MOLECULAR DYNAMICS STUDY OF BINARY MIXTURE LUBRICATING FILM IN HARD DISK INTERFACE

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Abstract

As the distance between the head-media spacing in hard disk drive shrink, there is a greater willingness for the usage of binary mixture of lubricants such as ZTMD and Zdol to overcome the problem of retention and replenishment of lubricants on the surface of the hard disk. Hence, in this work, lubrication performance of binary mixture will be modelled using molecular dynamics simulation based on a coarse-grain spring model using Euler Algorithm. Only preliminary results are shown here as the work is still in progress.

1. Introduction

Magnetic recording has become the main technology for the storage of digital data. With the introduction of hard disk drives (HDD) in consumer products, the demand for high performance HDD continues to increase at a rapid rate. With the continuous demand of increasing the areal recording density, lubricant film is expected to be 1 nm or less to fulfil 6.5 nm head-media spacing. Commercially used lubricant in HDD is PerFluoroPolyEther. Though it possess several advantages such as good lubricating and retention properties, it has the disadvantage of poor replenishment. To overcome this limitation, mixture of lubricants came into existence to enhance the performance and reliability of HDD.

2. Hard Disk Drive

HDD is a non-volatile, random access device for storing digital data and also allows quick access to large amounts of data on an electromagnetically charged surface or set of surfaces. A typical hard disk drive consists of a motor, spindle, platters, read/write heads, actuator and electronics as shown in Figs (1,2).

Fig.1 Hard Disk Drive

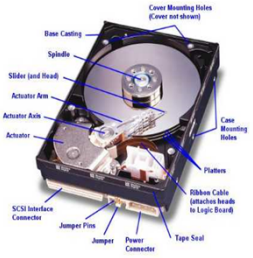

Fig.2 Nomenclature of HDD

It has one or more platters or disks and each platter usually has a head on each of its sides. In modern drives, the platters are made from glass or ceramic. The platters themselves are non-magnetic but have a magnetic coating which holds the magnetic impulses to represent the data. The platters are mounted on the spindle which is turned by the drive motor. Most current hard disk drives spin at between 5,400 and 10,000 RPM. The read/write heads float on a cushion of air only nanometers above the surface of the platters. As the read/write heads pass over the spinning platters they magnetize the surface in a pattern which represents the data in digital form. Storage of information in hard disk drives is accomplished by the relative motion between a rotating magnetic disk and a magnetic read/write element. The separation between the head and the hard disk during operation known as the flying height or floating height (FH), is one of the important parameters that controls the performance and durability of a hard drive (Fig. 3).

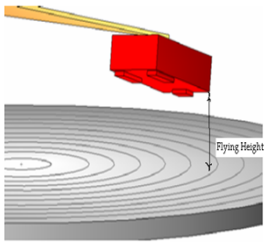

Fig.3 Flying Height

In order to increase the recording density it is necessary to minimize the FH. The current FH is approximately around 5 nm. Future recording will have lower FH below 3 nm. Such a low FH promotes intermittent head disk contact leading to the loss of data and even catastrophic failure of the drive. Moreover, at such a low spacing, the short range interactions caused by intermolecular force etc., becomes significant for the head disk interface. These interactions cause the head's flight to be unstable because these forces are highly dependent on the spacing and surface conditions between the slider and the disk. In order to eliminate intermittent head disk contact leading to the loss of data, Lubricant must be introduced in hard disk interface (HDI).

3. Binary Mixture Lubricant

In this work, our main intention is on the top most lubricant layer as shown in Fig. 4 since it plays vital role in separating hard disk interface with the read/write element, thereby preventing data loss and failure of HDD. The main functions of molecularly thin film of lubricant are to minimize friction, wear and also to prevent corrosion.

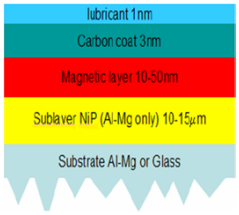

Fig.4 Layered structure of disk

While selecting lubricant, two performance parameters of lubricant are considered to be important.

