Mechanism of material removal on stainless steel through diamond abrasion: a molecular dynamics simulation study

Prabhat Ranjan[1,2], Anuj Sharma[3], Tribeni Roy[4,5,*]

[1]*Bhabha Atomic Research Centre, Mumbai, India*
[2]*Homi Bhabha National Institute, Mumbai, India*
[3]*Cardiff University, Cardiff, UK*
[4]*BITS Pilani, Pilani India*
[5]*London South Bank University, London, UK*

Presented in International Conference on Precision, Micro, Meso and Nano Engineering (COPEN - 12: 2022)
December 8 - 10, 2022 IIT Kanpur, India

ABSTRACT

A rough surface of any engineering material exhibits high surface energy which results in higher potential energy or cohesive energy of the material, and it affects both optical as well as chemical properties. In this paper, stainless steel 304 (or SS304) is selected for nano-finishing through diamond abrasive using MD simulations. It is found that the diamond abrasive creates new bonds with Cr and Fe atoms by rise in local temperature and stresses. Moreover, Ni atom diffuses inside the abrasive as it does not chemically bond with C atom. The abrasion on steel due to diamond also leads to phase transformation on both abrasive as well as the workpiece. Subsequently, the transformed phase is removed from the workpiece due to the newly formed chemical bonds, however, in the process, the abrasive particle deteriorates by phase transformation and materials loading. Thus, the present study is useful in optimising nano-finishing or nano-cutting process on stainless steel.

KEYWORDS

Nano-Finishing,
Polishing,
Molecular Dynamics Simulation,
Stainless Steel,
Corrosion Resistance.

1. Introduction

Stainless steel is widely used materials for various industrial applications due to their excellent properties such as high thermal conductivity, bio-compatibility, high melting point, high ductility etc. (Zaretsky, 2012). Comparing among all grades of stainless steel, SS304 with low carbon content is one of the most commonly used materials due to its weldability, machinability, etc. (Fatima, 2015). Whereas, there are some application areas in which optically polished surface is required such as pressure gauges, optical sensors, surgical tools, biomedical implants, etc. (Shih et al., 2004; (Sansone, 2013). To cater the nano-finishing requirement, mechanical polishing through traditional lapping is used as polishing. This also helps to reduce the risk of corrosion by reducing the amount of crevices on a metal surface that could promote corrosion. Moreover, nanofinishing can also rearrange atoms on the surface in natural way by using thermal or chemical processes that enhances corrosion resistance drastically.

*Corresponding author E-mail: tribeni.roy@pilani.bits-pilani.ac.in

https://doi.org/10.58368/MTT.22.3.2023.37-42

Nanofinishing is a final operation in manufacturing which reduces surface roughness value as low as a few nanometres or even less depending upon the type of nanofinishing process. In case of traditional lapping process, the finished surface finish obtained with various types of surface defects limit the corrosion resistivity beyond certain extent.

Advanced finishing process such as chemo-mechanical polishing (CMP) has been used to finish steel with surface finish up to 0.7 nm on SS304 using silica abrasive (Hu et al., 2012; Ranjan et al., 2018). In addition, chemo-mechanical magnetorheological finishing (CMMRF) process was also used to generate surface finish better than 0.2 nm on SS304 (Ranjan et al., 2018) with silica abrasive and it was also found that silica abrasives chemically assisted the material removal, thereby avoiding surface and sub-surface damages. Moreover, it is also found that the diamond is very good abrasive for its hardness to polish steel. However, there is a dearth of literature to implement diamond for polishing of steel. To investigate and establish the mechanism of material removal on steel using diamond abrasive, molecular dynamics simulation is carried out and the same is discussed in this paper.

Table 1
Parameters of molecular dynamics simulation.

