

Molecular dynamics studies of lubricant depletion under moving laser heating: Effects of laser power and film thickness

B. Li, C.H. Wong*

School of Mechanical and Aerospace Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore

ARTICLE INFO

Article history:

Received 3 February 2015

Received in revised form

10 May 2015

Accepted 13 May 2015

Available online 27 May 2015

Keywords:

Lubricant depletion

Molecular dynamics

Laser power

Film thickness

ABSTRACT

Molecular dynamics simulation is employed to study the depletion behaviors of perfluoro-lubricants under scanning laser heating for heat-assisted magnetic recording hard disk drives. A partial lubricant near the substrate is irradiated by the laser beam to mimic nano-scale heat transfer from disk to lubricant. The lubricant surface morphology and thickness profiles are examined to reveal the dynamic depletion behaviors. The localized temperature evolution is also evaluated to illustrate the direction-dependent ridge formation around the depletion zone. In addition, the effects of laser power and film thickness on lubricant depletion are explored. Although evaporation is enhanced significantly at high laser powers or for lubricant with thickness around one monolayer, thermodiffusion is the primary mode of lubricant depletion under scanning laser heating.

© 2015 Elsevier Ltd. All rights reserved.

1. Introduction

In hard disk drives, the writable magnetic grain size has to be scaled down to further increase areal density while preserving sufficient signal-to-noise ratio. Unfortunately, this would cause superparamagnetic instability of the recording bits. Heat-assisted magnetic recording (HAMR) has thus been proposed to suppress the thermal effect. It makes use of a very high anisotropy medium that is too high to be written for conventional write head. As such, a tiny laser beam is used to momentarily heat up the high anisotropy medium to its Curie temperature (about 700 K) during writing process. This technology can potentially achieve areal density up to 50 Tb/in². However, the use of femtosecond pulsed laser may cause some counterproductive effects on the performance and reliability of HAMR-based hard disk drive systems. One of such effects is the severe lubricant depletion occurring when subjected to rapid laser heating. It has been reported that the commercially used perfluoropolyether (PFPE) lubricants such as PFPE Zdol can be completely removed in less than 1000 laser shots [1]. Zhang et al. [2] numerically studied the effects of laser power and laser spot size on the recorded mark width in HAMR. It was shown that the mark width increases with the laser power nonlinearly due to the Gaussian distribution of the laser intensity. Moreover, they observed that, in certain power range, a wider mark width is induced with a smaller laser spot size when the laser power is constant. Ma et al. [3] theoretically investigated the

lubricant desorption caused by laser heating and found that the lubricant thinning rate could be decreased significantly by using lubricant with high molecular weight and lowering laser heating temperature. Li et al. [4,5] explored the lubricant evolution and degradation behaviors under static laser heating source using molecular dynamics (MD) simulation. It was shown that the lubricant film experiences severe depletion with time and forms raised ridges around the depleted zone due to imbalanced surface tension and non-equilibrium thermocapillary stress. They subsequently used the same technique to study lubricant adsorption and depletion instability on solid disk surfaces [6,7]. It was demonstrated that the lubricant end group functionality can greatly influence lubricant desorption, but show little effect on decomposition. Moreover, they examined the laser spot size effect on lubricant depletion [8] and observed the existence of a critical laser spot size at which the lubricant has the maximum thermodiffusion. In addition, Pacansky and Waltman [9] reported that PFPE lubricants degrade due to scission in the main chain when subjected to electron irradiation and pointed out that the response of PFPEs to high energy irradiation would differ greatly if exposure was performed under vacuum or atmospheric conditions. Heller [10] studied the effect of heating ultrathin PFPE films by a laser pulse with a heating rate of 10³ K/s to examine thermochemistry of lubricants. It was revealed that evaporation is the primary lubricant loss mechanism and the effective evaporation rate of PFPEs for laser heating is in orders of magnitude higher than that for oven heating. Tagawa et al. also performed a series of experimental studies on different PFPE lubricants under laser irradiation and clarified the effects of molecular weight, functional end groups, film thickness, and bonding ratio on lubricant depletion

* Corresponding author. Tel.: +65 6790 5913; fax: +65 6792 4062.

E-mail address: chwong@ntu.edu.sg (C.H. Wong).

during laser heating [11–13]. In all their tests, the laser beam had a large spot diameter of 900 nm and the maximum temperature achieved in most experiments was < 400 K. However, this may underestimate the lubricant depletion for a real HAMR system as the expected laser spot size is < 50 nm and the required temperature is about 700 K in order to lower the media coercivity. In other words, distinct characteristics of lubricant depletion might appear surface when different spot sizes and laser powers are used during laser heating. Moreover, it was shown that the lubricant depletion results in deep trenches whose width is comparatively small for lubricant films thicker than one monolayer. On the contrary, the depletion depth is shallower and the width is remarkably larger for lubricant films with thicknesses less than one monolayer.

