Int. J. Nano Dimens. 5(5): 453-462 (Special Issue) 2014
ISSN: 2008-8868

Contents list available at **IJND**

International Journal of Nano Dimension

Journal homepage: *www.IJND.ir*

Molecular dynamics simulation of a binary mixture lubricant for use in hard disk interfaces

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Received 23 September 2013
Received in revised form
02 December 2013
Accepted 26 December 2013

ABSTRACT

In Hard Disk Drives (HDD), it is necessary to decrease the Flying Height (FH) between the head and the disk (currently, FH is around 3-5 nm) so as to increase recording densities. Retaining the solid lubricant has become a difficult proposition owing to intermittent contact between the surfaces. ZTMD and Z are used as solid lubricant to lubricate these interfaces. In this paper, the behavior of the binary mixture lubricant such as ZTMD & Z is modeled and analyzed using Molecular Dynamics (MD) simulation with the help of GROMACS software. It can be observed from simulation studies that ZTMD has poor replenishment performance although it possesses good retention properties. Addition of Z molecules improves replenishment performance of whole system. When ZTMD molecules alone are modeled, final structure attains stable state only at -4800 $kJmol^{-1}$. After the addition of Z molecules, final structure (ZTMD+Z) attains more stable state at -6950 $kJ\ mol^{-1}$. When compared to ZTMD, binary mixture lubricants (ZTMD + Z) are considered as more stable and for use in HDDs for their efficient operation.

Keywords: *Bead-spring model; Binary mixture lubricant; Molecular dynamics; GROMACS; Hard disk.*

INTRODUCTION

With the introduction of HDD in consumer products, the demand for high performance HDD continues to increase at a rapid rate. In order to realize the ultra-high recording areal data density, a reduction in the FH is required which is considered as one of the important parameters that control the performance and durability of HDDs. Ideally, zero spacing is preferred. However, zero spacing would lead to higher friction and wear at the Head Disk Interface (HDI) which leads to further reduction in HDD performance. Currently FH is hovering around 3-5 nm. Such a low FH promotes intermittent head disk contact leading to the data loss and even catastrophic failure of the drive.

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In order to reduce the possibilities of intermittent head disk contact, a layer of lubricant is introduced in the HDI (Hard Disk Interface). Per Fluoro Poly Ether (PFPE) is one of the most commonly used lubricants.

With the continuous demand of increasing areal recording density with reduced FH, lubricant film is expected to be 1 nm or less to fulfill the requirement of 6.5 nm Head Media Spacing (HMS) for 1 Tbit/in^2 HDDs [1]. New types of lubricants have been recently reported to enhance the performance and reliability of HDDs. Dipropylamine group was introduced to one end of Demnum that can reduce the adhesive interaction between head and disk [2]. Multidentate functionalized PFPE lubricants were synthesized by introducing additional hydroxyl groups in the center of the backbone chain [3]. The single component of disk lubricant may not be sufficient to meet the harsh requirements of lubricants for ultra-small HMS. The mixture of lubricants with different properties can be feasible and promising for future HDDs by providing desirable conformation, adequate mobility, good tribological performance etc.

The essential idea to use binary mixture lubricants in HDDs are briefly introduced in [4]. It is a dual layer lubricant where the first layer comprises a lubricant mobility enhancer and the second layer comprises a lubricant. This dual layer lubricant showed faster mobility to ensure rapid healing of the depleted region in the lubricant. In addition, the phosphazene X1P improved the durability of head disk interface [5]. The retention and replenishment performance of ultra thin lubricant film was investigated [6]. Authors report that it possesses low mobility and results in intermittent head disk contact leading to data loss.

Nano level simulation was carried out by using various softwares such as NAMD as done by [7] and GROMACS [8-10] etc. The static and dynamic properties of PFPE were examined using MD simulation based on Coarse Grained Bead Spring (CGBS) model [11-16]. MD simulation based on CGBS model was used to investigate the static and dynamic properties of binary mixture lubricant film of ZTMD and Z [17] Through MD simulation, the nanostructure, conformation and dynamics of lubricant films with different molecular structures were investigated [18]. It was found that ZTMD had oblate flat conformation that is desirable for ultra-small HMS but possess low mobility.

However, no works have been found so far on modeling and analyzing of binary mixture lubricant using GROMACS. It is a modeling engine to perform MD simulation more efficiently. In this paper, binary mixture lubricant (ZTMD & Z) is modeled and analyzed using MD simulation with the help of GROMACS.

