**Title:** Dynamic Thermomechanical HDI Contact and Wear Model Accounting for Laser Heating and Contact Effects in HAMR and Planarized BPMR

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**Abstract**

We propose to develop and validate a nanoscale contact model with friction relevant to realistic HDIs to be used in HAMR and BPMR systems. A clear understanding of the nanoscale interfacial interactions and a readily usable physics-based model will allow us to also model nanoscale wear that is expected at these interfaces. The model will be based on both advanced computational finite element work (where we already have significant experience) as well as on molecular dynamic simulations. The model will then be validated with simplified quasi-static controlled scratch/wear experiments and realistic HDI flyability/contact experiments. This work builds on our recent (a) analytical and computational work that has resulted in nano-mechanical contact models for TFC technology HDDs that account for the presence of molecularly thin lubricant layers at the interface – including the effects of adhesion and friction, and (b) nanowear modeling of the nanometer thick carbon overcoat on TFC sliders. Moreover, these models have been implemented in simulation tools that can be used to investigate and optimize practical design parameters, such as size, geometry, roughness etc. The proposed work specifically aims to include thermal (HAMR) and morphological effects (BPMR) to the air bearing, dynamic microwaviness and contact and wear models. Experiments and molecular dynamics simulations will be used in conjunction with the computational work to verify the veracity of the models and measure model inputs such as roughness and material properties, as well as lubricant response to shearing. The resulting simulation tools would be provided to ASTC member companies for use in design optimization in an effort to achieve 2-10 Tbit/in² recording densities.
A. Subject of research and relevance to issue(s) to be solved.

1. Complete description of the research matter and its connection with ASTC stated goals

A combined HAMR-BPMR system may be the answer to further increasing the recording density in magnetic storage systems to 2-10 Tbit/in². However, both HAMR and BPMR technologies present enormous challenges in their realization. On one hand, the coupled effects of thermal, mechanical and contact with friction relevant to HAMR are not well understood nor modeled. Furthermore, BPMR poses challenges that directly affect/relate to tribology and involve the interaction of patterned media with TFC sliders that will operate in the fully flying or light contact recording regimes; These need to be clearly understood and modeled to enable success of such high recording densities.

Recent technological advances towards making HAMR a reality, describe a typical realization of this technology that involves sub-100 nm “rectangular pad” (as part of a lollipop-shaped Near-Field Transducer-NFT) that provides the necessary heating to enable bit-writing on high coercivity media [1]. This small protruding part will need to come to near contact and possibly contact with the rotating media for reliable high areal density recording. Compared to conventional recording with TFC technology, where the protruding bulge may experience sliding contact (mechanical stresses), in the case of HAMR, there is the additional complexity of transferring heat through the NFT to increase the temperature of the magnetic media to 400 °C during nanosecond-duration pulses. Understanding the dynamic thermomechanical interaction of the NFT with the rotating media and the effect of thermomechanical stresses on the NFT and media layers, as well as identifying the main failure modes is critical for robust HAMR design.

BPMR systems require extremely tight lithographic bit placement accuracy and a narrow size distribution to achieve good write synchronization between the recording head and the patterned media. Technologies have been proposed for fabrication of highly uniform magnetic dot patterns over large areas, while a narrow switching field distribution of the magnetic dots is critical to ensure exact bit addressability without overwriting adjacent bits [2]. Recent research suggested methods, such as simultaneously detecting the position and timing error, that would address the issues of position signal generation and timing recovery [3]. However, the tribological aspects of BPMR technology have not been sufficiently investigated. The modeling of possible contact between TFC technology sliders and bit-islands on the disk (or a planarized form of them) would require sophisticated contact models that would account for the inherent discontinuities at the interface both statically, and in a dynamic setting where disk vibrations could be detrimental to system performance.

Coupling HAMR with BPMR technologies would further complicate matters. The main issues that would need to be addressed in such systems are the thermal effects on the flyability and morphology of the interface, arising from changes in the air bearing and coupled structural deformations of the slider and disk, and the stresses present during possible contact with friction, especially in the presence of dynamics and a molecularly thin lubricant layer. Sufficient understanding of these complexities would allow for the design and optimization of HAMR/BPMR systems that would perform with stability and controllability to achieve recording densities of 2-10 Tbit/in². Note that based on our cooperation with the magnetic storage industry, it is our understanding that the critical need is not as much on the air-bearing simulation (which is still very important and needs further development) but on the nanocontact and wear mechanics, including thermal and topographical effects. Once such models are available they could be implemented
in existing proprietary air bearing codes (as was done in our past collaboration for op-shock impact, for example). The proposed research falls under the HAMR no. 4 Topic (HAMR Media Lubricant, Media Overcoat, and HDI), HAMR no. 12 Topic (Interaction of HAMR with BPMR) and BPMR no. 9 Topic (HDI Tribology for BPM).

