



Multi-functional Extreme Environment Surfaces: Nanotribology for Air and Space

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Nanostructured Multi-functional Surfaces Enabling Air and Space Tribology*

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Specialty

Nanotribology
Computational Tribochemistry
Computational Nanotribology
Nanomaterials Design
Material Physics & Coatings
Cryotribology
Cryotribology & Coatings
Computational Nanocomposites

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Specialty

Microtribology & MEMS
Tribocoating Analyses
Aerospace Tribocoatings

Industrial Partners

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Specialty

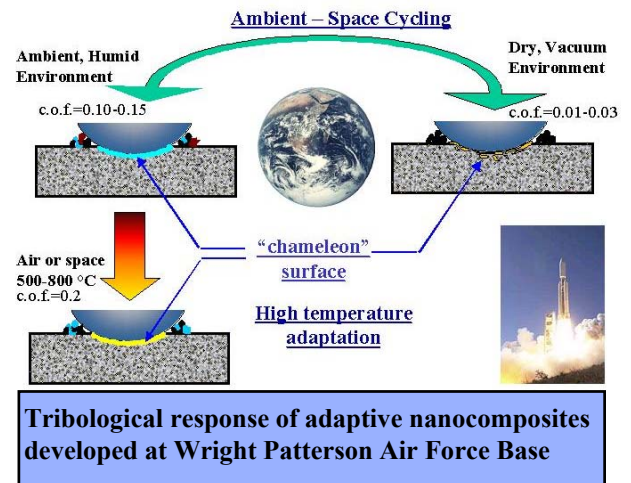
Space Materials Tribology
RF MEMS

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Executive Summary

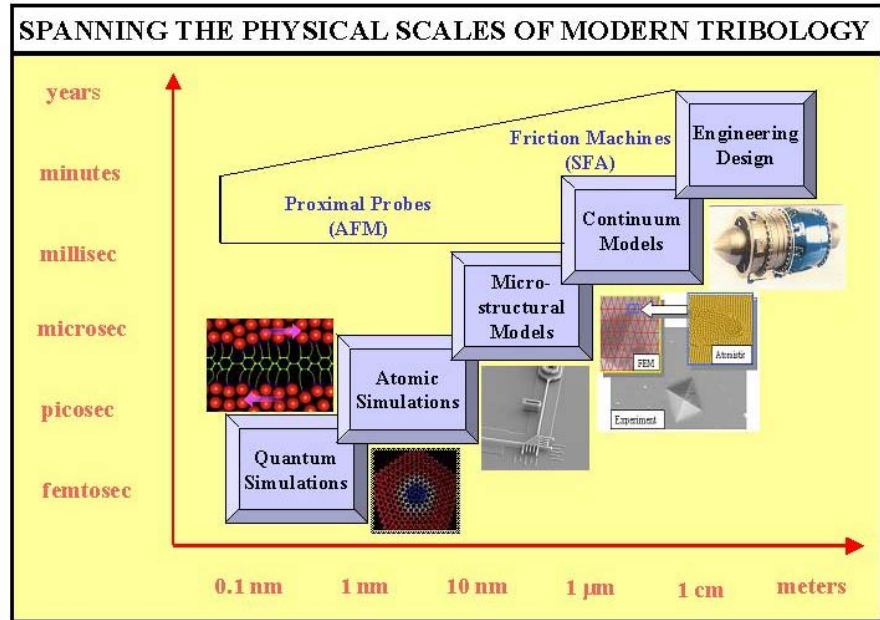
Tribological issues such as friction and wear are currently the limiting factors in the development and commercialization of a myriad of enabling technologies for advanced air and space applications, with surfaces and lubricants frequently being the weakest link in overall system reliability and performance. While no single lubricant/coating has been identified that can withstand the entire range of extreme environments encountered by these systems, multi-functional nanocomposite materials may be able to withstand such debilitating tribological conditions. Their widespread implementation will be limited, if not impossible, however without tribological design rules that are integrated with system design. To this end, we have assembled an unparalleled team of experts with wide ranging backgrounds but one common goal: Solution of Air Force/DoD and commercial tribological problems deemed paramount, while concomitantly training personnel and collaborating closely with Air Force researchers to carry forth these solutions in DoD and industrial settings. The following themes underlie our proposed work:



- **Nanosopic coating architectures:** Our team will prepare a wide variety of system architectures, include nanocomposite blends of materials that provide properties that are usually considered mutually exclusive, bound plus mobile phases, self-healing systems, fortified tribological materials, graded compositions and nanotribologically mobile systems.
- **Experimental-Modeling:** Our modeling team has pioneered new computational methods such as accurate interatomic force expressions, first principles/mesoscale defect strategies, and physically based finite-element defect/failure models. Our combined experimental and modeling capabilities allow closely coupled investigations over concurrent length scales, from the atomic to macroscopic scale.
- **Realistic, Real-time and Accelerated Test Methods:** Our test set-ups are designed to reveal the scientific basis for tribological performance of materials, focusing on thermal, chemical, and nano-dynamical attributes. Surface coatings' properties will be explored over a range of scales and operating conditions that span aircraft to molecular scale applications, cryogenic to high temperatures, and vacuum to moist/dry air environments. Highly innovative and unique test-devices will incorporate advanced characterization tools for accelerated identification and quantification of material failure mechanisms and will lead to new DoD performance measures to prevent failure.
- **Student training:** Upwards of thirty undergraduate, graduate and post-doctoral assistants will be immersed annually into a multi-disciplinary research environment, gaining unique perspectives on the insertion of new technology into defense mission applications. Many will train on-site in DoD, DOE, and industrial settings as part of their research activities.

