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Tribology

Low Friction Mechanisms of Solid Lubrication Film Formed by In-situ Tribo-coating

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Solid lubrication film formed by tribo-coating, which deposits a solid lubricant by evaporation to the contact interface during friction in vacuum, gives low friction coefficient below 0.03 that can not be observed by any other solid lubricants of soft metals in vacuum (Fig. 1).

Such superior friction properties are achieved by the combination of silicon nitride pin, stainless steel (SUS440C) disk and indium as lubricant. The tribo-coating film formed on the silicon nitride pin has nano-order composite structure which the crystalline indium of nano size are distributed in an amorphous matrix of silicon oxide and chromium oxide (Fig. 2). Because of the nano composite structure, a very thin indium film is formed without break down like conventional pre-coated thin film. The thinner indium film can give smaller value of friction coefficient than that of conventional solid lubricant.

In this presentation, unique tribological properties and structure of tribo-coated film are introduced. And the formation mechanism and low friction mechanism of the tribo-coated film are discussed.

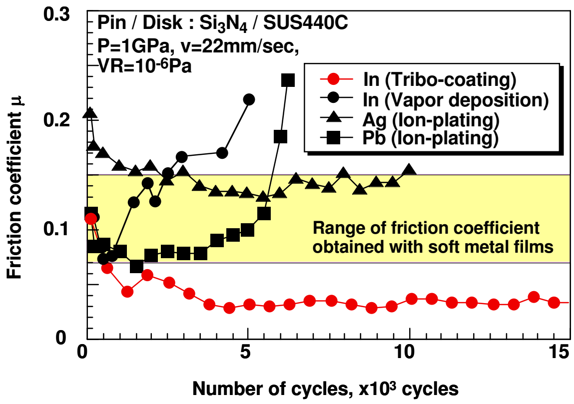
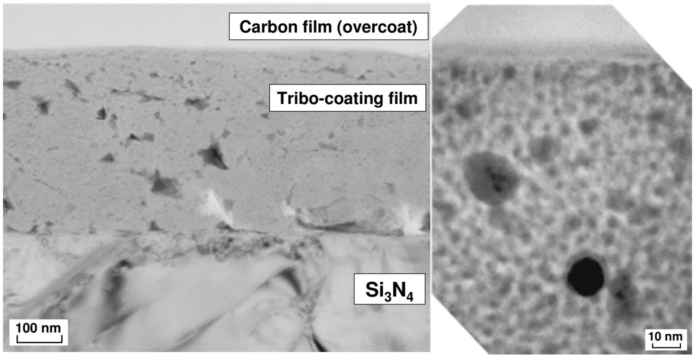


Fig. 1 Comparison of friction properties of tribo-coated In film and conventional soft metal films.



(a) (b)

Fig. 2 TEM images of the tribo-coated film formed on the pin surface in frictional pair of Si_3N_4 pin/SUS440C disk.

Super-low Friction of Carbon-based Coatings in Inert Gas

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Carbon-based coatings such as carbon nitride (CNx) coatings exhibit a wide range of very attractive properties such as low friction and wear, good thermal and chemical stability which make them very suitable for demanding mechanical applications.

In sliding of CNx-coatings in inert gas stream and/or atmosphere, it provides super low friction as show in Fig. 1. If the running-in process is taken place in oxygen for the initial sliding cycles, the following sliding in nitrogen gas gives the friction coefficient bellow 0.005 as shown in Fig. 2.

The beneficial effect of inert gas on reducing friction of carbon-based coatings is much more enhanced by selection of counter material, coating condition, surface roughness of the coatings, atmospheric humidity and running-in condition, which is pre-sliding before introducing inert gas to the sliding interface.

In this presentation, comprehensive overviews of the unique lubricious effects of "Inert gas" on friction with carbon-based coatings are introduced. And the mechanisms of low friction of CNx observed in inert gas are proposed. Finally, based on those attractive results high potential of carbon-based coatings for future successful tribological usage by controlling atmospheric gases is discussed.

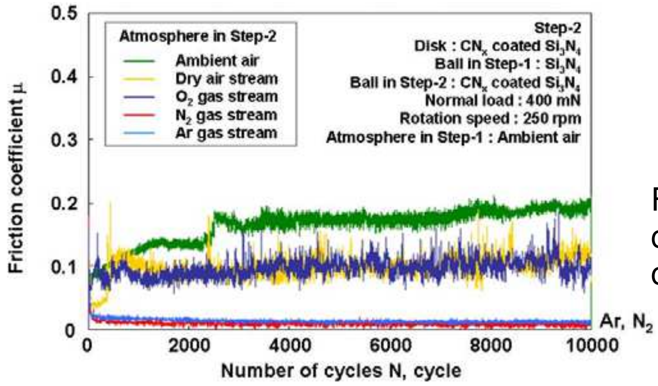

Fig. 1 Effect of atmospheric condition on friction of CNx coating slide against itself.

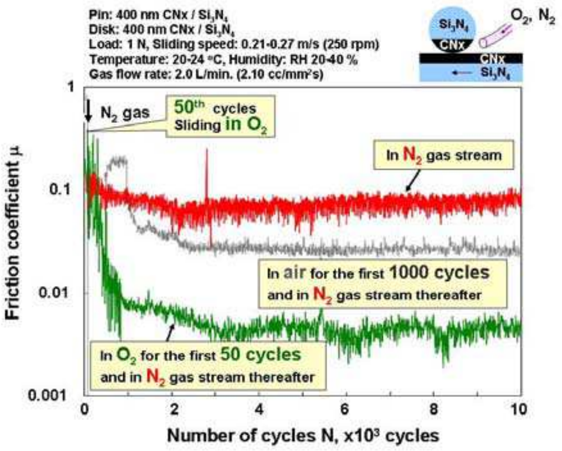

Fig. 2 The reduction in friction coefficient by supplying nitrogen gas at the first cycle in air, 100^{th} cycle after running-in in air , and 50^{th} cycle after running-in in oxygen stream in CNx/CNx.

Influence of a sliding velocity dependent friction law on the coupled effect of friction and surface roughness on shallow spherical nanoindentation

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ABSTRACT

Surface effects stemming from surface roughness and friction can become important in shallow indentation depths, potentially resulting in the variation of nanoindentation results. A numerical study is conducted aiming at a more complete understanding of the coupled influence of friction and sample surface roughness in nanoindentation of pure nickel, using a slip rate dependent friction law. Results confirm the strong interaction between these two contributions of surface effects, and their cumulative effect leads to significant variations in both the indenter load vs. displacement curves and in the evaluated elastic modulus.

1. Introduction

Nanoindentation is in principle a nanoscale hardness test, which results in a continuously sensed indenter load vs. indenter displacement curve from which the elastic modulus of the sample is derived using post–treatment methods. The nanoindentation response is composed of various contributions among which the geometry of the contact, and the contact interface behavior (both difficult to control experimentally) can play a significant role.

Generally only an estimation of the frictional behavior is given and its influence on the output data is unknown. The surface roughness of thin films can become comparable to the indenter penetration, especially when shallow indents are imposed to avoid spurious effects of the substrate[1]. In such configurations, surface effects related to the sample surface topography[2] and friction[3] are the most pronounced, potentially resulting in variations of the evaluated material parameters, which may wrongly be attributed to the thin film mechanical behavior.

This motivates numerical modeling efforts with the goal to investigate the influence of friction and its variation in indentation problems. Even though friction is naturally coupled with the effect of surface roughness in the experiments, numerical works analyzing both surface effects simultaneously are rather scarce[4], to the best knowledge of the authors. Findings using a Coulomb friction law suggest that the coupled effect of surface roughness and friction can be partially responsible for the dispersion otherwise attributed to the tested material behavior, or other sources of nanoindentation scatter[4]. As a general conclusion it can be shown that friction gives an important contribution to the physics of rough surface nanoindentation, therefore its significant interaction with surface roughness and its contribution to the energy balance of indentation should be accounted for in a thorough numerical analysis.