S.N.	Parameters	Value
1	Workpiece material	SS304L (Fe:70% Ni:10% Cr:20%)
2	Fixed base of workpiece	17.5 nm x 7.0 nm x 0.7 nm
3	Thermostat region of workpiece	A block of 17.5 nm x 7.0 nm x 4.9 nm
4	Newtonian region of workpiece	A block of 17.5 nm x 7.0 nm x 0.7 nm with a conical asperity of height = 3.5 nm, and base diameter = ϕ7.0 nm
5	Type of initial surface	Conical (sharp). It is incorporated to represent a rough surface
6	Lattice structure of workpiece	Face centre cubic (FCC) with Lattice constant =0.35 nm
7	Number of atoms on workpiece	78,030
8	Abrasive particles	Mono-crystalline Diamond (C)
9	Number of atoms on abrasive	11,522
10	Lattice structure of abrasive	Diamond cubic (DC) with lattice constant =0.357nm
11	Finishing medium	Water. It regulates temperature of workpiece and abrasive at 300K
12	Depth of cut by abrasive (*h*)	From 2.0 nm.
13	Time step	1 fs
14	Simulation time	47 ps
15	Viscous damping on abrasive	1.8×10^{-8} gm/s
16	Boundary	X: periodic, Y: periodic, Z: shrink

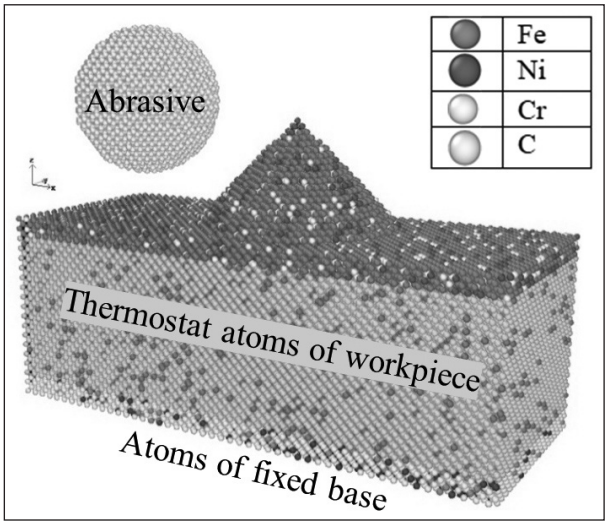

Fig. 1. MDS model for nanofinishing. Atom symbols are shown for Newtonian atoms and abrasive atoms.

2. Methodology

In this section, details of molecular dynamics simulation (MDS) are presented and discussed. Parameters of the simulation is shown in Table 1.

The MDS model consists of workpiece with a conical asperity, abrasive particle, and water medium, as shown in Fig.1. The conical asperity is modelled to study the abrasion process on a rough surface. The conical asperity has sharp geometry at apex which would help to correlate this MDS phenomena on highly rough surface to investigate material removal and surface modification.

Motion and position of the Newtonian atoms of Fig.1 are governed by Newton's second law of motion and fixed base atoms are frozen i.e. zero velocity. It was calculated by the direct integration of the classical Hamiltonian equations of motion using the Velocity-Verlet algorithm. Nanofinishing process was simulated using constant micro-canonical ensemble (NVE) under a constant number of atoms (N), the system's volume (V) and the total energy in the system (E).

To create inter-atomic forces, a hybrid pair potential was applied. This hybrid pair potential includes five types of pair potentials as shown in Table 2. Embedded atom method (EAM) type of pair potential was used to simulate stainless steel. For diamond abrasive particles, Tersoff potential was selected. Morse potential was used for the atoms of abrasive and workpiece. In the present work, LAMMPS software (Stadler et al., 1997) was used to perform a series of simulations

Table 2
Details of the pair potential to model and simulate materials in MDS.

S.N.	Atom-pair	Type of pair potential
1	Fe-Ni-Cr	EAM (G. Bonny, 2011)
2	C-C	Tersoff (Tersoff, 1989)
3	C-Fe and C-Cr	Morse (Xie, 2006)
4	C-Ni	Morse (A. V. Verkhovtsev, 2014)

as per the Table 1. To visualize the result of the simulation, OVITO software (Stukowski, 2009) was used, and further analysis was performed using post processing on the output data of the simulation. Towards better accuracy of the result with satisfactory computational efficiency, the computational time step was set to 1 fs. The abrasive particle was allowed to move under influence of an external force and viscous damping along x-axis. Size of the abrasive particle was selected as φ5 nm, and the size of asperity of workpiece was set to 3.5 nm as in nanofinishing, material removal is of the order of a few nanometre or less.