2. Proposed research approach

a. Experimental

Flyability experiments have verified the applicability of our contact model in predicting the nonlinear behavior of TFC technology sliders, especially close to light contact with the disk [4, 5]. Several parameters and inputs to our model were experimentally measured. These include the dynamic microwaviness (DMW) of the disk, roughness parameters, hardness and contact damping coefficients, and lubricant stiffnesses. For the latter, we have used the results of dynamic shearing experiments to calculate the lubricant forces as functions of separation and shear rate (recently submitted paper).

A combined HAMR/BPMR system will need to include thermal effects; hence, we propose to perform experiments to measure some of the input parameters to our model as well as verify its predictions.

i. We will perform detailed surface characterization and modeling of BPMR media. This work will provide improved topographical and dynamic microwaviness measurements. Working with the Nano-CEMMS center (http://nano-cemms.illinois.edu) at the University of Illinois we can obtain patterns to experimentally validate our contact models.

ii. Using the specialized sub-nanometer indentation systems (described below) we will measure the nanomechanical properties of the layered surfaces and examine their relationship to contact and wear. The measurements will be done at temperatures up to 400 °C (relevant to HAMR).

iii. Perform controlled nanofriction and nanowear experiments on provided or fabricated samples to investigate/validate the contact and wear models.

iv. In a separate National Science Foundation supported project titled “Synthesis and tribological behavior of metal diboride-nitride coatings: Optimizing the hard and compliant response,” along with Prof. Abelson we have been developing ultra-hard thin films and we will experimentally explore such films as a 1-2 nm thick films for magnetic storage.

v. Flyability experiments will be performed using ASTC-provided samples (if available) to investigate the effects of operating parameters, including roughness, dynamic microwaviness, slider geometry and dynamics on the flyability and reliability performance. These experiments will also be used to validate the improved analytical models proposed in this work. We have strong interactions and collaborations with the magnetic storage companies as well as DSI. Another option is that such experimental studies be done in collaboration/by our collaborators at one of the companies and publish the results together (as we have done in the past).

b. Computational

We have developed simulation tools and published our work on the modeling of TFC technology for extremely high density recording [4, 6]. Furthermore, we have recently published a model of the normal and shear forces developed during contact with molecularly thin lubricant (MTL) layer present on HDD disks [7]. We have recently proposed a comprehensive MTL contact model that includes improved formulations of adhesion and accounts for the contribution of the MTL layer to contact and friction. Also, current work aims to extend our dynamic model to three degrees-of-freedom (with slider pitch and roll
motions). Hence, our computational capabilities allow for accurate modeling of TFC technology sliders and the optimization of their performance for flyability and reduced contact [6]. As discussed below this work has been funded from a European research grant. Another significant body of work, relevant to the proposed research, is our recent work (sponsored by several magnetic storage companies) is (a) modeling and experimental validation of sliding/scratch of actual modern perpendicular recording media explaining both physical and magnetic erasures and (b) modeling of nanowear occurring on the overcoat material of a TFC slider in contact with “thermal/rigid” asperities (no temperature effects were considered).

In this research, we propose to build on our present models for HAMR/BPMR technology to create simulation tools that could be provided to ASTC member companies for internal use (such as integration on their own air bearing codes).

vi. Thermal effects will be incorporated into the contact modeling (and air bearing model) and coupled with structural deformations of the components. Similar to what happens with TFC technology systems, the applied heat is expected to increase the air bearing forces in the vicinity of localized heating, while, in addition to slider deformations (i.e. the TFC bulge in TFC technology sliders), heat applied through the NFT is expected to change disk morphology. Because structural deformations would be coupled to the air flow, we propose to combine the FEA modeling of BPMR [8] and smooth disks with an air bearing solver that would yield air bearing response as a function of various NFT and other parameters (thermal spot size, magnitude, and gradient).