The motivation of the present numerical work is to confirm these trends with a more complete description of the contact interface behavior, using a sliding velocity/slip rate dependent (SRD) friction approximation.

2. Numerical Model of Nanoindentation

Considering the complex physics which governs friction, the use of a single, constant coefficient of friction convoluting all friction related effects, may result in an exaggerated simplification for the representation of tip friction and potential stick–slip phenomenon. Experimental proof of slip rate dependent frictional behavior in conditions comparable to nanoindentation (contact pressure in the order of several GPa, sliding velocity of some nm /s induced by the plastic deformation of the sample material) is apparently scarce. This may be partially due to the particular contact conditions that are difficult to reproduce in other setups on this scale, such as nanoscratching. In numerical simulations however, the different contributions can be easily investigated separately to evaluate the potential influence of SRD friction on nanoindentation results. As a first extension of previous works[4], a SRD frictional behavior is included here using a simple bilinear evolution law of the coefficient of friction (Fig.1).

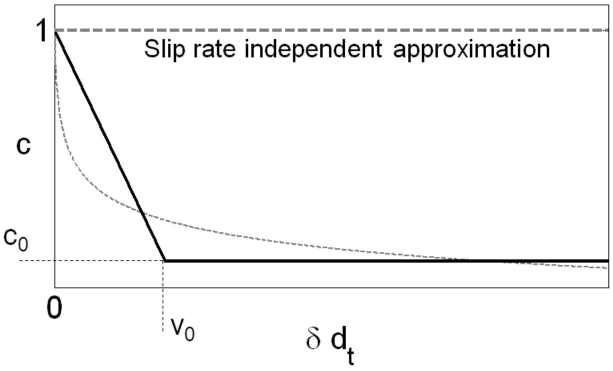

Figure 1: Simplified bilinear approximation of the evolution of the coefficient c multiplying the static coefficient of friction, μ_{static} = 0.5, as a function of the slip rate, δd_{t}, (thick solid line). v_0 = 2nm /s and c_0 = 0.4 stand for the cutoff slip rate of the velocity–weakening portion and for the constant value for slip rates larger than v_0, respectively.

The indentation setup (cube corner nanoindentation of pure nickel in 45 nm depth with a loading sequence of 5 s–5 s–5 s loading, holding and unloading time, respectively) is the one studied in[4], to allow a straightforward comparison with the previous results. Pure polycrystalline bulk nickel is modeled as an elastic–viscoplastic material[4]. The spherical part of the indenter tip is modeled as a rigid spherical body of 100 nm radius. For each studied case, different 2D finite element meshes of 8 noded quadratic quadrilateral elements with an axisymmetric modeling assumption were used. The bottom nodes of the mesh are prescribed a horizontal planarity condition and the side nodes of the model are blocked in the radial direction.

$$\Delta E = \frac{E_{\mathrm{eval}}}{E_{\mathrm{ref}}} - 1 \tag{1}$$

Two post-treatment methods[5,6] are applied to evaluate the variation of the resulting elastic modulus with respect to the reference indentation of a flat, frictionless surface (Eq.1).

3. Slip Rate Dependent Friction in Rough Surface Nanoindentation

The surface roughness, inspired from an experimental surface scan, is chosen to have a relatively simple representation here, considering only four levels of a protuberance–on–protuberance type roughness description. The surface profile depicted in Fig.2 is described by the sum of four sine functions with different amplitudes, wavelengths and phase shifts (increasing amplitudes are associated to increasing wavelengths).

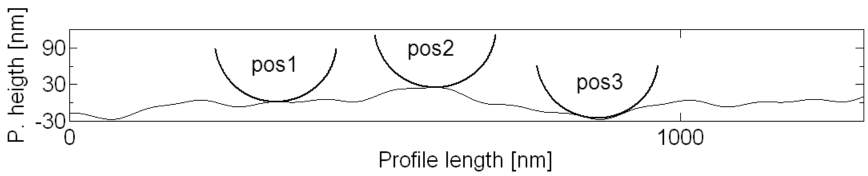

Figure 2: Representation of the surface roughness profile.

Three different indentation positions are considered (Fig.2) with an indentation depth of 45 nm after initial contact. Surface roughness can have a twofold effect resulting in either a higher or a lower peak load (Fig.3) and contact stiffness (Oliver and Pharr results in Fig.4), whether the indentation is performed in a roughness valley or on the tip of an asperity, respectively.
Friction results in a general increase in the load level with respect to the frictionless case, coupled to displacement bursts when using SRD friction (Fig.3). When indenting the highest peak (position 2) the overall effect of friction is the smallest, and no displacement burst appears. Conversely, when indenting in the deepest valley (position 3) frictional effects are the most important and up to 5 displacement bursts, increasing in length with increasing load are observed. When activating friction, the dispersion in nanoindentation results shows a general increasing trend for both Coulomb (μ = 0.5) and SRD friction approximations. This is due to the topography dependency of the frictional effects, illustrated in Fig.4 by the varying increase in the evaluated elastic modulus with respect to the frictionless case. This non–homogeneous and topography–dependent variation caused by friction results in a general increase in the average value of the evaluated elastic modulus. Even though adding the SRD frictional behavior can have a significant influence on the potentially induced displacement bursts, it affects to a lesser extent the evaluated elastic modulus, with respect to the values obtained for the Coulomb friction approximation (up to roughly 10% increase is observed).

4. Conclusions

Results confirm that neglecting frictional and surface roughnes effects may be a debatable assumption when the indentation depth becomes comparable to the size of the surface asperities. The cumulative effect of friction and surface roughness on the dispersion in nanoindentation

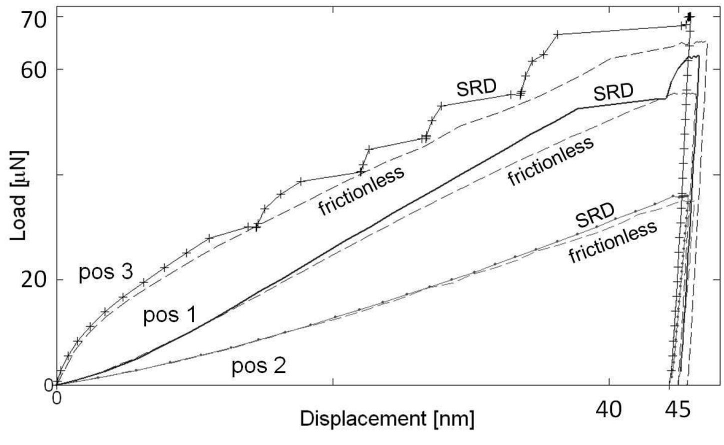

Figure 3: Computed load–displacement curves.