3. MDS and Analysis Techniques

3.1. Common neighbor analysis

Structure analysis is an essential aspect to characterize arrangement of atoms for discriminating between several structures like FCC, BCC, HCP, DC, etc. through adaptive common neighbor analysis method (Stukowski, 2009).

3.2. Forces between abrasive and workpiece

Since Morse pair-potential is used between abrasive and workpiece, the interaction force between them has been computed by taking negative derivative of the Morse potential function within the cut-off range.

3.3. Atomistic stress

Interaction between atoms of abrasive and workpiece leads to stresses for deforming material. In general, virial stress (Subramaniyan & Sun, 2008) is used to compute stress on individual atoms. From the analysis point of view, von-Mises stress has been computed which tells about equivalent stress on a specific atom instead of having a set of stress matrix.

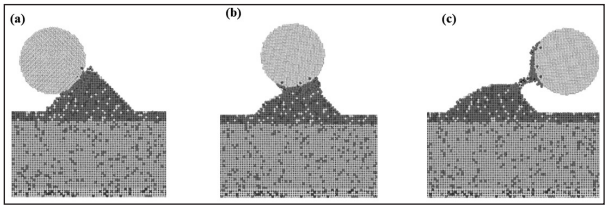

Fig. 2. Atomic configurations during nanofinishing at the time of (a) 8 ps, (b) 15 ps and (c) 29 ps.

3.4. Temperature

In general, material removal zone in mechanical abrasion polishing is relatively low and it is experimentally difficult to measure the temperature. Hence, molecular dynamics simulation is used to calculate kinetic energy of the work-piece atoms for mapping the temperature at every time-step.

4. Results & Discussion

After carrying out all simulations, suitable processing method was also implemented to analyse and investigate the process or behaviour of components. Afterwards, all results are discussed in the following sections.

4.1. Material movement

The atomic configuration of abrasive and workpiece during abrasion is shown in Fig. 2 at different times. Fig. 2(a) shows initial contact at 8 ps. At 15 ps, abrasive reached the centre of the conical peak as shown in Fig. 2(b). After 29 ps, material from work piece is getting removed by attachment with the abrasive as shown in Fig. 2(c). It also indicates that Fe and Cr atoms are getting spread on the surface of abrasive. Additionally, Ni atoms are diffusing inside the abrasive particle since it is highly inert metal as far as chemical reactivity is concerned. Thus, simulation results reveal that diamond performs chemical assisted abrasion on steel, however, it is not possible with Ni-based materials.

4.2. Stress

Von-Mises stress is computed at different times of nanofinishing and the same is presented in Figs. 3&4. Fig. 3 shows the stress distribution during initial contact of abrasion. Magnitude of stress becomes higher than 70 GPa which is more than enough to transform the lattice structure of abrasive and workpiece as the material's lattice gets changed at the stress level more than their

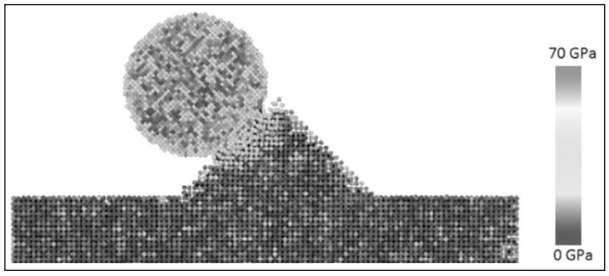

Fig. 3. Von-Mises stress during nanofinishing at the time of 8 ps.