EXPERIMENTAL

Molecular dynamics simulation

In this work, GROMACS is used for conducting MD simulation. The flowchart of a typical GROMACS MD run is shown in Figure 1. In GROMACS, it is necessary to create pdb files for Z and ZTMD to perform MD simulation. The chemical structure of Z and ZTMD are listed in Table 1.

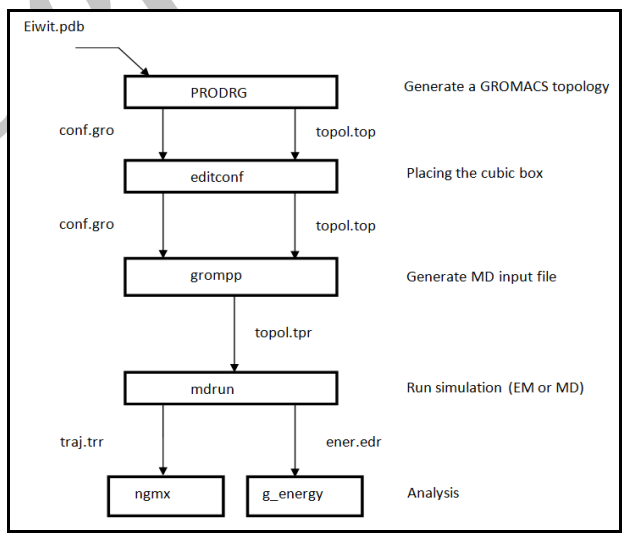

Fig. 1. Algorithm of GROMACS MD run

In ZTMD model, besides the functional beads in both chain ends, two functional beads are introduced in the centre of the chain. The .pdb files containing the molecular structure of Z and ZTMD are created using Accelrys discovery studio software. Rasmol and Pymol softwares are used to view the 3D structures of pdb files. In this work,

five different structure configurations of pdb files are created and are listed in Table 2. PRODRG server [19] is used to convert the coordinates in pdb file to GROMACS topology format. Once the GROMACS topology files are created, cubic box has been placed around the lubricant molecules. Input parameters such as number of steps, time step, cut-off, integrator algorithm etc. are mentioned in the file md.mdp.

In this work, MD simulation is carried out for the time period of 2000 picoseconds to simulate the Newtonian equations of motion for systems with pre-determined numbers of particles are shown in (1).

$$\frac{d^2 r_i}{dt^2} = \frac{F_i}{m_i}, \qquad (1)$$

Where F_i the force is exerted by the atoms and m_i is the mass of the atom. Periodic boundary conditions with minimum image convention are used. Only the nearest image of each particle is considered for short-range non-bonded interaction terms. For long-range electrostatic interactions, a lattice sum method named Particle Mesh Ewald (PME) is used. The entire atoms in the simulation system have dispersive interactions described by the 12-6 Lennard-Jones (LJ) potential [20-21] as shown in (2).

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \qquad (2)$$

Where, ε is the depth of the potential well, σ is the (finite) distance at which the inter-particle potential is zero and r is the distance between the particles. Leap-frog algorithm is used for integrating Newton's equations of motion. The position at $r(t+\partial t)$ is calculated from (3 & 4).

$$r(t+\partial t) = r(t) + \partial t v(t+\frac{1}{2}\partial t), \qquad (3)$$

$$v(t+\frac{1}{2}\partial t) = v(t-\frac{1}{2}\partial t) + \partial t a(t), \qquad (4)$$

Steep descent algorithm is used for energy minimization [22]. Berendsen temperature and pressure algorithm are used for temperature and pressure coupling respectively as shown in (5 & 6).

$$\frac{dT}{dt} = \left(\frac{T_0 - T}{\tau}\right), \qquad (5)$$

$$\frac{dP}{dt} = \left(\frac{P_0 - P}{\tau_p}\right), \qquad (6)$$

Where T the temperature of the system containing atoms is, T_0 is the room temperature, P is the pressure of the system containing atoms, P_0 is the atmospheric pressure. Then, grompp command makes gromacs preprocessor to read molecular topology file, checks the validity of the file, expands the topology from a molecular description to an atomic description. Bonds and bond-angles are converted into constraints. It also reads input parameters from md.mdp for the mdrun. Eventually, a binary file is produced that can serve as the sole input file for the MD program. The command mdrun is used to perform MD simulation. The command ngmx is used to view the trajectory and the command g_energy, g_rms, g_gyrate are used to generate outputs such as energy, root mean square deviation, radius of gyration respectively in xvg file format. Xmgrace software is used to view the xvg file format.