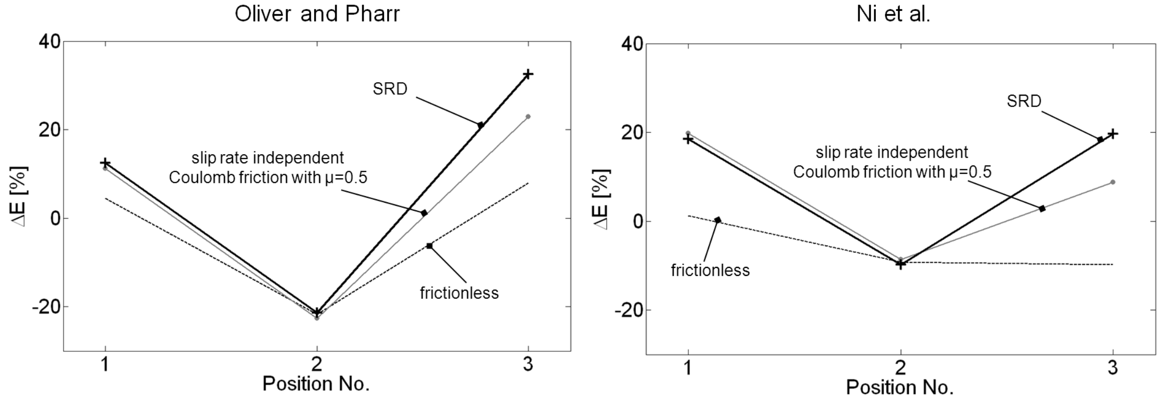

Figure 4: Variation of the evaluated elastic modulus as a function of the indentation position.

results was confirmed in this set of simulations for both slip rate dependent and slip rate independent friction approximations. Considering friction in a numerical model with roughness increases the scatter because of the high sensitivity of the frictional effects on the contact geometry, resulting in an additional variability of the results.

Slip rate dependent friction may generate displacement bursts in the loading curves in some cases. This effect is potentially related to the velocity–weakening behavior of the postulated friction law and the induced a stick–slip phenomenon. Taking slip rate dependent friction into account can lead to potential convergence issues and high computational cost. It was observed to play a particularly important role when the stick–slip behavior of the contact is in the focus of the study, and it also results in an increase in the dispersion of the evaluated elastic modulus with respect to a Coulomb approximation.

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The influence of particle shape on granular lubrication

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Conventional liquid lubricants fail to perform adequately in extreme environments, i.e. at high temperatures and loads. As an example, modern turbine engines require bearings which can operate at up to 800 °C under loads of several MPa at relative velocities of up to 50 m/s. Granular lubricated bearings are promising candidates for such applications [1]. Figure 1 depicts a granular lubricated contact. In order to provide a bearing capability, the function of the grains is threefold: First, they separate the 1st and 2nd body. Second, they transmit load between them. Third, they accommodate the relative velocity.

Experimental and numerical research on granular lubrication has been conducted over the past two decades [1]. The discrete element method (DEM) has proven to be a powerful simulation tool to relate microscopic grain properties to the macroscopic lubrication behaviour [2]. So far, the grains have been modelled mostly as spheres while the granular contact properties such as adhesion and coefficient of restitution were varied [3,4]. In the present study, we focus on the influence of grain shape. Rod-like and plate-like shapes with varied aspect ratio are compared to spheres with respect to load transmission and macroscopic friction coefficient.

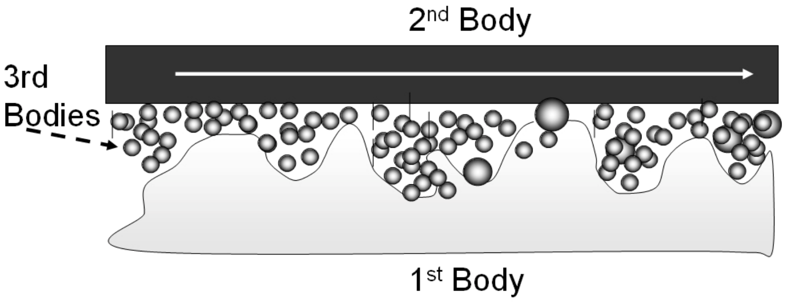

Figure 1: Schematic of a granular lubricated contact. The grains act as 3rd bodies between the 1st and 2nd body in relative motion. From: http://www.me.cmu.edu/faculty1/higgs/powder.html

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Compressible kinematic modeling of granular flow

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Discrete Element Method (DEM) simulations are used to obtain detailed velocity and volume fraction distributions of a granular material which discharges from a hopper due to gravity (see Fig. 1a). A comprehensive theoretical framework for granular flow in this regime is not yet discovered. Yet, a continuum approach to describe the velocity field is given by *kinematic modeling* [1-3]. It constitutes a partial differential equation for the vertical velocity component v_z using a coupling constant B which has the unit of length,

$$\frac{\partial v_z}{\partial z} = B\frac{\partial^2 v_z}{\partial x^2}\,.$$

This model is comparably simple as it requires merely B as a fitting parameter. However, measured velocity fields can only be described with moderate accuracy. In the present work, the basic kinematic modeling assumption of incompressibility of the granular material is replaced by explicitly considering the volume fraction field in the hopper (see Fig. 1b). Consequently, the extended approach is referred to as *compressible kinematic modeling*. It is found that B is a monotonically increasing function of the local volume fraction up to 95% of the maximum volume fraction of the system (see Fig. 1c). The only relevant length-scale in the vicinity of the hopper orifice is the width of the orifice. Thus, B scales with the size of the orifice.

It is demonstrated, that the proposed compressible kinematic modeling is able do reproduce the DEM velocity profiles at a high level of detail. Thus, an improved continuum description of granular flow is given by the present work.

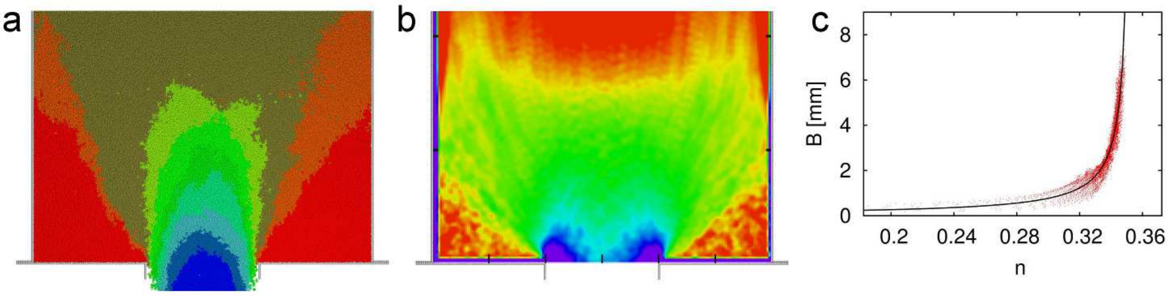

Figure 1: Color coded velocity magnitude (a) and volume fraction (b) distributions from DEM simulations; blue means high velocity/low volume fraction and red means low velocity/high volume fraction. (c): Kinematic modeling parameter B as a function of the local volume fraction n.

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From atomic membranes to molecular adsorbates: How interfacial atomic structure influences nanotribology in carbon-based systems

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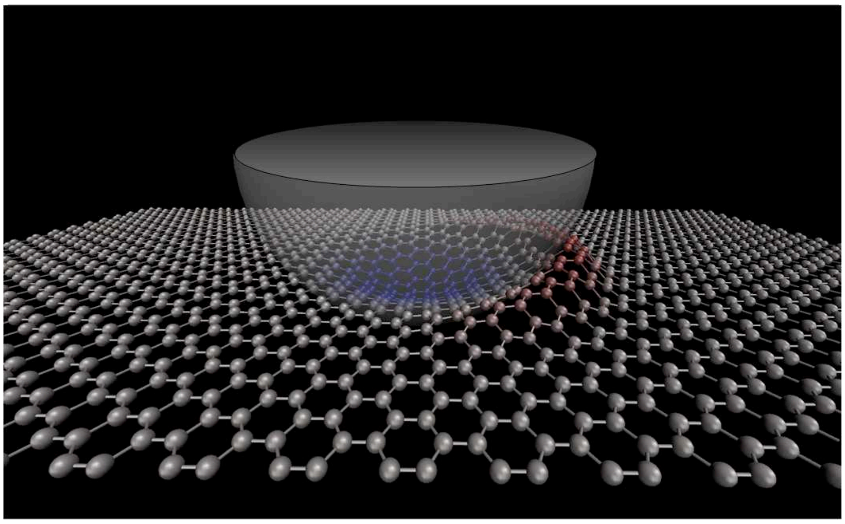
Many carbon-based materials, including diamond, carbon nanotubes, diamond-like carbon (DLC), graphite, and graphene, exhibit unusual and extreme material properties. The tribological behavior of these materials is no less interesting: diamond can function as an abrasive or a solid lubricant; DLC can exhibit extremely low macroscopic friction, yet shows rather high nanoscale friction; DLC has lower friction when dry, while diamond has lower friction when wet. I will briefly review some of the important and at times contradictory behavior that is seen in these materials. I will also mention the application areas where these materials can be applied. I will then focus on the atomistic origins of two particularly interesting effects: (1) the critical environmental sensitivity of friction and wear for diamond interfaces[1]; and (2) the unusual stick-slip friction behavior seen in thin graphene sheets[2].