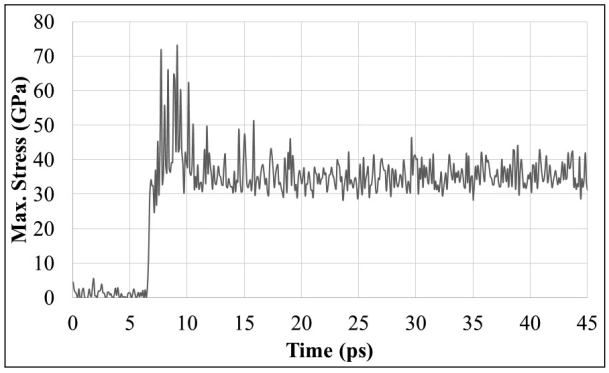

Fig. 4. Maximum value of the von-Mises stress during nanofinishing at different time.

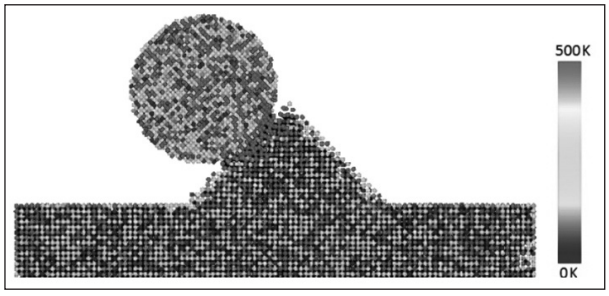

Fig. 5. Temperature distribution at the time of 8 ps.

theoretical tensile strength (E/2π). In addition, it is observed that initial stress level during the contact of abrasive and workpiece shows higher stress which may occur due to impact loading. Thereafter, the peak or maximum stress becomes constant at 30-40 GPa which is the theoretical tensile strength of steel as shown in Fig. 4. This happens due to the neck formation between abrasive and the workpiece as shown in Fig. 2(c). This neck formation is responsible for inducing tensile stress on the steel workpiece.

4.3. Temperature

In the similar way, temperature during nano-finishing was computed as presented in Figs. 5&6. Fig. 5 shows the temperature distribution at the time of 8 ps where the maximum temperature is getting localised near the contact zone. This

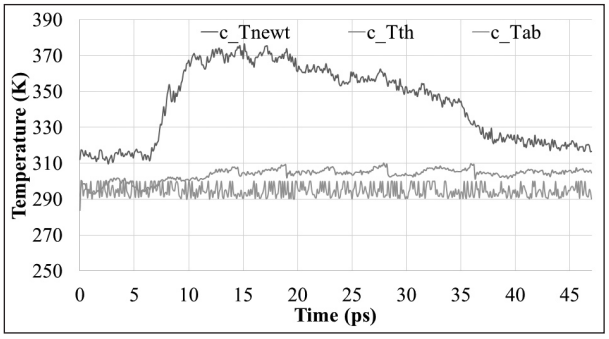

Fig. 6. Average temperature variation on Newtonian atoms (c_Tnewt), thermostat atoms (c_Tth) and abrasive atoms (c_Tab) at different time.

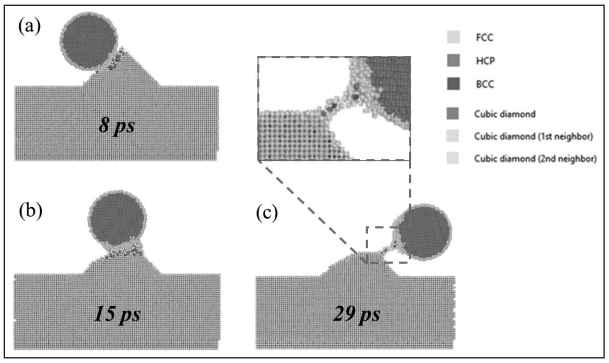

Fig. 7. Lattices transformation of workpiece and abrasive atoms at different time.

might occur due to the plastic deformation and the lattice transformation.

Fig. 6 shows the average temperature variation with time. In case of workpiece, Newtonian atoms show rise in temperature due to the abrasive action. In addition, the thermostat atoms also show a very minimal rise in temperature that happens due to heat transfer within the workpiece. After the completion of abrasion, the system including abrasive and workpiece tries to converge at 300K which indicates that the thermodynamics of MDS is correctly modelled.