For conventional non-HAMR-based hard disk drives the main concentration on lubricants is their tribological and mechanical properties, while for emerging HAMR applications thermal and tribological behaviors of PFPEs are essential to explore. Until now, incomplete and the lack of understanding of lubricant failure due to laser heating still remains a critical issue that retards the rate of introducing HAMR into engineering applications. If laser-induced lubricant depletion cannot be addressed appropriately, lubrication investigation relevant to tribology might not be so urgent and practical for HAMR and laser-based systems associated with the use of ultrathin PFPE lubricants. Therefore, the present work details the investigation of local heat dissipation and lubricant evolution under moving laser heating for HAMR applications. The factors that influence lubricant depletion such as laser power and lubricant film thickness will be thoroughly examined to understand the lubricant depletion instabilities under moving laser heating.

2. Molecular dynamics simulation and methodology

2.1. Molecular model

Following our previous work [4,8,14], the perfluoropolyether (PFPE) Zdol2000 molecule is described by a coarse-grained bead-spring model as shown in Fig. 1, which neglects the detailed atomic information but still captures the essence of internal molecular structure [15]. Frequently used coarse-grained bead-spring models for PFPEs can also be found in literatures [15–23] to clarify the choice of potential functions and parameters used in this research work. Although these models cannot provide 100% accurate and/or dimensional interpretation of real physical lubricant systems, they provide fundamental knowledge and understandings on properties and phenomena that are difficult to examine using current available experimental techniques.

As shown in Fig. 1, the PFPE lubricant is modeled as a pure material and each chain consists of 8 backbone beads and 2 end

beads to represent a molecular weight of about 2000 g/mol. In the simulations, the disk particles are assumed not to enter into lubricant phase when subjected to laser heating and vice versa. In this way, the disk particle fluctuates around its equilibrium position and maintains stability under laser irradiation. Though, the fluctuation of disk particles reflecting the temperature can change the disk surface roughness, it has a slight influence on the interaction between the lubricant and disk [24]. Furthermore, the heat transfer to lubricant film mainly comes from the underlying magnetic medium, which absorbs most of the laser beam to reduce its magnetic coercivity. Therefore, to save computation time, the disk is modeled as a thermally inert, infinitely long and deep flat surface, and is located at $z=0$ in the simulation cell, to provide external forces exerting on lubricant beads (see Eq. (2)) as well as serve as an external heat bath to lubricant film.

In the MD simulations, all the beads interact with one another through a truncated-shifted 12-6 Lennard-Jones (LJ) potential computed as

$$U_{LJ}(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 - \left(\frac{\sigma}{r_c} \right)^{12} + \left(\frac{\sigma}{r_c} \right)^6 \right] \quad (1)$$

where σ refers to the diameter of the bead (reduced unit of length), ϵ is the potential depth (reduced unit of energy), and r is the bead distance. The cutoff r_c for the non-bonded LJ potential is set to be 2.5σ to improve computation efficiency.

The van der Waals interaction between the bead and disk is described by a 9-3 LJ potential, which is derived by summing the interaction of a single bead with a semi-infinite smooth surface and is given as

$$U_{wall}(z) = \epsilon_w \left[\frac{2}{15} \left(\frac{\sigma}{z} \right)^9 - \left(\frac{\sigma}{z} \right)^3 \right] \quad (2)$$

where ϵ_w denotes the potential depth for the interaction between the bead and the disk, and z is the distance between the bead and the surface.

The bonded interaction of neighboring beads along a lubricant chain is normally governed by the finitely extensible nonlinear elastic (FENE) potential, which is computed as [16,17]

$$U_{FENE}(r) = -\frac{1}{2}KR_0^2 \ln \left[1 - \left(\frac{r}{R_0} \right)^2 \right] \quad (3)$$

where $r \leq R_0$, $K = 30k_B T / \sigma^2$ is the spring constant, k_B is the Boltzmann constant, T is the absolute temperature, $R_0 = 1.5\sigma$ is the maximum extension of the spring, and r is the bond length.

The end group functionality for PFPE Zdol is described by a short-range exponential decay function [4,8,14,15,18–22]. The interaction $U_{eb-wall}$ between the end bead and the disk, and the interaction U_{eb-eb} between the end beads can thus be expressed as

$$U_{eb-wall}(z) = -\epsilon_w^p \exp \left(-\frac{z-z_c}{d} \right) \quad (4)$$

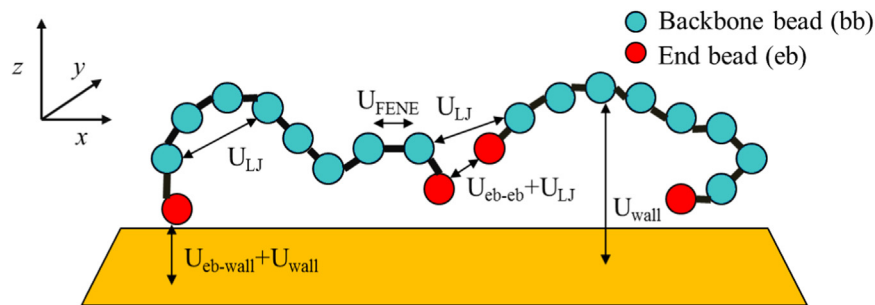


Fig. 1. Schematics of the coarse-grained bead-spring model together with 5 potentials used in MD simulations. The cyan beads are backbone groups, the red beads are end groups, and the yellow flat wall is the substrate surface. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Download English Version:

<https://daneshyari.com/en/article/614424>

Download Persian Version:

<https://daneshyari.com/article/614424>

[Daneshyari.com](https://daneshyari.com)