Deliverables include a new generation of design rules and new multi-functional coatings of appropriately scaled and blended constituents to be custom tailored for operation in extreme environments, accompanied by a fundamental understanding of the scale-dependent mechanisms that control their performance, as well as new accessibility to the nascent field of **cryotribology**.

Statement of Work: Our MURI team consists of three highly overlapping sub-groups focusing on air, space, and MEMS applications. Our overarching objective is to establish the **scientific foundation** of the tribological properties of multi-functional surface treatments in terms of scale-dependent thermal, chemical, and mechanical processes. We will employ the knowledge gained to introduce a **new generation of multi-functional coatings** comprised of constituents that are optimally scaled and blended for life-cycle service in the extreme environments associated with air, space and MEMS applications. To accomplish these goals, our team will combine methods for synthesizing advanced materials, highly innovative and **unique test-devices**, and predictive **multiscale modeling** to identify and exploit the critical physical mechanisms that underlie the successful performance of structures, for service in a widely varying range of extreme environments. This **strong coupling between synthesis, testing, and modeling**, which is a **hallmark of our team**, will provide unprecedented new scientific insights and engineering capabilities not possible through individual efforts. Our proposed work spans all length and time scales of modern tribology.



The specific tasks to be performed are as follows:

Thrust I: Terrestrial Applications - High Temperature & Moist/Dry Air Environments

(Ia) Synthesize nanocomposite blends of materials, including WC-WS₂ in diamond-like carbon and MoS₂ in Al₂O₃, that exhibit adaptive/smart abilities to lower friction and resist wear through environmentally induced changes in surface chemistry.

(Ib) Perform *in situ*, real-time characterization of tribocontact materials evolution with a Raman tribometer, to document in-use tribological performance at the mesoscale, and to establish fundamental lubrication mechanisms beyond the materials processing stage.

(Ic) Perform *in situ*, real-time imaging studies of tribocontact materials by means of scanning probe-quartz crystal oscillator combinations in a variety of extreme environments, to document in-use tribological performance at the nanoscale, and to establish fundamental lubrication mechanisms beyond the materials processing stage.

(Id) Utilize a multi-scale modeling hierarchy that couples first-principles structure and dynamics at the atomic scale, large-scale molecular dynamics simulations at the submicron scale, and macroscopic-scale advanced finite element modeling, to guide experiments, by accurately predicting materials systems with custom tailored properties for specific applications.

(Ie) Expand current modeling capabilities to allow for humid environments, by adding oxygen atoms in addition to hydrogen in existing molecular dynamics codes to form water molecules.

(If) Utilize specialized finite element microstructural modeling of nanocomposite and nanocrystalline materials to examine the impact and interrelation of grain-size, interface strength, and grain boundary sliding on macroscale deformation, wear, and failure modes.

Thrust II: Space Applications - Cryogenic and Vacuum Environments

(IIa) Synthesize diamond film nanocomposite coatings, to increase the tribological operating temperature range of conventional hard carbon-based coatings by 100's of degrees.

(IIb) Obtain comprehensive measurements of static and sliding friction coefficients on well-characterized interfaces over the temperature range 4 – 1100 K, to characterize fundamental physical materials mechanisms and establish the foundations of cryotribology.

(IIc) Perform on-chip MEMS tribometer measurements of well-characterized interfaces, for direct comparisons with atomistic modeling efforts, and measures of low-contact stress geometries characteristic of space applications.

(IId) Perform parallel studies with lateral force microscopy to provide information on shear strength, static and sliding friction, and adhesion over wide-ranging length scales.

(IIe) Perform large scale molecular dynamics simulations coupled to finite element continuum methods to model surface dynamics, energy transfer mechanisms, lubrication modes, chemical wear, and contact stresses spanning the atomic to the micron scale.

(IIIf) Perform Quartz Crystal Microweighing (QCM) mobility studies of bound plus mobile phases to document nanodynamical behavior of candidate lubricates at picosecond to nanosecond time scales that directly overlap with the modeling efforts.

Thrust III: Silicon and RF MEMS Contacts

(IIIa) Perform silicon MEMS tribometer measurements of static and sliding friction coefficients from 4-700K in controlled environments, to assess lubricant performance in realistic conditions.

(IIIb) Identify bound plus mobile phases of self-healing and nanotribologically mobile lubricants for silicon MEMS that resist decomposition at high temperature in variable atmospheres.

(IIIc) Synthesize polycrystalline silicon films with improved tribological performance and to provide silicon sample materials for accelerated test set-ups such as the QCM.

(IIId) Synthesize electrically conducting multifunctional materials, based upon noble metal alloys, with nanoparticle dispersion strengthening (nanodiamond, oxides and nitrides), that significantly extends the range of operating conditions for RF MEMS switch applications.

(IIIe) Investigate RF MEMS switch performance in a variety of environmental conditions and at cryogenic temperatures, to single out, separate and identify contact failure mechanisms.

(IIIIf) Investigate the mechanical and electrical evolution of RF MEMS switch contacts by means of scanning probe microscopy, to gain nanometer scale topological and mechanical and contact resistance information at various stages of contact lifetime.

(IIIg) Perform first principles molecular dynamics simulations of sliding interfaces (both silicon and conducting nanocomposites), to characterize trends and specify energy transfer and failure/wear mechanisms as a function of surface termination, surface roughness, load, relative velocity, near-surface structure, nanoparticle volume fraction, and particle-matrix interactions.