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Interface Friction in Carbon-Nanotube/Diamond Nanocomposites

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Diamond/carbon-nanotube nanocomposites have a broad range of applications because of the exceptional mechanical properties of both matrix and fibers. The interface plays a key role in determining strength and toughness of ceramic composites, and so here we use molecular dynamics to examine interface adhesion and friction in this system. As expected to arise during processing, interstitial C atoms are placed at random positions between matrix and CNT in order to capture interface adhesion and remaining dangling bonds are terminated with H. We use the modified C-C REBO potential introduced by Pastewka and coworkers that includes an environmental screening coefficient to better capture bond breaking and reforming of C-C bonds, and extend this to C-H. The deformation of the interface, and the pullout forces, are investigated during quasistatic pullout of the carbon nanotube as a function of the percentage of interstitial atoms and the degree of interwall coupling between walls inside the CNT. The pullout force exhibits "frictional" sliding wherein the pullout force is nearly constant after an initial elastic response and fracture of initial interface bonds. The mechanism for the friction is the successive breaking and re-forming of bonds between the interstitials and matrix or CNT. The friction force is found to be linearly proportional to the number of interstitial C atoms, indicating that each interstitial provides, on average, a characteristic resistance to sliding deformation. Implications for design and performance of CNT-based nanocomposites are discussed.

In-Situ Observation of Metallic Tribosystems

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In this talk we will present novel tools and methods to observe and analyze metallic tribocontacts. For this purpose we have constructed a multitechnique tribometer which allows us to follow topographical changes, friction forces and wear particles under lubricated sliding [1]. Information on the topography of one of the two surfaces is gathered in-situ with a 3D holography microscope at a maximum frequency of 15 fps and higher resolution images are provided at defined time intervals by an atomic force microscope (AFM). We present first results of iron and copper surfaces using a poly-alpha-olefin lubricant.

In the second part of the talk we present observations of friction induced subsurface changes in metallic multilayers. While the multi-layer serve as a marker structure it is possible to investigate them after the friction experiment using Focused ion beam (FIB) analysis and Scanning Transmission Electron Microscopy (STEM). These experiments are compared to Molecular Dynamics (MD) Simulations in order to unravel mechanisms of material mixing.

[1] S.Korres, M. Dienwiebel, submitted to Rev.Sci.Instrum., arXiv: 1003.1638v1

Tribology of Diamond-Like Carbon coatings: multi-scale and multi-physical processes

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Diamond-Like Carbon (DLC) films are getting more and more popular in industrial applications, especially thanks to their unique tribological properties. Most tribological coatings are either hard wear resistant materials but exhibiting high friction, or soft with easy shear and thus low friction but exhibiting higher wear rates. How to account then for the paradoxical combination of hard DLC coatings exhibiting low wear together with low friction?

Thanks to high hardness, high strain tolerance and smoothness achieved with most DLC deposition techniques, plastic flow is not likely to occur in the contact area, neither as abrasive phenomena nor as shearing of contacting asperities. Nevertheless, adhesive interactions with DLC surfaces can vary significantly depending on counterface nature and environment, from strong covalent bonding to weak Van-der-Waals interactions between passivated surfaces, especially with hydrogen. Adhesion appears then as the major phenomenon controlling friction and wear of DLC films.

From various experimental results obtained with different DLC in several environments, the key-role of adhesive phenomena will be discussed, highlighting their consequences on velocity accommodation modes. These results will point out that formation, behavior and release of adhesive junctions are critical for contact evolution. The strength of adhesive junctions is affected not only by tribochemical reactions with counterface and/or environment, but also by their size and hence by surface topography. The release of these junctions will finally depend on mechanical properties of the contacting surfaces.

Understanding friction and wear of DLC coatings requires thus the study – or the modeling – of multi-scale and multi-physical processes, from molecular level to apparent contact size and from tribochemistry to surface mechanics.

Making and breaking of atomic bonds in tribocontacts

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Modelling friction and wear processes has to be chemically accurate to correctly describe bond breaking events and must yet be suitable for engineering application which requires description of macroscopic materials degradation and materials losses on the scale of an engine. This must be combined with the chemical complexity of the involved materials: metals, ceramic coatings and lubricants, to name just a few. Our aim is to reduce this complexity as much as possible and to study a few model systems, which allow one to demonstrate the usefulness of modelling approaches in this context.

I will describe our first approaches towards the simulation of wear processes of diamond and diamond-like carbon (DLC) films. Ab initio methods and simpler tight binding approaches are used to assess the relative importance of certain chemical changes or reactions. These methods also form the basis for the development of empirical potentials that can accurately represent bond breaking processes. They are then used for atomistic simulations of the immediate tribocontacts. Phase transitions and structural changes in these contacts are important for the understanding of the polishing of diamond and the wear of DLC.

Smooth Particle Hydrodynamics for Tribological Applications

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The suitability of the numerical method Smooth Particle Hydrodynamics (SPH) is tested for tribological applications. Smooth particle hydrodynamics is a meshless Langranian method. The method was first applied to astrophysical and cosmology problems and is now also applied in the area of fluid dynamics and solid dynamics as well as in coupling problems of both media. The method offer substantial potential for problems which include moving discontinuities, like cracks and defragmentation, and large deformations. These problems are encountered by modeling tribological systems, i.e. surfaces in moving contact with each other and optionally lubrication. Wear occurs in the contact region, where material can be removed. If this is happening in a non controllable fashion the performance of the part is unreliable.

In the present work the shear behavior of a multilayer is investigated using SPH. The multilayer consists of three layers, namely the wear debris between two layers of material. A pressure is imposed on the top layer and a horizontal velocity on the bottom one. A parametric study is done for different material combinations and diverse material constitutive laws. The SPH results are assessed by means of comparison with the discrete element method which is reported as a suitable simulation technique for tribological systems.

Measuring the glass-transition temperature in thin atactic polystyrene films: molecular dynamics approach

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ABSTRACT

We have performed molecular-dynamics simulations to explore the influence of confinement on the glass-transition temperature (T_g) for supported atactic-polystyrene thin films of different thicknesses, $(1 \div 10)$ nm, and different strengths of attraction to the substrate, $(0.1 \div 3.0)$ kcal/mol. For each film we define three different (substrate, middle and surface) layers using the simulated density. We calculate the T_g by measuring the density variation with a temperature both for each film and corresponding layers. We find that for the whole film the T_g remains almost constant for films down to 2 nm where the middle layer vanishes, and drops down for thinner films. We claim that the redistribution of mass in the three film layers may explain the change with film thickness of the average T_g, if the latter is determined from linear fits of the average glass and melt densities

1. Introduction

The the glass-transition temperature (T_g) is still a much-discussed subject in condensed matter physics. In the case of confined polymer films the physical picture is getting even more complex since it involves different relaxation processes of polymer-chain segments on different timescales. There is evidence that the presence of a supporting surface and a free interface in a film may change both the static and dynamic behavior of polymer chains. Therefore, it is important to explore the influence of the confinement on the glass-transition temperature. To determine the T_g in films with different thicknesses many experimental studies have been employed [1-4]. The first ellipsometry studies showed that the value of T_g in polystyrene (PS) films deviates from that in bulk, and decreases maximally ca. 25 K, [1]. This effect does not strongly depend on the PS molecular weight but rather on the thickness of film: the thinner the film, the larger the reduction of T_g. Lately it was shown that the deviation of T_g in supported films may depend on the strength of the polymer interaction with a substrate: for a strong attraction, a small decrease (or even the increase) of T_g can be observed [2]. However, no thickness dependence of T_g was observed when different experimental methods were used instead of ellipsometry [3,4]. Since the experimental methods, in principle, define the glass-transition temperature as the average property of a whole film, the local effects of supporting surfaces or free interfaces and their local influences on the average T_g can not be fully recognized.