Table 1. Chemical structure of Z and ZTMD

PFPEs name	Chemical Structure
Z	$CF_3[(OCF_2CF_2)_m\text{-}OCF_2)_n]OCF_3$
ZTMD	$HOCH_2(OH)CHCH_2OCH_2\text{-}Y\text{-}CH_2OCH_2CH(OH)CH_2OCH_2CH(OH)CF_2CF_2$ $CF_2CH(OH)CH_2OCH_2CH(OH)CH_2OCH_2\text{-}Y\text{-}CH_2OCH_2CH(OH)CH_2(OH)$ Where $Y = -CF_2[(OCF_2CF_2)_m\text{-}OCF_2)_n]OCF_2-$ and m/n = 2/3

Table 2. Various types of structural configurations

Sl.No	Various types of structural configurations
1	Single ZTMD molecule
2	Combination of Z and ZTMD
3	Combination of six ZTMD molecules
4	Six times replication of combination of Z and ZTMD
5	Addition of six Z molecules to combination of six ZTMD

RESULTS AND DISCUSSION

GROMACS MD run is conducted for the time period of 2000 picoseconds for five different structure configurations of Z and ZTMD. After MD run was finished, graphs are generated between potential energy Vs radius of gyration and RMSD Vs time for all the various structural configurations of Z and ZTMD.

The structures of single ZTMD molecule before and after MD simulation are shown in Figure 2a & 2b and the combined structure of Z and ZTMD molecules before and after MD simulation are shown in Figure 3a & 3b respectively. The combined structures of six ZTMD molecules before and after MD simulation are shown in Figure 4a & 4b and the structures of six times replication of combination of Z and ZTMD molecules before and after MD simulation are shown in Figure 5a & 5b respectively. The structures of addition of six Z molecules to combination of six ZTMD molecules before and after MD simulation are shown in Figure 6a & 6b respectively.