4.4. Phase transformation

Based on common neighbor analysis, lattice of workpiece and abrasive were computed and presented in Fig. 7 at different times of abrasion. Grey coloured atoms represent amorphous and non-lattice structures. Fig. 7(a) shows that initial contact lead to major amount of lattice transformation on the workpiece in HCP, BCC and amorphous. As time progresses, abrasive atoms also get affected as the circular shape of cubic diamond phase changes from Fig. 7(a-c). While removal of material from workpiece, all transformed phases are taken away by abrasive

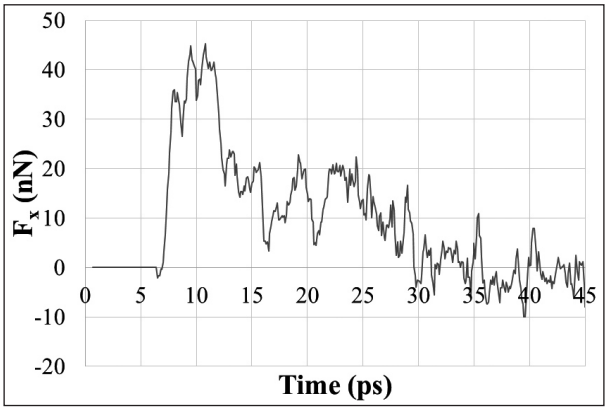

Fig. 8. Force along abrasion on the workpiece at different time.

as shown in the inset of Fig. 7(c). But the deformed lattice on the abrasive remains in it with atoms adhered from workpiece. Fig. 2(c) and Fig. 7(c) show that the processed workpiece gets smoothened on the sharp conical asperity without any altered lattices which indicates that nanofinishing with diamond leads to smooth surface without any sub-surface damages. However, the abrasive gets affected by its phase transformation and materials loading that needs attention to improve the nanofinishing process.

4.5. Force

Finally, forces along abrasion (x-axis) were computed and is presented in Fig. 8. It shows that the initial force at the contact (at 10 ps) is higher due to impact loading and thereafter it reduces due to the neck-formation. The neck applies a contact stress as shown in Fig. 5, but its cross-section reduces with time which results in reduction of the forces.

5. Conclusions

In this paper, simulations at molecular scale were carried out to investigate the effect of diamond abrasion on stainless steel. The conclusions are summarised as follows.

- Diamond forms chemical bond with Fe and Cr atoms which helps for chemical assisted nanofinishing on steel. It is not applicable for Nickel based materials.
- Material removal takes place by diamond abrasive through formation of new chemical bonds, and it results in nanometric smooth surface without any sub-surface damage.
- The abrasive gets damaged due to phase transformation of cubic diamond and loading of workpiece atoms on the abrasive.

References

Bonny, G., Terentyev, D., Pasianot, R. C., Poncé, S., & Bakaev, A. (2011). Interatomic potential to study plasticity in stainless steels: the FeNiCr model alloy. *Modelling and Simulation in Materials Science and Engineering, 19*(8), 085008. https://doi.org/10.1088/0965-0393/19/8/085008

Fatima, S., Khan, M., Jaffery, S. H. I., Ali, L., Mujahid, M., & Butt, S. I. (2015). Optimization of process parameters for plasma arc welding of austenitic stainless steel (304 L) with low carbon steel (A-36). Proceedings of the Institution of Mechanical Engineers, Part L: *Journal of Materials: Design and Applications, 230*(2), 640-653. https://doi.org/10.1177/1464420715584392

Hu, X., Song, Z., Liu, W., Qin, F., Zhang, Z., & Wang, H. (2012). Chemical mechanical polishing of stainless steel foil as flexible substrate. *Applied Surface Science, 258*(15), 5798-5802. https://doi.org/10.1016/j.apsusc.2012.02.100

Ranjan, P., Balasubramaniam, R., & Jain, V. K. (2018). Investigations into the mechanism of material removal and surface modification at atomic scale on stainless steel using molecular dynamics simulation. *Philosophical Magazine, 98*(16), 1437-1469. https://doi.org/10.1080/14786435.2018.1439191

Sansone, V. (2013). The effects on bone cells of metal ions released from orthopaedic implants. A review. *Clinical Cases In Mineral And Bone Metabolism*. https://doi.org/10.11138/ccmbm/2013.10.1.034