Such a separation can be carried out in a dynamic computer simulation. The existing simulations for model polymers also report significant deviations of T_g from the bulk values if polymers are spatially confined [5]. It was suggested [6] that the role of a free interface is to increase the segmental mobility there, and, as a consequence, to reduce the average T_g value for the whole film. The free interface behaves as a melt (i.e. it has lower T_g) in contrast to the frozen glassy middle (bulklike) layer of the film.

In this article we present the results of molecular-dynamics simulations of supported atactic polystyrene (aPS) films. The main purpose is to study the possible variation of the average T_g with film thickness, as well as the variation of T_g in three different layers - substrate, middle and surface.

2. Polymer model and simulation details

In the present simulations we have chosen the united-atom representation of aPS. For the model description and more details of the force-field we refer to [7]. We have performed simulations for supported aPS films of different thicknesses (1÷10) nm. Each film consists of 4, 8, 16, or 32 chains, with 80 monomers per chain (molecular weight $\sim$ 8400 Da, below the entanglement molecular weight of 1.3×10^4 Da), and 2564, 5128, 10256, 20512 united atoms, respectively. The average gyration radius of these chains is found to be about (1.5÷2.0) nm. Periodic boundary conditions are implemented in the x and y directions only (the box size is fixed to 7×7 nm). In order to simulate supported films we introduce a completely smooth, structureless substrate. To simulate the monomer-substrate interactions a truncated 9-3 Lennard-Jones (LJ) potential is chosen:

$$U_{sub}(z) = \frac{1}{2}\varepsilon\left[\left(\frac{z_{min}}{z}\right) - 3\left(\frac{z_{min}}{z}\right)\right] \tag{1}$$

Here z denotes the distance from the monomer to the substrate and ε is the strength of the attraction to the substrate. $z_{min} = 0.3$ nm is the distance at the minimum of the potential. In the present simulations the potential strength ε varies from 0.1 kcal/mol (non wetting) to 3.0 kcal/mol (complete wetting).

Each film was equilibrated at an initial high temperature of 540 K in a high-mobility melt state, and subsequently cooled with a constant cooling velocity of 0.01 K/ps down to the room temperature, 300 K, well below the T_g.

3. Glass-transition temperature

In the present simulations we measure the glass-transition temperature for the whole film and for three separate (substrate, middle and surface) layers inside the film. The definition of the layers is shown in Fig 1 (left). To calculate the T_g we measure the variation of density with temperature for the whole, film resp. in the layers. In Fig 1 (left) the ”GDS” abbreviation denotes the position of the Gibbs dividing surface, and ρ_{md} denotes the density in the middle of a film. The glass-transition temperature is measured by selecting two linear regions of the data corresponding to high and low temperatures, fitting them by straight lines and finding the intersection point, Fig 1 (right).

In Fig 2 we present the thickness dependence of the glass-transition temperature for the whole film (left) and middle layer (right) for different strengths of attraction to the substrate. The glass-transition temperature in the middle layer practically does not depend on the total film thickness. It also weakly depends on the strength of attraction. Its average value (for different films, and different degrees of attraction), 405 ± 12 K, is shown in Fig 2 by the dashed lines. This temperature can serve as an indication of the glass-transition temperature in bulk aPS. For the whole film some decrease of T_g with decreasing film thickness is observed, but only for very thin films, less then 2 nm.

We fitted the simulation data in Fig 2 (left) by the empirical formula [2]:

$$T_g(h) = T_g^{bulk}\left[1 - \left(\frac{A}{h}\right)^{\delta}\right] \tag{2}$$

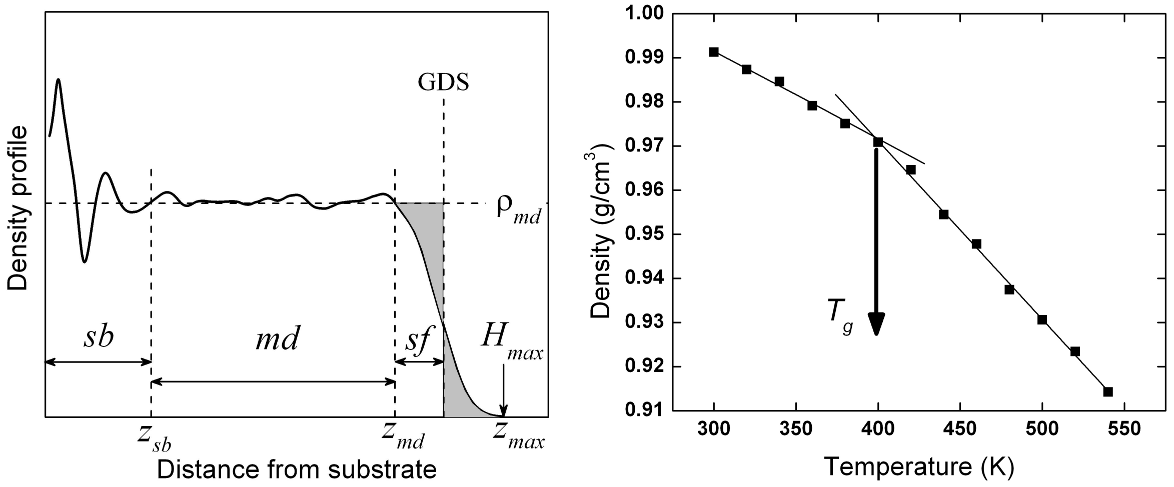

Figure 1: (Left) The density profile for a supported aPS film and the definition of three layers with different density behavior: substrate (sb), middle (md) and surface (sf). (Right) Density variation with temperature of a film with 32 chains and the glass-transition temperature as a point of intersection of two straight lines.

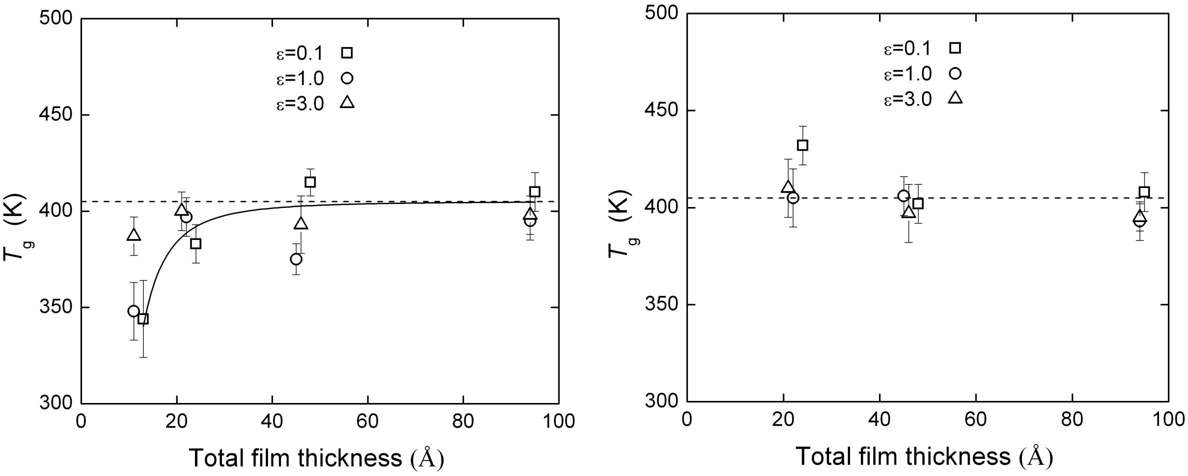

Figure 2: Thickness dependence of T_g for the whole film (left) and middle layer (right) for the case of weak (0.1 kcal/mol) and strong (1.0, 3.0 kcal/mol) attraction to the substrate.

