

Atomistic simulation method in head-disk interface of magnetic data storage systems

Robert L. Smith, Pil Seung Chung, Sessa Hari Vemuri, Geun-Young Yeom, Lorenz T. Biegler et al.

Citation: *J. Appl. Phys.* **111**, 07B717 (2012); doi: 10.1063/1.3679386

View online: <http://dx.doi.org/10.1063/1.3679386>

View Table of Contents: <http://jap.aip.org/resource/1/JAPIAU/v111/i7>

Published by the [American Institute of Physics](#).

Related Articles

Micromagnetic simulations of sweep-rate dependent coercivity in perpendicular recording media
J. Appl. Phys. **111**, 123905 (2012)

Ultra-high coercivity small-grain FePt media for thermally assisted recording (invited)
J. Appl. Phys. **111**, 07B729 (2012)

Influence of magnetic viscosity on the first order reversal curves of antiferromagnetically coupled perpendicular recording media
J. Appl. Phys. **111**, 07B728 (2012)

Analysis and design of shingled magnetic recording systems
J. Appl. Phys. **111**, 07B716 (2012)

Modeling for write synchronization in bit patterned media recording
J. Appl. Phys. **111**, 07B918 (2012)

Additional information on *J. Appl. Phys.*

Journal Homepage: <http://jap.aip.org/>

Journal Information: http://jap.aip.org/about/about_the_journal

Top downloads: http://jap.aip.org/features/most_downloaded

Information for Authors: <http://jap.aip.org/authors>

ADVERTISEMENT



Special Topic Section:
PHYSICS OF CANCER

Why cancer? Why physics? [View Articles Now](#)

Atomistic simulation method in head-disk interface of magnetic data storage systems

Robert L. Smith,¹ Pil Seung Chung,¹ Sessa Hari Vemuri,¹ Geun-Young Yeom,² Lorenz T. Biegler,¹ and Myung S. Jhon^{1,2,a)}

¹Department of Chemical Engineering and Data Storage Systems Center, Carnegie Mellon University, Pittsburgh, Pennsylvania 15213, USA

²School of Advanced Materials Science and Engineering, Sungkyunkwan University, Suwon 440743, South Korea

(Presented 31 October 2011; received 23 September 2011; accepted 7 December 2011; published online 12 March 2012)

The conventional modeling paradigm of head-disk interface (HDI) in magnetic data storage systems was based on meso/macro scale modeling. We investigate inter-molecular interaction energy for four sets of model PFPE dimers and elucidate the importance of hydrogen bonding between the hydroxylated functional endgroups in interaction strength. We found that for these model dimers representing PFPEs, the DDPA-DDPA (non-hydroxylated) dimer demonstrates the least stable interaction. We further investigated binary blends of hydroxylated and non-hydroxylated model PFPE lubricant and observed diminished interaction strength as compared to pure hydroxylated dimers. Our atomistic interaction energy study reported here will provide insight for tuning physiochemical properties of lubricant film by controlling blending ratios and chain end functionality to obtain desired lubricant performance. © 2012 American Institute of Physics. [doi:10.1063/1.3679386]

I. INTRODUCTION

The reliability of the hard disk drive system (HDD) at the head-disk interface (HDI) is primarily determined by performance of the lubricant layer. A molecularly thin layer (~1.2 nm) of perfluoropolyether (PFPE) lubricant protects the carbon overcoat layer from the slider's rapid flight occurring at 1.5 nm above the lubricant surface. PFPEs have the following fluorinated ether backbone structure that provides thermal and chemical stability under harsh HDI conditions: X-[(OCF₂-CF₂)_p-(OCF₂)_q]-O-X, where p/q ~ 2/3.¹ Several efforts at molecular design of lubricant performance have led to the synthesis of PFPEs with specialized functional endgroup structures, X. In contrast to first generation Fomblin Z, which contains a -CF₃- endgroup, the Zdol (-CF₂CH₂OH) and Ztetraol (-CH₂OCH₂CHOHCH₂OH) forms contain hydroxyl groups capable of interacting more strongly with each other as well as with a hydrogenated or nitrogenated surface. DDPA serves as an alternative functional lubricant which has the ability to adhere strongly to the surface due to its dipropylamine endgroup structure (see Fig. 1(d)).

Although the functional endgroups have the advantage of strong adhesion during disk rotation, the dynamic property of lubricant replenishment, or self-healing, capability must be addressed to ensure constant surface coverage after head-disk contact. Superior lubricant replenishment is linked to high molecular mobility which is influenced by the strength of intermolecular interaction. In practice, lubricants with strong molecular interaction may have sluggish self-healing

performance as was shown experimentally when comparing the mobility of nonfunctional and functional PFPE.²

Previous studies used molecular and mesoscale simulation techniques to model lubricant films at the HDI.³⁻⁸ Thus, in this work we evaluate the intermolecular interaction as a function of endgroup structure using *ab initio* theory to make inferences regarding the lubricant replenishment performance. In addition, we will highlight the force field parameters needed for many-body molecular simulation where temperature effects can be incorporated.