Shih, C.-C., Shih, C.-M., Su, Y.-Y., Su, L. H. J., Chang, M.-S., & Lin, S.-J. (2004). Effect of surface oxide properties on corrosion resistance of 316L stainless steel for biomedical applications. *Corrosion Science, 46*(2), 427-441. https://doi.org/10.1016/s0010-938x(03)00148-3

Stadler, J., Mikulla, R., & Trebin, H. (1997). IMD: A Software package for molecular dynamics studies on parallel computers. *International Journal of Modern Physics C, 8*, 1131-1140

Stukowski, A. (2009). Visualization and analysis of atomistic simulation data with OVITO–the Open Visualization Tool. *Modelling and Simulation in Materials Science and Engineering, 18*(1), 015012. https://doi.org/10.1088/0965-0393/18/1/015012

Subramaniyan, A. K., & Sun, C. T. (2008). Continuum interpretation of virial stress in molecular

simulations. *International Journal of Solids and Structures, 45*(14-15), 4340-4346. https://doi.org/10.1016/j.ijsolstr.2008.03.016

Tersoff, J. (1989). Modeling solid-state chemistry: Interatomic potentials for multicomponent systems. *Physical Review B, 39*(8), 5566-5568. https://doi.org/10.1103/physrevb.39.5566

Verkhovtsev, A. V., Schramm, S., & Solov'yov, A. V. (2014). Molecular dynamics study of the stability of a carbon nanotube atop a catalytic nanoparticle. *The European Physical Journal D, 68*(9). https://doi.org/10.1140/epjd/e2014-50371-4

Xie, J. (2006). Atomistic Simulations and Experimental Studies of Transition Metal Systems Involving Carbon and Nitrogen. Stockholm: Royal Institute of Technology.

Zaretsky, E. V. (2012). Rolling bearing steels – a technical and historical perspective. *Materials Science and Technology, 28*(1), 58-69. https://doi.org/10.1179/1743284711y.0000000043

Dr. Prabhat Ranjan has completed his bachelor's in science in mechanical engineering from NIT Patna in 2007. Subsequently, he obtained his M.Tech from IIT Kanpur in 2009, and Ph.D in 2019 from HBNI Mumbai. He is working as a Scientific Officer at BARC Mumbai since 2009 till date. His research field are micro and nano manufacturing, rotor dynamics, molecular dynamic simulations, etc. Till date, he has published 24 articles in peer reviewed international journal and more than 20 conference papers. One patent is granted, and one is filled. He has also contributed as a book chapter.
(E-mail: pranjan@barc.gov.in)

Dr. Anuj Sharma is presently working as a postdoctoral research associate in Cardiff University, UK, where he is working on SPH modelling to understand the nano-scratching process since November 2020. Prior to joining the Cardiff University, he has worked as a Senior Project Scientist at IIT Delhi for over a year. There, he worked in an IIT-DRDO project related to investigation of blast wave interaction with energy absorbing materials. He obtained his Ph.D from Bhabha Atomic Research Centre, Mumbai in the year 2019. In Ph.D, he carried out numerical and experimental techniques to study the nano regime diamond turning process. He has published number of journal and conference papers through his Ph.D work. For his work in Ph.D, he was awarded with "Outstanding Doctoral Student" award in engineering domain by HBNI Mumbai.
(E-mail: anuj30026@gmail.com)

Dr. Tribeni Roy earned his Bachelor's and Master's Degrees in Mechanical Engineering from Assam Engineering College, India, in 2010 and 2014, respectively. In 2019, he earned a Ph.D in Engineering Sciences from the Homi Bhabha National Institute (Bhabha Atomic Research Centre). He has carried out his postdoctoral research at Imperial College London on hybrid energy storage devices for electric vehicles, a project financed by Innovate UK in conjunction with five UK industries. Dr. Roy is a currently an Assistant Professor at BITS Pilani, with nearly 25 publications in peer-reviewed journals, 10 conference presentations, He is also a Visiting Academic at London South Bank University, UK.