where T_g^{bulk} is taken equal to T_g in the middle layer and h is the film thickness. The fit results $A = 0.18$ nm for the characteristic length and $\delta = 1.1$ for the exponent are quite different from the values obtained by Keddie from ellipsometry experiments ($A = 3.2$ nm, $\delta = 1.8$), but are rather close to those from dielectric studies by Fukao ($A = 0.39$ nm, $\delta = 0.96$) [1,8]. Lattice MC simulations results for a model PS give $A = 6.2$ nm and $\delta = 1.71$ [9].

While the glass-transition temperature of the middle layer only weakly depends on the strength of attraction to the substrate, T_g for the whole film fluctuates considerably; however, no regular trend with the strength of attraction is observed. Obviously, the overall decrease of the glass-transition temperature with the film thickness for the whole film can not be explained by the thickness dependence of the T_g values of the middle layer. Therefore, we have tried to study the thickness dependencies of the T_g values in the substrate and surface layers. For the majority of the simulated films the T_g values of the substrate layer increase above the bulk value (by $\sim 20 \div 70$ K, depending on the strength of attraction to the substrate). For the thicker (h $\sim$ 10 nm) simulated film with a strong ($\varepsilon = 1 \div 3$ kcal/mol) adsorption to the substrate the largest increase is observed, about 80 K. For the surface layer we were not able to identify the glass transition since the density remains almost constant with decreasing temperature. We can only speculate that either the surface T_g is below the simulated temperature window, or the fluctuations in the results are so big that the surface T_g can not be defined with reasonable precision. Due to the influence of a substrate and the presence of a free surface the density itself changes through the film in such a way that the film becomes stratified with different densities in different layers. In [13] we show that such stratification can be expressed in terms of mass that redistributes itself under the influence of the substrate and the free surface and that this cause a change of the average glass-transition temperature when the film thickness is reduced.

Acknowledgements

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Multiscale Computations – three examples in nanomechanics

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After a brief review on multiscale computations, three examples of different categories are discussed, and the effectiveness and limitation of each approach is addressed. Quasicontinuum is the first example, which shows two simulations of a nanoscale indentation and of fracture of carbon nanotubes in the uniaxial tension. The second example is about a hybrid method of QM/QC (quantum mechanical and quasicontinuum) for the fracture simulation of carbon nanotubes. This turns out to improve the solution from the foregoing QC method. The last example belongs to a hierarchical multiscale approach, aiming at looking into the rate effect on the adhesion behavior of a thin metal layer, such as gold or copper, onto two different materials. One of the two materials is modeled as a punch made of silicon or silicon dioxide, and the other as a substrate made of polymer such as PMMA. A hierarchical multiscale simulation is developed to study the role of the rate effect in the adhesion and decohesion from the quantitative view. To capture the atomic origin of the viscous force and to establish a phenomenological constitutive equation on the continuum scale, the molecular simulation is utilized to obtain the constitutive parameters of the polymer substrate. Then, the resulting constitutive equation is implemented into finite element code to examine the dynamic behavior of adhesion and decohesion. The rate effect is discussed with the aid of the results from this simulation and from the material testing.

Atomistic Investigation of Asperity Contact:
A study of Two Configurations

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Tribological phenomenon is central for the study of contact mechanics and many aspects of engineering applications. Recent development of nanotechnology opens unique opportunities to explore nano-scale mechanisms for the understanding of an asperity contact. This study discusses nanomechanics investigation of two asperity contact conditions — a hard asperity indenting a soft surface and a soft asperity indenting a hard surface. A hard asperity indenting a soft surface has enabled the measurement of hardness of materials to become commonplace. Material characterization is an integral part of tribological study. Previous investigations of the indentation size effect in metals indicate that the hardness increases with a decreasing indentation depth, particularly for indentation in the submicrometer regime. The results show that the increase in hardness is inversely proportional to the square root of the indentation depth. In this regard, the indentation size effect is similar to the Hall-Petch relationship describing the grain size effect on the strength of metals and alloys. However, the Hall-Petch equation does not apply at the nanoscale, as indicated by a recent study. The simulation results show that the nanohardness does not have a strong dependence on the indentation depth when the indentation depth falls into the nanometer regime. The indentation size effect and void effect from the molecular scale up to the macro-scale is discussed.

The behavior of the soft asperity contacting a relatively hard surface plays a central role of in a variety of surface phenomena such as tribological behaviors, electrical and thermal contact conductance. Moreover, an understanding of interfacial phenomena at nano-scale is fundamentals for the atomic origins of macroscopic friction and wear. We examine the full range of asperity contact behaviors and show that the results are in good agreement with those predicted by continuum theory in the elastic, elastic-plastic and plastic regimes. When two contact surfaces have relative motion, a sliding contact takes place. Tabor (1959) introduced the concept of “junction growth” based on the experimental finding that implies an increase of the contact area as the result of an increasing tangential load. Our study shows that the onset of lateral junction growth in the nanometer regime is primarily the result of the slips of atoms within the asperity, which causes new asperity atoms come into contact with the flat. This result substantiates the assertion of Tabor that junction growth is essentially a plastic deformation process. Moreover, the simulation results reveal that the presence of an adsorbed layer on the asperity surface significantly delays the onset of lateral junction growth until the adsorbed layer is splayed out from the interface. Comparisons among molecular simulations, continuum approach and experimental findings are conducted to elucidate the underpinning of the tribological mechanisms and shed light on how to build durable systems to fulfill the compelling energy saving trend.

Dynamic Green's function approach for solid friction and contact-size effect

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To investigate the relationship between solid friction and energy dissipation due to phonons, we analytically derived a dynamic Green's function of a harmonic square lattice that consists of infinitely large bulk atoms. The inclusion of the infinite degrees of freedom enables to capture the energy dissipation mechanism due to phonons [1]. We also developed a self-consistent scheme used for achieving a steady state, and introduced a fast convolution method [2] that dramatically reduces the computational overhead.

The approach is applied to a simple friction model, as shown in Fig. 1 (a). In the system, normal force per surface atom does not change with the variation of *N* at the same normal pressure, because the ratio of the contact area is fixed at 1/4. Figure 1 (b) shows dependence of the friction coefficients on the contact size. As *N* becomes larger, the friction coefficients first decrease and then increase.

In analysis of the friction system, energy transfer from the sliding upper solid to low-frequency phonon of the lower solid is observed. The energy dissipation leads to friction. It is also found that phonons of non-zero wave number play channels of the energy dissipation, that account for the friction dependence on the contact size.