II. ESSENCE OF ATOMISTIC MODELING

Endgroups detached from the backbone were truncated into model structures which retain the characteristic endgroup functionality. The model structures used for the analysis are shown in Figs. 1 and 2. The relaxed molecular geometries and configurations of the endgroup monomers and dimers were obtained with density functional theory (DFT) with the B3LYP exchange-correlation functional with the Aug-cc-pVDZ Dunning basis set in Q-Chem 3.2.⁹ The augmented basis set adds diffuse functions to allow for greater accuracy in calculating the intermolecular interaction. The functional is corrected for dispersion effects using the Grimme correction.¹⁰ Our DFT provides a qualitative evaluation of the strength of the interaction as a function of endgroup structure while requiring minimal computational time.

III. RESULTS AND DISCUSSION

The relaxed configurations of the pure dimers for Z, Zdol, Ztetraol, and DDPA are given in Fig. 1. The shortest intermolecular bond among the hydroxylated endgroups is 1.94 Å for Zdol and 2.06 Å for Ztetraol occurring between

^{a)}Author to whom correspondence should be addressed. Electronic mail: mj3a@andrew.cmu.edu.

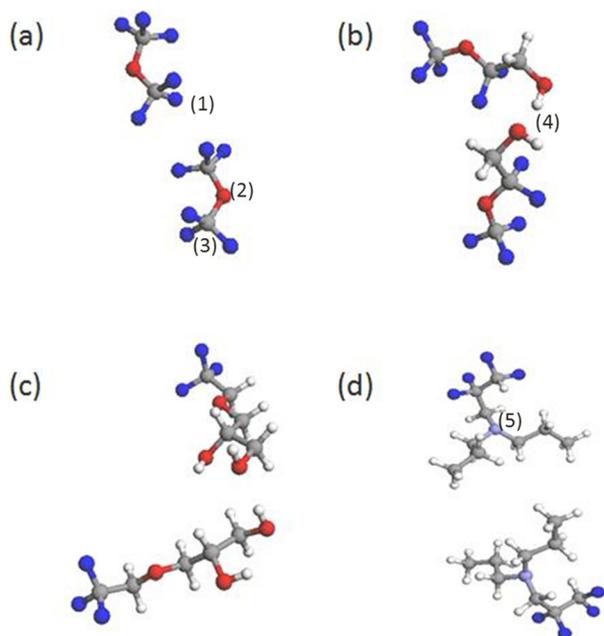


FIG. 1. (Color online) Pure relaxed lubricant dimers for (a) Z, (b) Zdol, (c) Ztetraol, and (d) DDPA. (1)-Fluorine, (2)-Oxygen, (3)-Carbon, (4)-Hydrogen, and (5)-Nitrogen.

the hydrogen and oxygen of the OH groups. This indicates that interaction between the monomers is influenced by hydrogen bonding where the positively charged hydrogen is attracted to the electron density of the oxygen. As shown in Fig. 1(d), for DDPA, the shortest intermolecular bond of 3.86 Å occurs between the hydrogens of the propyl groups on each monomer. This orientation provides a basis for the small magnitude of the attraction between DDPA monomers since the hydrogens would have a repulsive contribution to the interaction. This is contrary to the case where there is a significant interaction between polar atoms as we observed for the hydroxylated endgroups. For Z forms, the shortest intermolecular bond of 2.92 Å is between fluorine atoms as opposed to the ether oxygens. Similar to DDPA, the interaction between the equivalent F atoms would lead to a less attractive interaction. Thus, the structures of the relaxed dimers illustrate preferred orientations of the monomers as they form complexes and provide a basis for the interaction energy behavior.

Table I shows the energies of interaction for the pure dimers. For the pure complexes which correspond to Fig. 1,

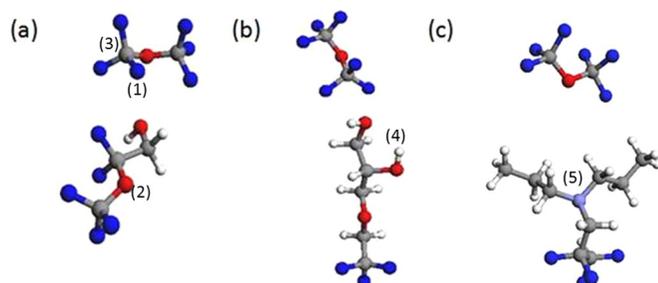


FIG. 2. (Color online) Z blended with functional lubricants: (a) Z-Zdol, (b) Z-Ztetraol, and (c) Z-DDPA. (1)-Fluorine, (2)-Oxygen, (3)-Carbon, (4)-Hydrogen, and (5)-Nitrogen.