vii. We propose to perform FEA work on the modeling of BPMR media sliding contact (thermomechanical model) for use with the dynamic contact model. Quasi-static results of spherical contact, friction and adhesion forces with respect to separation could be extrapolated into a rough surface contact model [9, 10]. The resulting model would include the effect of Bit Aspect Ratio and media grain size.

viii. BPMR media will also contribute dynamically to the system. Hence, we propose to include the effect of BPMR morphology into the dynamic microwaviness that serves as the dynamic input into our model and compare these to experimentally measured values.

ix. Once we have reliable contact/friction/yield models then we can work on a nanowear model.

x. The proposed simulation tools will use a systems approach for the investigation of component performance to understand and optimize their design.

xi. The 3-DOF model currently under development will allow for more realistic results such that the effect of the skew angle on flyability and contact will also be investigated thoroughly.

xii. The resulting simulation tools would allow for the variation of different system parameters to observe their effect on flyability (clearance and vibrations) and contact. Contact is possible with HAMR and BPMR; hence, our model will be able to accurately characterize the severity of contact and wear at the interface as per previous work [4]. The model will not depend on arbitrarily selected parameters, but will use physics-based formulations for the contact, friction (not dependent on assumed, constant friction coefficient) and adhesion forces – including lubricant contact – to predict system behavior while experiments and simulations will be used to define the model inputs of dynamic microwaviness and air bearing forces.

In addition to the computational (continuum) work summarized above, we propose to perform molecular dynamics (MD) simulations to investigate lubricant contact under heating effects for BPMR media. The initial purpose would be to verify the recently developed MTL model by replicating the results of dynamic shearing experiments. Specifically, given a certain lubricant morphology and treatment that would affect the percentage of molecules bonded to the substrate, we propose to perform MD simulations of an MTL layer sheared between a sphere and a rigid substrate and extract the bearing and shearing
forces acting on the sphere, both for the shearing velocities encountered in the experiments (~200 μm/s) and the very high velocities occurring in magnetic storage. Once the veracity of the MTL model is checked, heating effects can be applied and substrate morphology altered to simulate HAMR and BPMR conditions respectively.

3. Likely outcome of research

The proposed research will provide simulation tools to predict the flyability, contact and wear (reliability) of novel HAMR/BPMR systems using a mechanics and systems-level approach. The validity of these simulation tools that will make use of experimentally measured parameters as well as computational inputs (to predict air bearing and BPMR contact forces) will be verified experimentally via controlled and flyability experiments. In addition, MD simulation results are expected to verify and/or correct our continuum-based modeling approach for use within the MTL contact model. The simulation tools could be used to perform design optimization for various system parameters to improve system performance and achieve 2-10 Tbit/in² recording densities.

References


B. Resources required to perform project

a. Personnel, students, etc.: In this project we request support for a PhD student to work on the technical component of the project. In addition we will also employ one undergraduate student to support the graduate student in developing the computer codes for the contact and wear models.
b. **Equipment, lab, etc.:** The Microtribodynamics laboratory at the University of Illinois that has been funded in the past by INSIC, the National Science Foundation and several hard disk drive companies on research related to contact mechanics, friction and wear of the HDI is equipped with the following equipment that will be used in this project: (a) Atomic Force Microscope for detailed topographical measurements, (b) Flyability measurements using LDV, (c) Specialized sub-nm Nanoindentation system for measuring properties of very thin films, (d) recently acquired PicoIndetner, where indentation inside a TEM can be performed to better understand film damage and thus wear.

c. **Computational:** Illinois is home to the National Center for Supercomputing Applications (NCSA) and we have an ongoing grant/computer time for the last 7 years. We plan to use the NCSA to perform the computations related to wear, as multilayer contact simulation requires such resources.

### C. Resources other than ASTC funding dedicated to perform project

The proposer has recently secured a three year grant from the European Union (Cyprus Research Promotion Foundation) that directly supports former INSIC-supported PhD student Antonis Vakis that has been working on the contact model of TFC accounting for molecularly lubricant contact (including MD simulations) [4-7]. Antonis will continue to work on this issue and a new PhD student will be hired directly on the new project as described above. Also, the proposer has an ongoing NSF grant on HfB$_2$ coatings (along with Materials Prof. Abelson) to develop new hard coatings, with one of their application being magnetic storage overcoats. On this project two PhD students are supported (Jungkyu Lee and Andy Cloud) and their work will be complementary to this project.