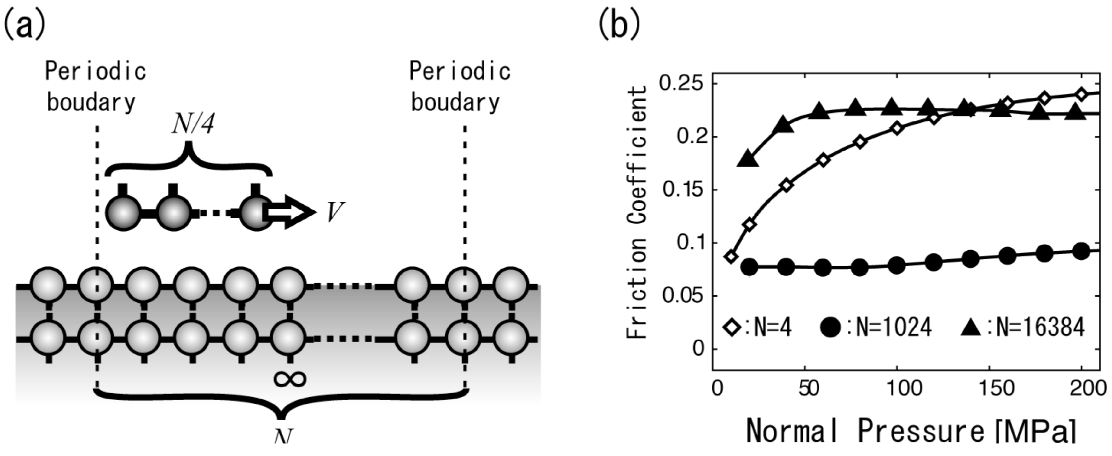

Fig. 1: (a) Image of the solid friction system between periodically contacting surfaces. The lower body consists of infinite bulk atoms. The upper body slides at 10m/sec and the atomic bonds are frozen. The lattice constants of the both bodies are same. (b) Dependence of friction coefficients on contact size: i. e., *N*.

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Molecular dynamics simulations of microstructural evolution during sliding interactions

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Microstructural evolution during sliding interactions between ductile metals is the result of several dynamic and interacting phenomena that are strongly driven by the high strain-rate, stress, strain and temperature experienced near the sliding interface. The aim of this study was to gain insights into these dynamic events via molecular dynamics simulations. Fe-Cu, Fe-Ni and Cu-Ni tribopairs, described by embedded atom potentials, were studied to probe the effect of mechanical forcing on friction and microstructure evolution in clustering, ordering and miscible binary tribopair systems. Lennard-Jones potentials were also employed to model tribopairs with different hardness ratios and enthalpies of mixing. The variables studied included sliding velocity, crystal orientation, enthalpies of mixing, hardness ratios, and presence of crystal defects.

Plastic deformation in the subsurface material was found to contribute to friction and adiabatic heating. Crystal orientation and presence of preexisting dislocations, interfaces and asperities play an important role in determining the deformation processes. Intriguingly, unexpected deformation modes such as dynamic recrystallization leading to nanocrystallization (Fig 1.), amorphization and twinning in high stacking fault energy materials are observed in addition to dislocation activity. Formation of vortices is observed in the amorphous layer near the sliding interface. Material flow due to plastic deformation, in particular, vorticity is observed to cause mechanical mixing. While the extent of mixing is affected by the enthalpy of mixing, even clustering systems could be forced to mix if the velocity is high enough suggesting that mixing is a highly driven process. The hardness ratio between the counterparts has a stronger influence on mixing kinetics than the thermodynamics of mixing.

Comparisons with experiments suggest that such simulations can provide valuable mechanistic insights into the experimentally observed formation of the mechanically mixed, nanocrystalline layer and transfer film during sliding in ductile metals.

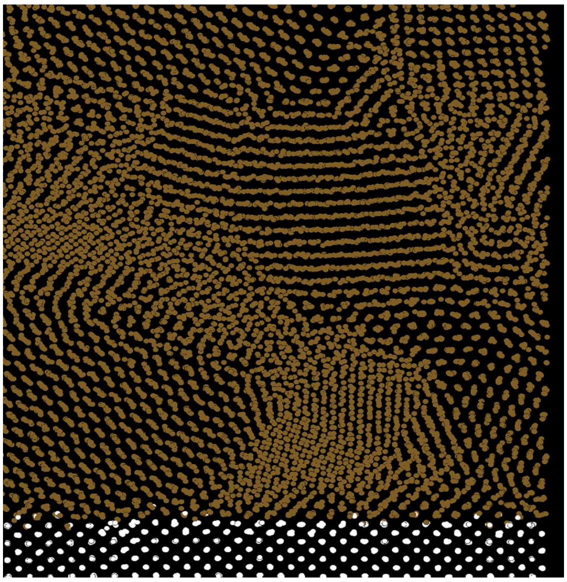

Fig 1. Nanocrystallization of Cu due to dynamic recrystallization in a Cu-Fe tribopair

Is shear induced dispersion of carbon nanotubes in aluminum matrices feasible?

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Tensile strengths of carbon nanotubes (CNTs) are typically an order of magnitude higher than that of carbon fibers, which are well established reinforcements for organic materials. It has been shown experimentally that the addition of CNTs instead of carbon fibers can lead to significant improvements of mechanical properties [1]. Despite these promising results in the field of organic composites there are comparatively few studies dealing with reinforcement of metal matrices by CNTs.

CNTs tend to form bundles via van der Waals interactions. Splitting them is necessary in order to enlarge the contact area between CNT and matrix. We carried out molecular dynamics studies of pristine CNTs in sheared aluminum melts. These reveal that splitting these bundles by shear is almost impossible. In organic materials dispersion can be supported by chemical functionalization [2]. Since Al_4C_3 is easily wet by aluminum [3], the formation of aluminum carbide particles at CNT walls might play a similar role for CNTs in aluminum. We used density functional theory to investigate the reactivity of pristine and defective CNT walls. Graphene has been used as a model for large diameter CNTs. It turns out that pristine surfaces are almost unreactive. Binding of small aluminum clusters is mainly of an ionic nature while the magnitude of charge transfer decreases with increasing cluster size. Binding energies drastically increase when aluminum atoms on vacancies in graphene are considered. This indicates that carbide formation can start at defects in CNT walls. Typical CNTs from chemical vapor deposition processes contain many defects and if necessary they can be created artificially for example by ball milling of a mixture of CNTs and metal powder [4].

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Quantum Chemical Molecular Dynamics Simulation on Tribochemical Reaction Dynamics of Diamond-Like Carbon

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Recently classical molecular dynamics simulation is frequently employed to investigate the tribological phenomena. In addition, more recently the electronic level understanding of the tribochemical reactions is strongly demanded. However, the classical molecular dynamics method cannot simulate the chemical reactions. Hence, we developed a tight-binding quantum chemical molecular dynamics simulator1) and it was applied to the tribochemical reactions of diamond-like carbon. Experimentally, the friction coefficients of diamond-like carbon are significantly changed by the synthesis process and then in this study we investigated its reason.

Fig. 1 shows the simulation model for the tribology process of diamond-like carbon. In this model, H atoms are incorporated to terminate the dangling bonds of diamond-like carbon. Fig. 2 shows the change in the charge of two H atoms and the bond population between the above two H atoms. Here, the bond population indicates the bond strength, which is calculated by the number of electrons in bonding and unti-bonding orbitals between two atoms. The charge and bond population cannot be obtained by the classical molecular dynamics method and then these are the merit of quantum chemical molecular dynamics method. The increment of the bond population at 3 ps shows the formation of H_2 molecule at the interface by the tribochemical reaction. Moreover, the change in the H charges from 0.2 to 0.0 indicates that the electron transfer led to the above tribochemical reactions. Moreover, the formation of H_2 molecule was found to increase the friction coefficient of the diamond-like carbon because the loss of the terminated H atoms led to the formation of new C-C bonds at interface. Finally, we concluded that the experimental fluctuation of the friction coefficient of the diamond-like carbon is due to the dynamic behavior and tribochemical reactions of H atoms.