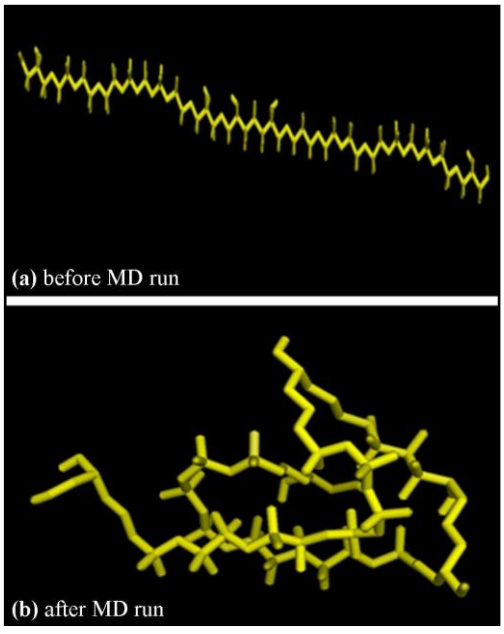

Fig. 2. (a- b) Structure of ZTMD

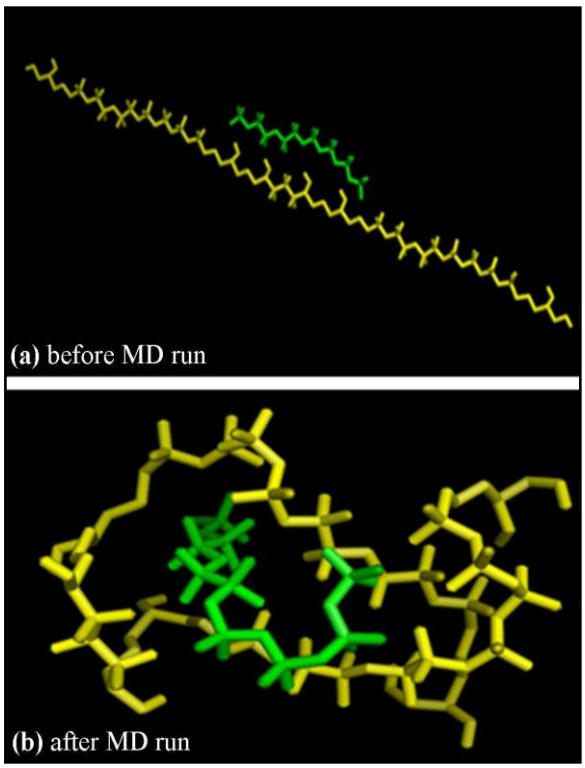

Fig. 3. (a- b) Structure of combination of Z and ZTMD

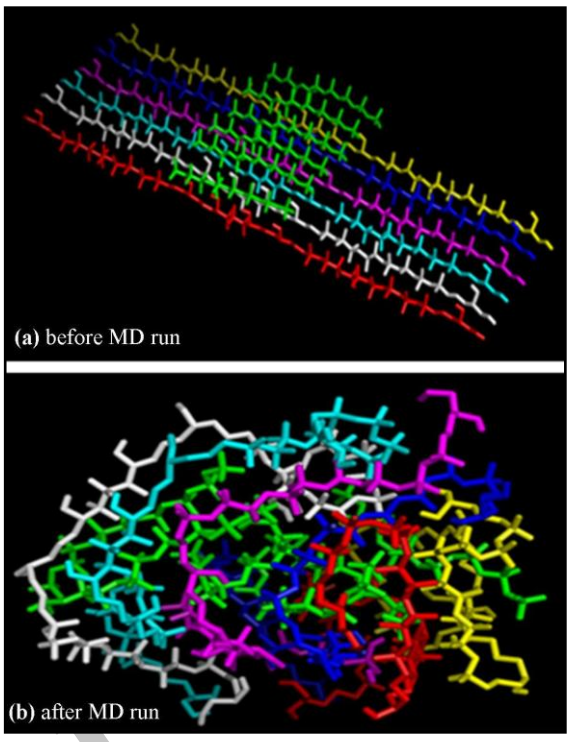

Fig. 5. (a- b) Structure of six times replication of combination of Z and ZTMD

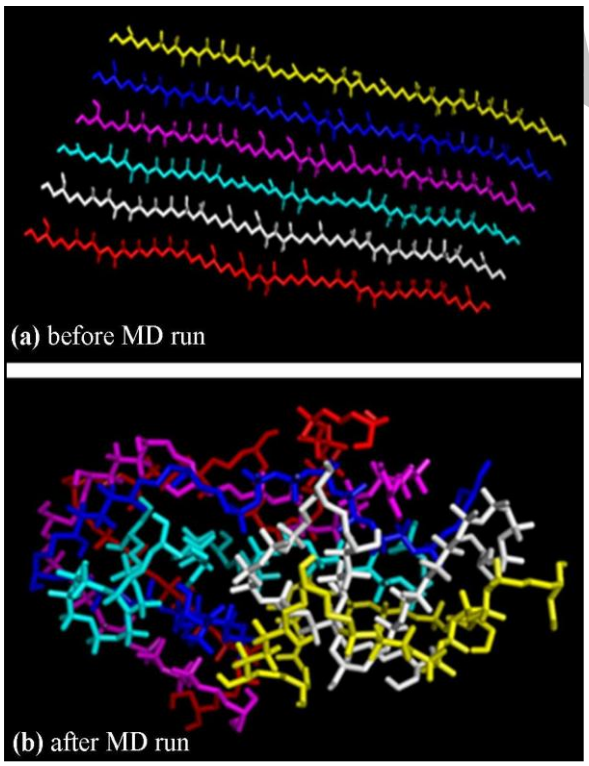

Fig. 4. (a- b) Structure of combination of six ZTMD molecules

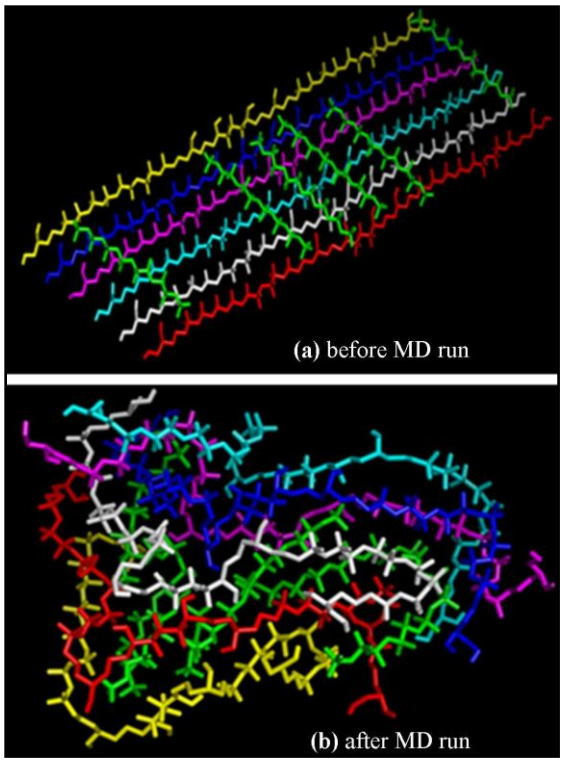

Fig.6 (a- b) Structure of addition of six Z molecules to combination of six ZTMD molecules

From Figure 7a, it is clear that potential energy decreases gradually and attains steady state at -630 kJmol^{-1} from 700 ps onwards. It represents the stable nature of intermolecular association and aggregation of a ZTMD molecule. In analyzing lubricant molecules, the radius of gyration is indicative of the level of spreading of the structure. In Figure 8a, Radius of gyration remains constant at 0.573 nm indicating spreading of ZTMD is uniform at reduced thickness. In general, the root mean square deviation (RMSD) is the measure of the average distance between the atoms of superimposed lubricant molecules. From Figure 9a, RMSD value remains constant at 0.26 nm which represents the structural stability of ZTMD molecule.

Figure 7b shows that potential energy decrease gradually and attains steady state at -790 kJmol^{-1} from 300 ps onwards. From Figure 8b, Radius of gyration remains constant at 0.639 nm representing spreading of com_1mer is uniform at reduced thickness. From Figure 9b, RMSD value remains constant at 0.24 nm which represents the structure stability of combination of Z and ZTMD molecules.