the Zdol and Ztetraol have the strongest strength of interaction with energies of -8.23 kcal/mol and -14.1 kcal/mol, respectively, where the negative value denotes a stable interaction. The similarity between the interaction for Zdol and Ztetraol despite the extra OH group on Ztetraol indicates only one strong hydrogen bond between the OH groups of the Ztetraol monomers. The secondary OH groups on both Ztetraol monomers do not show direct intermolecular bonding. A much weaker interaction is observed for the Z and DDPA dimers with values of -2.38 kcal/mol and -0.950 kcal/mol. Compared to DDPA and Z, the hydrogen bonding for Zdol and Ztetraol among the hydroxylated endgroups provides a greater capacity to form more strongly bound dimer complexes. This result could indicate that the hydroxylated lubricants have diminished self-healing potential due to intermolecular interactions that hinder lubricant diffusion. However, many-body simulations must be performed to establish a more concrete link between the strength of endgroup interaction and molecular diffusion.

Relaxed configurations for blended dimers are shown in Figs. 2 and 3. When blending Z with the functional lubricants, the intermolecular distances are all longer than for the pure functional endgroups. This indicates less stable complexes when comparing to pure functional clusters highlighting the ability of Z to form weaker intermolecular bonds. For the blends of functional lubricants in Fig. 3, the closest intermolecular bond for the Zdol-Ztetraol dimer is between the hydrogen and oxygen of the hydroxyl group similar to the pure Zdol and Ztetraol cases. This similarity in orientation between the pure and blended cases indicates that the mechanism of interaction is still driven by hydrogen bonding when the hydroxylated lubricants are blended. The configuration of the Zdol-Ztetraol dimer also highlights the extra OH group available on the Ztetraol which would be free to form a hydrogen bond with an OH group on a third monomer. Figure 3(b) shows the dimer complex for Zdol and DDPA. The closest interaction here takes place between fluorines on each monomer. The orientation of the dimer represents the case where the portion of the endgroup closest to the backbone interacts. Since the fluorines would repel each other, this is expected to be a less stable interaction than if the hydrogens were in close contact with fluorines. Alternatively, as shown in Fig. 3(c), the Ztetraol-DDPA dimer has a close contact between the hydrogen of the first OH group and the fluorines of DDPA. This type of orientation is expected to produce a more stable interaction than for the Zdol-DDPA orientation.

The interaction energies for the blended dimers are also listed in Table I. The inclusion of Z with the functional

TABLE I. The interaction energies for pure and blended PFPE endgroups where a negative value represents a stable interaction.

PFPE Dimer	ΔU (kcal/mol)	PFPE Dimer	ΔU (kcal/mol)
Z	-2.38	Z-Ztetraol	-4.09
Zdol	-8.23	Z-DDPA	2.43
Ztetraol	-14.1	Zdol-Ztetraol	-8.51
DDPA	-0.950	Zdol-DDPA	1.25
Z-Zdol	-3.98	Ztetraol-DDPA	-1.56

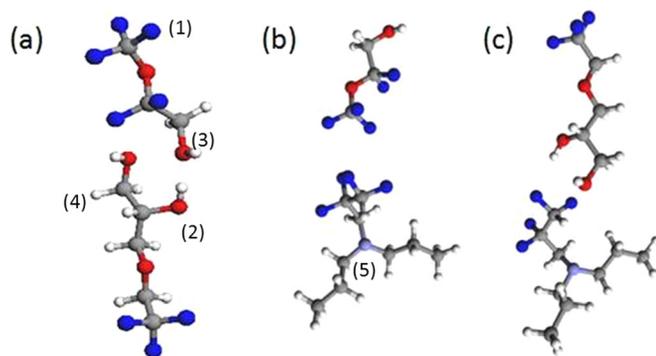


FIG. 3. (Color online) Blended functional lubricant dimers for (a) Zdol-Ztetraol, (b) Zdol-DDPA, and (c) Ztetraol-DDPA. (1)-Fluorine, (2)-Oxygen, (3)-Carbon, (4)-Hydrogen, and (5)-Nitrogen.

endgroups diminishes the strength of the interactions for all three functional groups. In the case of Zdol and Ztetraol blends with Z, the interaction energy decreases to -3.98 kcal/mol and -4.09 kcal/mol, respectively, indicating the interaction is still attractive. However, for the case of Z blended with DDPA, the interaction becomes repulsive with a value of 2.43 kcal/mol. This combination of Z and DDPA results in the most repulsive interaction for any lubricant dimer.