1. Retention performance
2. Replenishment performance

Retention performance is staying property of lubricant. Replenishment performance is the ability of lubricant to move to the location where lubricant film was ruptured due to the intermittent contact between the slider and the head. Mostly the selected lubricant possesses 50 % Retention and 50 % Replenishment. Commercially used lubricant in HDD is PerFluoroPolyEther(PFPE). Liu et al. [1] studied the retention and replenishment performance of ultra-thin lubricant film (PFPE) and also studied head touch-down and take-off hysteresis. Authors observed that ultra-thin lubricating film possesses low mobility and results in intermittent head disk contact leading to the loss of data. Due to limitation of poor replenishment, mixture of lubricants with different properties came into existence.

Binary mixture lubricant consist of two lubricants which do not react with each other. It comprises a lubricant mobility enhancer and a lubricant. Compared to pure single lubricant, It shows faster mobility which ensures rapid healing of depleted region in the lubricant, thereby improving durability and preventing the failure of HDD. Chung et al. [2] investigated the static and dynamic properties of the binary mixture lubricant films of ZTMD and Zdol. Authors found that binary lubricant films have higher mobility than pure ZTMD monolayer. Here ZTMD has very strong attraction with the overcoat and exhibits very low mobility. Zdol has weak interaction with the overcoat and shows high mobility.

In this work, binary mixture lubricant (ZTMD & Z) is employed and coarse-grained bead spring model is applied to describe the spreading of binary mixture lubricant molecules. All the beads in the simulation system have interactions described by the 12-6 Lennard-Jones (LJ) Potential. Molecular dynamics (MD) simulation is employed to investigate the short range interaction between the head and the lubricant film. It is possible to carry out MD simulation on desktop computers. Chembeti [3] carried out MD simulation on a dual core Dell XPS computer installed with Linux and the simulation results are statistically and physically equivalent and it is compared with MD simulation carried on IBM RISC/6000 workstations.

4. Molecular Dynamics Simulation using Euler Algorithm

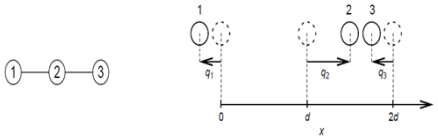

Fig. 5(a) Linear chain of three interacting particles

Fig. 5(b) Linear chain after the change of variables $q_i = x_i - (i-1)$

MD is a form of computer simulation in which atoms and molecules are allowed to interact for a period of time by approximations of known physics, giving a view of the motion of the particles. It follows the classical time evolution i.e. the positions and velocities after each of a series of time steps of a collection of virtual interacting particles by means of their integrated equations of motion. The dynamics are derived from Newton's second law as given by Eq. 1. Here the three-particle system shown in Fig. 5(a) is considered. It is assumed that there are no external forces acting upon the system and that each particle interacts with only two other particles, namely, its nearest neighbours. In addition, all particles have the same mass m and that all interactions have a common force constant k.

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

$$F_i = -\frac{\partial V}{\partial r_i} \qquad (2)$$

Here Hooke's law (HL) potential is used to model the system as a collection of masses and springs. It is especially popular for a first approximation because its visualization in terms of springs provides a natural model for chemical bonds.

For any particle i, force is given by Eq. 2. If r_{eq} designates the equilibrium position of a particle, then the HL potential energy of that particle at any position r is given by Eq.3. the force acting on each particle i is given by Eq.4. The equilibrium points of particles 1, 2, and 3 are now 0, d, and 2d respectively, and any vanishing q_i means that particle i is at its equilibrium position. The relevant coordinate system is shown in Fig. 5(b).

$$V(r) = \frac{k}{2}(r - r_{eq})^2 + V_{min} \qquad (3)$$

$$V(x_1, x_2, x_3) = \frac{k}{2}[(x_2 - x_1 - d)^2 + (x_3 - x_2 - d)^2 + V_{min} \qquad (4)$$

the force acting on each particle is obtained by Eq. 5.