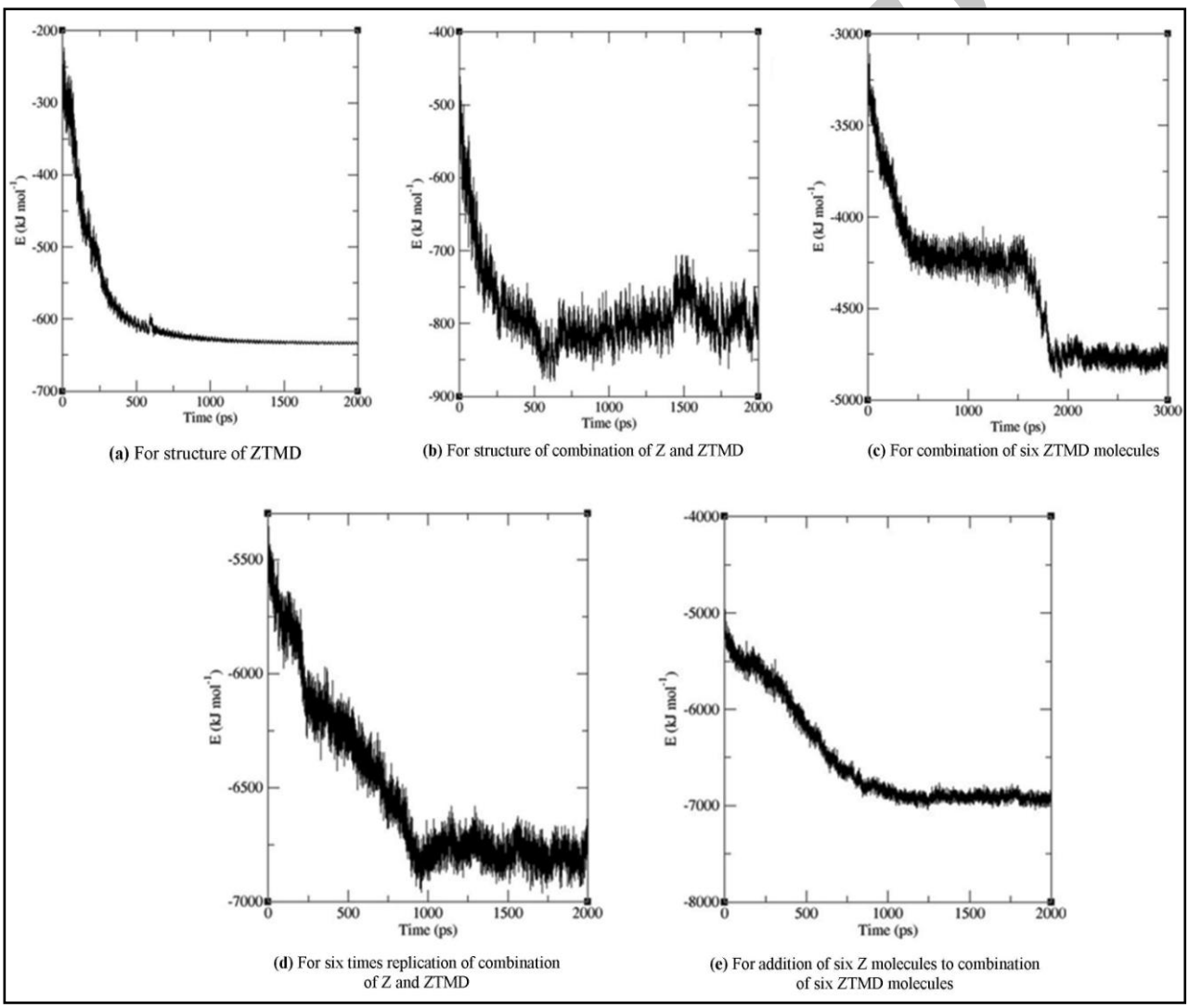

Fig.7 (a- e) Potential energy Vs. time for various structural configurations

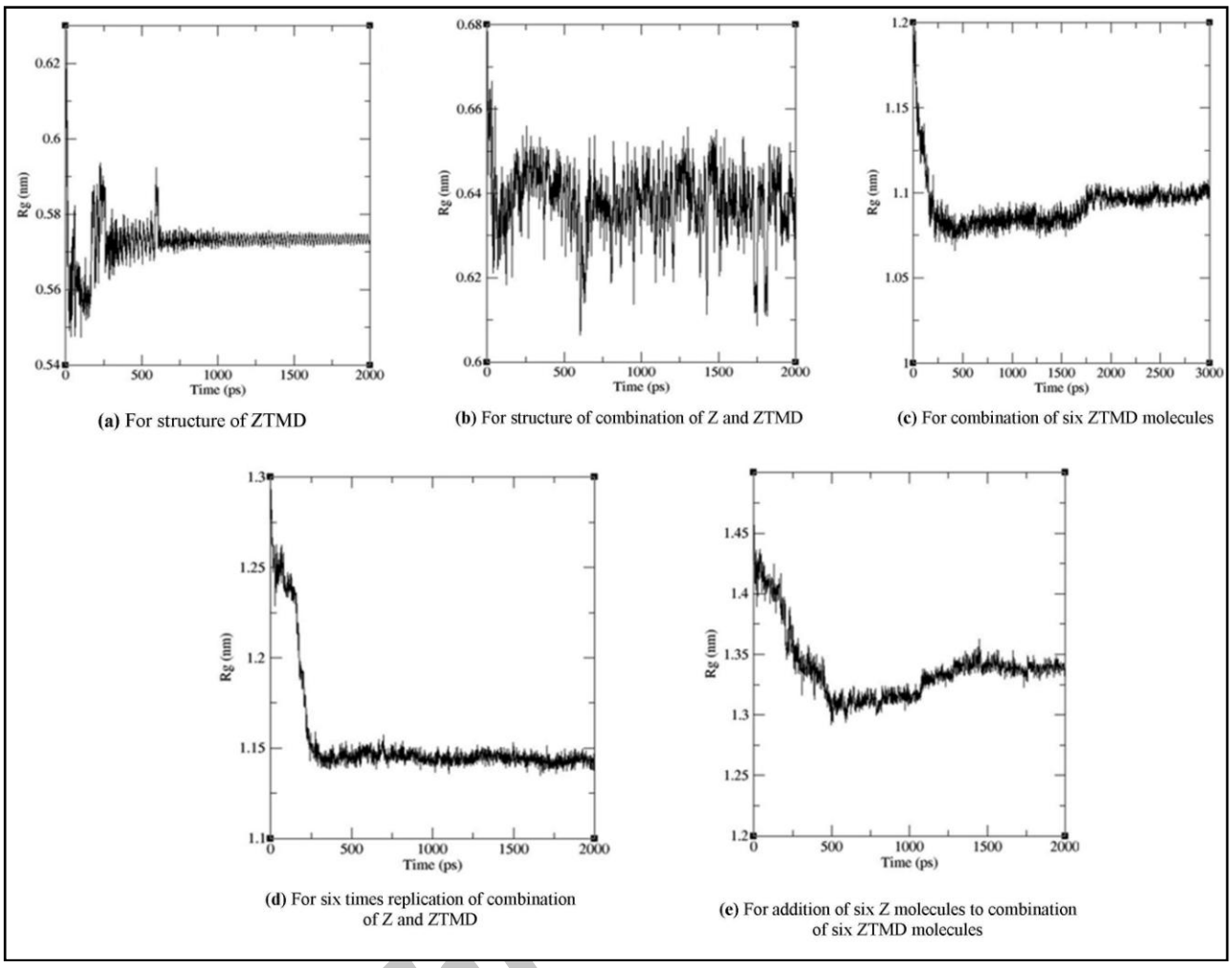

Fig. 8. (a- e) Radius of gyration Vs. time for various structural configurations

Figure 7c indicates the gradual decrease in the potential energy as well as the attainment of an intermediate stable structure at -4250 kJmol^{-1} from 450 – 1500 ps and reaches another stable structure at -4800 kJmol^{-1} from 1900 – 3000 ps. It represents the more stable nature of intermolecular association and aggregation when compared to single ZTMD molecule. However, there is unstable structure between 1500 – 1900 ps due to less mobility. It can be seen from Figure 8c that Radius of gyration remains constant at 1.08 nm up to 1500 ps and 1.09 nm from 1900 ps onwards. Problem of instability is well captured between 1500 and 1900 ps. From Figure 9c, it can be seen that RMSD value remains constant at 0.31 nm which represents the structural stability of combination of six ZTMD molecules.

From Fig. 7d, it is clear that potential energy gradually decreasing and attains stable structure at -6800 kJmol^{-1} from 950 ps. It represents the more stable nature of intermolecular association and aggregation when compared to single ZTMD and combination of six ZTMD molecules. Problem of mobility is also vanishes. Here Z molecules in the final structure i.e. at 2000 ps diffuses, hence they form stabilized ZTMD & Z mixture. From Fig. 8d, Radius of gyration remains constant at 1.145 nm representing spreading of ZTMD & Z molecules is uniform. From Fig. 9d, RMSD value remains constant at 0.48 nm which represents the structure stability of six times replication of combination of Z and ZTMD molecules.

