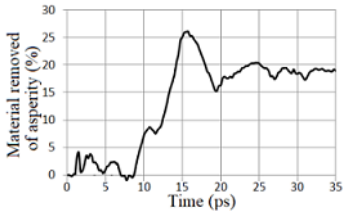


Fig.6. (a-d) Material removal at different level of polishing time. (e) Plot of 'total amount of removed material from asperity of the w/p' with the polishing time during single stroke of polishing in silicon.

The final finished surface after one stroke of polishing seems as smother surface. Moreover, the material removal from the workpiece is quantified and plotted in Fig.6e, in which the percentage of removed material from the workpiece asperity is 20%. Hence, it can be stated that the material removal is less during polishing of hard material like silicon with respect to a ductile material. The material removal behavior on aluminium and silicon can be conceived by compare of Fig.3d and Fig.6e. It reveals that the MRR on 'Al' is 2.75 times higher with respect to 'Si'. Material removal on 'Al' material is smooth as the plot shows smooth lines. However, silicon shows large fluctuation on material removal as polishing time progresses, which might be happening because of material's hardness.

4.2.3. Temperature of polishing zone

Average temperature near the polishing zone has been computed and plotted as shown in Fig.7. Average temperature of the polishing zone goes upto 1100 K which is enough to soften the workpiece material for deformation followed by material removal. In general, mono-crystalline silicon gets soften drastically when temperature increases beyond 800 K, and this is why the workpiece and abrasive particle deform during the mechanical polishing as shown in Fig.6c.

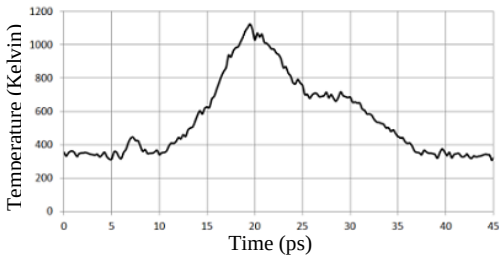


Fig.7. Variation in average temperature of the asperity of the workpiece with varying polishing time.

5. CONCLUSIONS

In this paper, MD simulation has been carried to investigate about mechanical polishing process at atomic scale. For this investigation, two types of workpiece materials are taken. Present study concludes following important outcomes;

- During mechanical polishing of aluminium, metallic bond gets formed with abrasive particle followed by material removal. The removed material gets permanently adhered with the abrasive particle.

- Lattice structure of Al-workpiece material alters during the polishing process. After polishing, the altered phase gets recovered. Lattice structure during polishing of silicon shows formation of amorphous phase during the polishing. And this amorphous phase does not recover back.

- Material removal in aluminium is 2.75 times higher as compared with silicon.

- Temperature of the polishing interface gains beyond softening temperature, and it goes upto half of materials' melting point.

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