### D. Resources requested from ASTC and how they will be utilized

a. **Funding: Total request of $ 70,000. Primarily to support one PhD student**

   a. **Overhead:**
      i. 56% of grad student stipend (tuition remission) $13,435
      ii. 58.5% of all costs (direct project cost) $20,877
   
   b. **Direct project cost** $35,688
   
   c. **Facility use fees (use of Center of Microanalysis of Materials for use of analytical tools such as Auger, XPS, TEM, SEM etc)** $ 2,000
   
   d. **Materials (consumables)** $ 2,018
   
   e. **Student stipends:** $ 26,070
      i. 11 months for PhD student: $ 23,991
      ii. 100 hours for Undergraduate student $ 1,000
      iii. Benefits for Graduate student $ 1,079
   
   f. **Travel (for travel by two people to the ASTC meetings)** $ 5,600

b. **Expected technical cooperation with sponsor(s): materials to be provided by sponsor(s) (e.g., targets, devices, engineering support, etc.)**

The proposer and his research team have a long history of technical cooperation with ASTC industrial partners. Tangible outcomes of these interactions include the following: (a) sponsoring of research projects by several of the ASTC members; (b) providing magnetic storage samples (standard and
specialized builds Head and Disks; (c) joint presentations in conferences; (d) joint archival journal publications (with Seagate, HGST and SISA); (e) several summer internships by graduate students at the companies and (f) several of my former graduate students employed by ASTC companies. We do plan to continue these collaborations and cooperation as we have already done in preparing this proposal. Some specifics of the proposed interactions for this project are described below (which could change depending on the constant feedback with our colleagues in the industry).

Assuming BPMR/HAMR media and components could be provided by ASTC member companies, then we will characterize these samples using unique tolls we have in Illinois and the measure parameters would be used in the contact models. Such characterization includes roughness, dynamic microwaviness and nanomechanical property measurements. If such samples are not available, then we can either obtain them from DSI (which we also have collaboration) or based on input from the member companies fabricate them ourselves for the surface characterizations. Also, to verify our contact/wear models, we would like to do both flyability experiments as well as simpler “scratch-type” experiments (for wear validation). Samples for flyability could either be provided to us to perform the test in Illinois or we can collaborate with one of the member companies to perform the tests internally (or part of an internship) and compared to our models.

To account for heating effects, we will obtain cantilever/heating tips from our collaborator Prof. Bill King (at the University of Illinois) to perform such studies, since samples from ASTC members are unlikely to be provided to us.

c. Sponsors’ facility utilization

As described above, we will use the AFM, sub-nanoindentation, Picoindeter, and flyability set ups to perform the experimental components of this work at Illinois. The only uncertainty is that the flyability experiments could be performed at one of the ASTC members, if samples could not be provided to Illinois. Note that we have, in the past, performed surface characterization (roughness, material properties and dynamic microwaviness) and flyability (clearance and vibrations) experiments in the MicroTriboDynamics Laboratory at the University of Illinois.

d. Expected students’ internships

As in the past, with the cooperation of our industrial partners, the student(s) working on this and similar projects would be available (and delighted) to do internships.

E. Timeline

The main research tenets and their expected duration are summarized in the following table.

<table>
<thead>
<tr>
<th>Description</th>
<th>Duration</th>
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<tbody>
<tr>
<td>1. Surface characterization studies (roughness, DMW, etc)</td>
<td>Continuously</td>
</tr>
<tr>
<td>2. Nanomechanical property measurements</td>
<td>Continuously</td>
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<tr>
<td>3. Contact model development for BPMR media (FEA)</td>
<td>Months 1-6</td>
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<tr>
<td>4. Contact model development for HAMR</td>
<td>Months 3-9</td>
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<tr>
<td>5. Optimization studies for HAMR/BPMR design parameters</td>
<td>Months 9-12</td>
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<tr>
<td>6. Experiments to verify contact and wear models</td>
<td>Months 6-12</td>
</tr>
<tr>
<td>7. Lubricant dynamic shearing experiments and MD simulations</td>
<td>Months 9-12</td>
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F. Home Institution and Resources