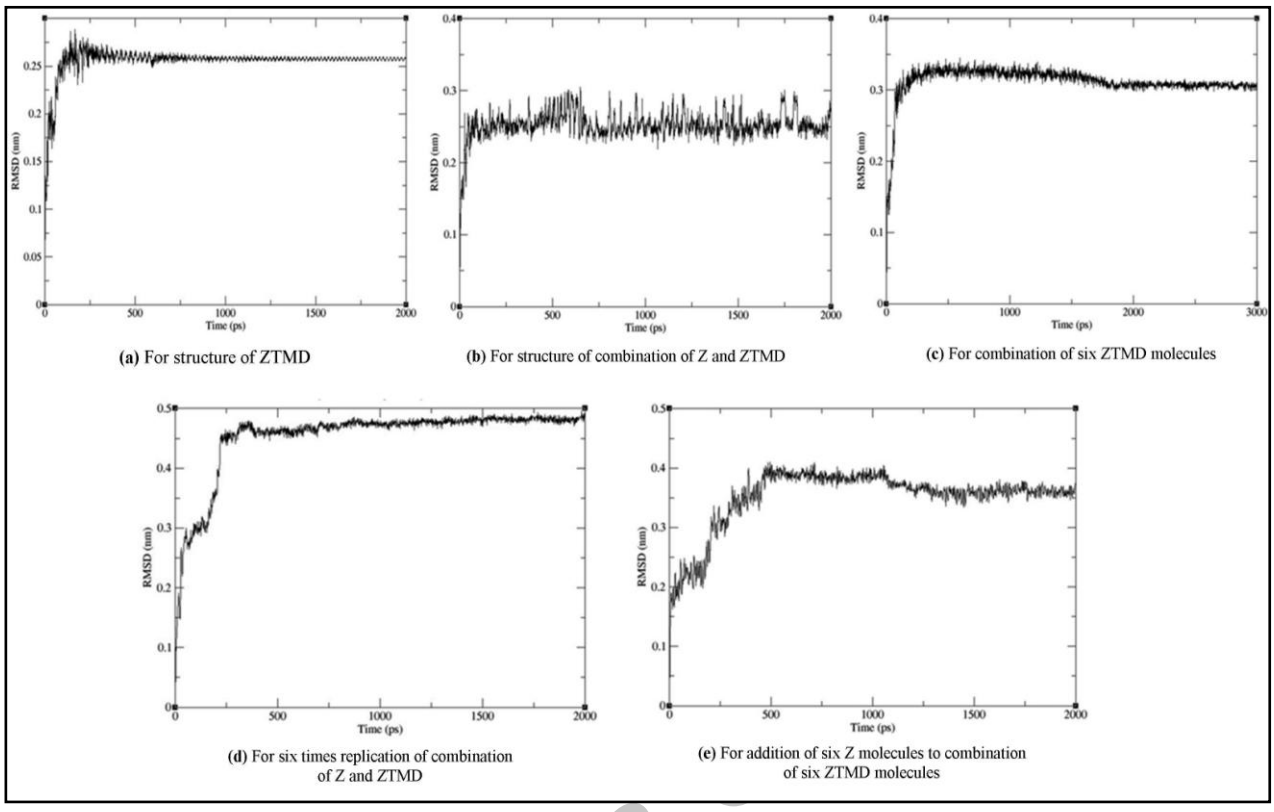

Fig. 9. (a- e) RMSD Vs. time for various structural configurations

From Fig. 7e, it is clear that potential energy gradually decreasing and attains stable structure at -6950 kJmol^{-1} from 900 ps. It represents the more stable nature of intermolecular association and aggregation when compared to single ZTMD, combination of six ZTMD molecules and six times replication of combination of Z and ZTMD molecules. Problem of mobility also vanishes. Here Z molecules in the final structure i.e. at 2000 ps diffuses, hence they form stabilized ZTMD & Z mixture. From Fig. 8e, Radius of gyration remains constant at 1.134 nm representing spreading of ZTMD & Z molecules is uniform. From Fig. 9e, RMSD value remains constant at 0.360 nm which represents the structure stability of addition of six Z molecules to combination of six ZTMD molecules.

CONCLUSIONS

The binary mixture lubricant films of ZTMD and Z are investigated via MD simulation using GROMACS software package. From the simulation results, it can be concluded that, intermediate stable layer is formed before reaching final stable structure when ZTMD molecules alone are simulated. This intermediate layer is harmful and it is formed due to poor mobility (replenishment) of ZTMD. Because of poor replenishment, ZTMD alone cannot be used as lubricant in HDD. If used, it leads to data loss or even failure of HDD may happen. In order to improve replenishment performance of system, Z molecules are added to ZTMD molecules. As a result, aggregation of ZTMD is more stabilized by Z molecules and also mobility performance of whole system is improved. When ZTMD molecules alone are modeled, final structure attains stable state at -4800 kJmol^{-1}. After addition of Z molecules, final structure (ZTMD+Z) attains stable state only at -6950 kJmol^{-1}. When compared to ZTMD, binary mixture (ZTMD + Z) are considered as more stable and for use in HDDs for their efficient operation.

Notations

a	Acceleration of the atom (nm ps^{-2})
F	Force exerted by the atom interaction (kJ mol^{-1} nn
i	Atom number
m	Mass of the atom (amu)
P_0	Atmospheric pressure (kJ mol^{-1} nm^{-3})
P	Pressure of the simulated system (kJ mol^{-1} nm^{-3})
r	Position of the atom (nm)
T	Temperature of the simulated system (K)
T_0	Room temperature (K)
t	Time (ps)
v	Velocity of the atom (nm ps^{-1})
V	Potential function (kJmol^{-1})
ε	Energy of potential well (kJmol^{-1})
σ	Inter-particle potential distance (nm)
τ_p	Pressure coupling constant (ps)
τ	Thermal coupling constant (ps)

ACKNOWLEDGMENTS

The computational facilities provided by Center for Bioinformatics, Pondicherry University, India are gratefully acknowledged.

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Cite this article as: N. Anandan *et al.*: Molecular dynamics simulation of a binary mixture lubricant for use in hard disk interfaces.
Int. J. Nano Dimens. 5(5): 453-462 (Special Issue) 2014.