$$F_1(q_1, q_2) = k(q_2 - q_1) \qquad (5)$$

$$F_2(q_1, q_2, q_3) = k(q_1 - 2q_2 + q_3) \qquad (6)$$

$$F_3(q_2, q_3) = k(q_2 - q_3) \qquad (7)$$

After substituting the eqn. 5, 6 & 7 in Eq. 1 to give the final equations of motion which is given by Eq. 8, 9 & 10 respectively.

$$m\ddot{q}_1 = k(q_2 - q_1) \qquad (8)$$

$$m\ddot{q}_2 = k(q_1 - 2q_2 + q_3) \qquad (9)$$

$$m\ddot{q}_3 = k(q_2 - q_3) \qquad (10)$$

The simplest time integration algorithm is based on Euler's method for ordinary differential equations Eq. 8, 9 & 10 is given by Eq. 11 & 12 as follows,

$$q_i(t+h) \approx q_i(t) + hv_i(t) \qquad (11)$$

$$v_i(t+h) \approx v_i(t) + \frac{h}{m} F(q_i(t)) \qquad (12)$$

5. Results and discussions

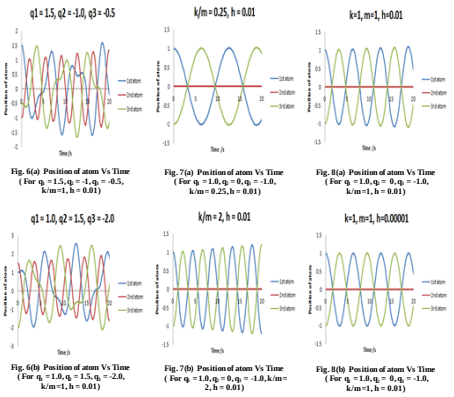

Fig. 6(a) Position of atom Vs Time (For $q_1 = 1.5, q_2 = -1, q_3 = -0.5$, k/m=1, h = 0.01)

Fig. 7(a) Position of atom Vs Time (For $q_1 = 1.0, q_2 = 0, q_3 = -1.0$, k/m = 0.25, h = 0.01)

Fig. 8(a) Position of atom Vs Time (For $q_1 = 1.0, q_2 = 0, q_3 = -1.0$, k/m=1, h = 0.01)

Fig. 6(b) Position of atom Vs Time (For $q_1 = 1.0, q_2 = 1.5, q_3 = -2.0$, k/m=1, h = 0.01)

Fig. 7(b) Position of atom Vs Time (For $q_1 = 1.0, q_2 = 0, q_3 = -1.0$, k/m = 2, h = 0.01)

Fig. 8(b) Position of atom Vs Time (For $q_1 = 1.0, q_2 = 0, q_3 = -1.0$, k/m=1, h = 0.01)

Program is written and compiled using FORTRAN 95. Execution parameters include number of atoms in the chain, force constant (k),particle mass (m), integration time increment (h), time interval between printings (hp), length of the simulation (len). Any self-consistent set of units can be employed. Graphs are drawn between position of atoms and time for various input parameters. In the Fig. 6(a) & (b), a graph is drawn between position of atom and time by varying only the positions keeping other variables constant. In the Fig. 7(a) & (b), a graph is drawn between position of atom and time by varying only k/m ratio keeping other variables constant. From this graph, it is clear that the number of maxima and minima increases when k/m ratio increases. In the Fig. 8(a) & (b), a graph is drawn between position of atom and time by varying time steps keeping other variables constant. From this graph, it is clear that the computation time increases when the value of time step increases.

6. Conclusion

Molecular dynamics simulation of binary mixture lubricant performance on a HDD is being studied. In this work, only Hooke's law potential model of MD was carried out using Euler Algorithm and further modelling is required to simulate the exact behavior of binary mixture of lubricant, that work is currently under progress.

References

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