Consistent with the configuration of Fig. 3(a), the Zdol-Ztetraol dimer has the strongest interaction of -8.51 kcal/mol. This is also similar to the strength of the interaction for the Zdol and Ztetraol pure dimers providing further support for the point that hydrogen bonding is the key binding mechanism in both the pure and blended cases when pairs of hydroxyl groups are present. Thus, the strongest interactions are still observed when going from the pure case to the blended case for the hydroxylated endgroups. As the orientation in Fig. 3(b) indicates, the interaction for the Zdol and DDPA is unstable with a value of 1.25 kcal/mol. In contrast, the dimer of Fig. 2(c) has a stable interaction of -1.56 kcal/mol most likely due to the interaction between the fluorines and hydrogens. Thus, we have obtained both moderately repulsive and more strongly attractive dimer configurations for hydroxylated endgroups with DDPA.

In order to translate the strength of the endgroup functionality to lubricant self-healing performance we are obtaining intermolecular force field parameters for molecular dynamics simulation where temperature effects can be evaluated. In addition to the intermolecular potentials, intramolecular potentials are needed, and these were obtained in a previous work where we observed the stiffest bonds to be the between O and H with C-C bonds being the most flexible.¹¹

IV. CONCLUSIONS

We have examined intermolecular interactions among various model PFPE lubricants which complement our earlier studies of intramolecular interactions. For the pure lubricant complexes, we found superior intermolecular interaction between lubricant endgroups with hydrogen bonding capabilities. However, the pure Z and DDPA complexes display the longest intermolecular bond lengths as well as weaker interactions. The binary lubricant blends demonstrated strong interaction between blended hydroxylated lubricants and diminished strength of interaction when adding Z and DDPA to hydroxylated lubricants. The most repulsive interaction was observed for Z blended with DDPA. Therefore, we have identified the ability to tune lubricant interaction by introducing blends of various functional and nonfunctional endgroup types. This result indicates that self-healing properties may be tailored by selecting optimal blend ratios which can be investigated using optimization formulations. Our capabilities in determining force constants that govern both intermolecular and intramolecular degrees of freedom allow us to make a linkage between atomistic descriptions and molecular/meso scale condensed phase models via coarse-graining procedures and we are currently extending our lubricant analysis to include temperature effects applicable for the heat-assisted magnetic recording system.

ACKNOWLEDGMENTS

This work was supported by Korea Science and Engineering Foundation through the WCU Project.

- ¹D. Kim, P. S. Chung, P. Jain, S. H. Vemuri, and M. S. Jhon, *IEEE Trans. Magn.* **46**, 2401 (2010).
- ²M. S. Jhon, D. M. Phillips, S. J. Vinay, and C. T. Messer, *IEEE Trans. Magn.* **35**, 2334 (1999).
- ³P. S. Chung, H. Park, and M. S. Jhon, *IEEE Trans. Magn.* **45**, 3644 (2009).
- ⁴Q. Guo, P. S. Chung, M. S. Jhon, and H. J. Choi, *Macromol. Theor. Simul.* **17**, 454 (2008).
- ⁵H. Chen and M. S. Jhon, *J. Appl. Phys.* **103**, 07F536 (2008).
- ⁶P. S. Chung, H. Chen, and M. S. Jhon, *J. Appl. Phys.* **103**, 07F526 (2008).
- ⁷Q. Guo, P. S. Chung, H. Chen, and M. S. Jhon, *J. Appl. Phys.*, **99**, 08N105 (2006).
- ⁸X. Ma, J. Gui, L. Smoliar, K. Grannen, B. Marchon, C. L. Bauer, and M. S. Jhon, *Phys. Rev. E*, **59**, 722 (1999).
- ⁹C. Kong, A. White, A. I. Krylov, C. D. Sherrill, R. D. Adamson, T. R. Furlani, M. S. Lee, A. M. Lee, S. R. Gwaltney, T. R. Adams, C. Ochsenfeld, A. T. B. Gilbert, G. S. Kedziora, V. A. Rassolov, D. R. Maurice, N. Nair, Y. Shao, N. A. Besley, P. E. Maslen, J. P. Dombroski, H. Daschel, W. Zhang, P. P. Korambath, J. Baker, E. F. C. Byrd, T. Van Voorhis, M. Oumi, S. Hirata, C.-P. Hsu, N. Ishikawa, J. Florian, A. Warshel, B. G. Johnson, P. M. W. Gill, M. Head-Gordon, and J. A. Pople, *J. Comput. Chem.* **21**, 1532 (2000).
- ¹⁰S. Grimme, *J. Comp. Chem.* **27**, 1787 (2006).
- ¹¹R. Smith, P. S. Chung, J. A. Steckel, M. S. Jhon, and L. T. Biegler, *J. Appl. Phys.* **109**, 07B728 (2011).