The University of Illinois at Urbana-Champaign, is ranked among the top engineering universities in the United States. The college of engineering is one of the largest colleges in the United States with 420 faculty and 170 million dollars per year in research expenditures. The Microtribodynamics laboratory has strong collaborations with major hard disk drive industries and major research centers (e.g., the Data Storage Institute in Singapore). Facilities for conducting nanoscale mechanics research, including research on the head-disk interface (HDI) of magnetic storage drives, include laboratory equipment and computational facilities capable of conducting sub-5 nm and contact HDI research. State-of-the-art experimental and computational facilities are also available for this research:

The Center for Microanalysis of Materials, F. Seitz Materials Research Laboratory: This is a DOE-supported national facility housed within the FS-MRL (http://cmm.mrl.uiuc.edu/). The PI holds a research professor appointment with MRL. It maintains an extensive set of characterization tools for the analysis of advanced materials from the atomic level to the macroscale. The instrumentation includes Auger 2-D depth profiling, RBS, UPS, XPS, STM, AFM, XRD, SEM, TEM, ToF-SIMS and FEG-TEM/STEM equipped with EDS and PEELS capabilities. The proposer makes extensive use of these facilities and there is a nominal charge (budgeted in the project). New instruments obtained by the proposer and housed at MRL include a Hysitron TI-950, a Hysitron PI-95 Picoindenter inside a TEM and specialized custom-made sub-nanometer indentation systems. Refer to the Figures below.

National Center for Supercomputing Applications/National Computational Science Alliance: State-of-the-art supercomputing facilities that are available to UIUC faculty with no-cost internal proposals. We are currently using these facilities to HDI contact and nano wear.

AFM, sub-nanoIndenter systems integrated with a multimode AFM and stand alone, Hysitron TI-950 TriboIndenter (includes high temperature stage (400 oC)), Hysitron PI 95 TEM PicoIndenter
G. Biographical sketch of researchers

Andreas A. Polycarpou received his PhD from the State University of New York at Buffalo in 1994 in Mechanical Engineering. His specialization is in the fields of tribology, nanotribology, nanomechanics, and nanomechanical properties with applications to conventional engineering systems and miniature devices such as microelectromechanical systems and magnetic storage hard disk drives. Dr. Polycarpou has published extensively in the abovementioned research areas and his portfolio includes over 130 peer-reviewed journal papers, many dozens of conference papers, numerous patents and dozens of invited lectures. Dr. Polycarpou has won numerous national and international awards, such as the ASME Burt L. Newkirk Award (2001), the NSF Faculty CAREER Award (2003), the Xerox Award for Faculty Research (UIUC, 2005, 2007), the STLE Edmond E. Bisson Award (2007), a Fulbright Scholarship, The J. William Fulbright Foreign Scholarship Board, Cyprus (2007), the ASME K.L. Johnson Best Paper Award in Contact Mechanics (2007) and the STLE Walter D. Hodson Award (2008). Dr. Polycarpou is an Associate Editor for the ASME Journal of Tribology (2005-2011) and on the Editorial Board of Review of Scientific Instruments (2006-2009) and Microsystem Technologies (2006-2009). He has been funded from INSIC, and many of the magnetic storage companies with focus on the contact mechanics, friction and wear of HDI, including roughness effects, multi-layer film structures and dynamic effects.

Antonis I. Vakis is a Ph.D. candidate in the Mechanical Science and Engineering Department of the University of Illinois at Urbana-Champaign. He works on nanoscale tribology with emphasis on application to magnetic storage at the Microtribodynamics Lab under Professor Andreas A. Polycarpou. His work is currently funded through a Young Researchers of Cyprus (PENEK) Grant administered between the University of Illinois and the University of Cyprus. Through this grant he currently also holds the position of Researcher at the Department of Electrical Engineering of the University of Cyprus. He has also taught the course ME371: Mechanical Design II as an Instructor, for which he received the Mechanical Science and Engineering Alumni Association Teaching Fellow Award. Mr. Vakis has thus far authored 4 peer reviewed journal papers and 3 conference papers for his current research. He received his M.S. Degree in Mechanical Engineering from the University of Illinois in 2008 for his work on the biomechanical modeling of trap-jaw ant mandible strikes, for which he co-authored 1 peer reviewed journal paper and 1 conference paper. He studied at the New Jersey Institute of Technology between 2002 and 2005, where he earned his B.S. Degree in Mechanical Engineering – graduating Summa Cum Laude – during which time he was a CASP (Cyprus-America Scholarship Program) Fulbright scholar.