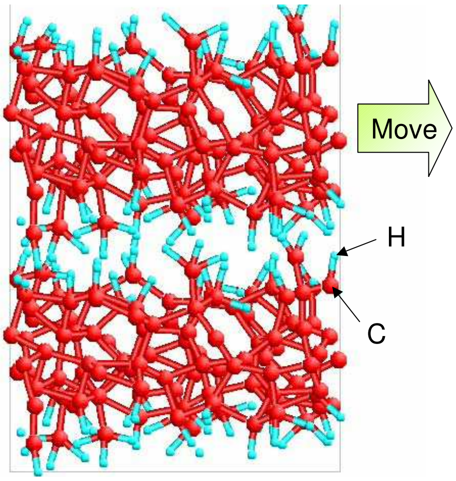

Fig. 1 Simulation Model

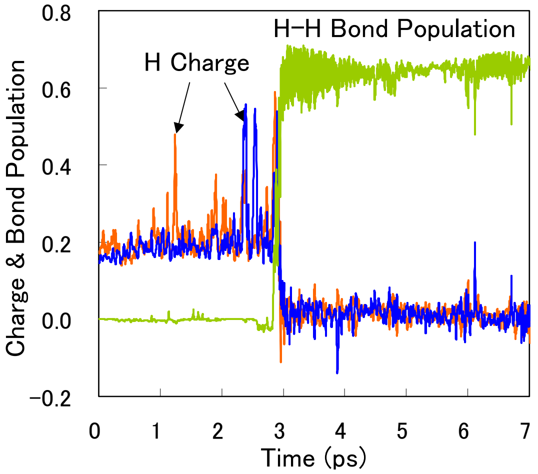

Fig.2 Charge and bond population

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Oxygen-induced degradation of carbynoid structures on carbon surfaces: a DFT study

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Carbynoid structures - *sp*-bonded carbon chains - have recently attracted interest due to their promising one-dimensional properties and to their presence in many nanoscale processes. In particular, they have been reported to form during the growth of nanostructured carbon films, as well as during the *mechanical polishing of diamond* surfaces. The interaction of these structures with air is crucial to the final structure of the deposited or polished surfaces. Crucially, oxygen was found to cause the degradation of carbynoid strutures. This may play an important role in the wear mechanism of the diamond polishing.

Here we present a DFT study of the oxidation mechanisms of carbynoid structures. Due to the lack of reference experimental studies specifically devoted to the oxidation mechanisms of supported carbon chains, the accuracy of our simulations is assessed by studying the oxidation of small cationic carbon cluster in the gas phase, for which detailed experimental data exist. This allows us to gain insight into unclear oxidation mechanisms of cyclic cationic carbon clusters. Moreover, the extension of our simulation approach to supported linear carbon clusters yields possible mechanisms for the oxygen-induced degradation of such structures.

Modeling of self-sharpening knifes using the Discrete Element Method

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Cutting is an important process in everyday life and industrial processes. Since every cutting process is a specific and highly complex tribological system a lot of different types of cutting processes exist.

In the current project new cutting devices for the cutting of highly filled abrasive polymers are developed following a biomimetic approach: Rodents have developed rootless incisors consisting of a soft core and a hard lamella of enamel, which constantly grow and during lifetime the rate of growth is in equilibrium with abrasion which leads to a steady sharp cutting edge through directed wear. Therefore, a Discrete Element Method (DEM) approach is used to model this process: The cutting edge as well as the polymer is discretised and simulated by individual elements (spheres) in three dimensions with periodic boundary conditions. DEM is particularly suitable for the representation of abrasive applications, since an overload of individual joints leads to their rupture, so that individual elements can be detached from the matrix and the deformation gets visible. A key issue is the careful calibration of the microscopic interaction parameters (viscous spring-damper systems (compressive and tension-springs) and bending beams) to real material properties. Furthermore only small areas can be simulated in full detail due to the high computational burden. These areas are supported by coarser models in the back. The calibration of the model is carried out by comparing the simulation results of tension-, pressure and impact tests with real experiments. Still a realistic amount of cuts (> 10 000) cannot be simulated. Therefore, the damage of the material is taken into account by load-collective fatigue models with an implemented multiscale statistical approach: The tolerable force which may act on the bonding of the spheres is interpolated due to the force load after each simulated cut to reduce the required steps.

From electronic DFT to continuum mechanics descriptions of sliding contacts

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In this talk we present sequential multi-scale simulations of a tribological contact, which consists of two rough surfaces that are lubricated by olefins. The various techniques involved include first-principle, density functional theory calculations, force field based molecular dynamics simulations as well as coarse-grained simulations of two sliding elastic walls separated by a fluid layer. In the latter case, interactions within the solid walls are modeled with elastic Green's functions while the fluid is treated with a mesoscale (lattice Boltzmann) method. In order to avoid artifacts near the interface in the continuum description, square gradient theory corrections are included into the mesoscale description of the fluid.

We start out by discussing the parameterization of a classical force field describing the interaction between an aluminum substrate and olefins. This step involves an iterative scheme in which a guess for the interaction potential is improved iteratively by running a medium-scale, tribological molecular dynamics simulation for typical shear rates and local pressures from which new molecular configurations are produced. For subsets of these configurations we calculate the forces with first-principle calculations, which are used to optimize the force field parameters. Once sufficient convergence has been achieved, large-scale molecular dynamics simulations are performed with which pressure and shear rate dependent viscosities as well as slip length are determined as well as the wavelength dependent compressibility, which is the key quantity in the square gradient theory. Molecular dynamics simulations are also used to determine the Green's function coefficients for the elastic walls. Lastly, we consider geometries of linear dimensions of micrometer scales to ascertain realistic estimates for normal and shear pressures for rubbing aluminum surfaces.

A study of chemical mechanical polishing on CeO_2 nanocrystals based on classical and tight-binding quantum chemical molecular dynamics simulations

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CeO_2 has an important role in existing and potential applications as an abrasive grain for polishing glass. Thus, it is important to investigate polishing processes of CeO_2 depending on its grain size, density, degree of hardness and lattice defect. Therefore, we have studied chemical mechanical polishing processes of CeO_2 nanocrystals using theoretical approaches such as classical and tight-binding quantum chemical molecular dynamics simulations. In this study, we focused on La-doped CeO_2 nanocrystals which indicate excellent chemical mechanical polishing properties. Then, we investigated some characteristics of the La-doped CeO_2 ($Ce_{1-x}La_xO_{2-x/2}$) *via* classical molecular dynamics simulations. When x value is 0.4, we constructed a sphere model of 40% La-doped CeO_2 ($Ce_{0.6}La_{0.4}O_{1.8}$) comprising 675 Ce, 450 La and 2025 O atoms as shown in Fig. 1. Here, there are 225 vacancies in this model. The oxygen atom distributions based on the results of the molecular dynamics simulations as shown in Fig.2 presents increasing peaks of the oxygen distributions where the oxygen atoms locate near the center of the nanocrystal. These rising peaks suggest that the oxygen atoms diffuse into the vacancy sites around the center of the nanocrystal. At the conference, we will present typical chemical mechanical polishing processes of CeO_2 particles based on the tight-binding quantum chemical molecular dynamics[1], and discuss how the oxygen defects of the La-doped CeO_2 nanocrystal affect the chemical mechanical polishing processes.

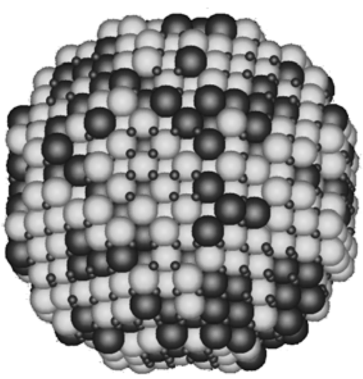

Fig.1 A sphere model representation of the atom positions for $Ce_{0.6}La_{0.4}O_{1.8}$. Big white, black and small spheres present Ce, La and O atoms, respectively.

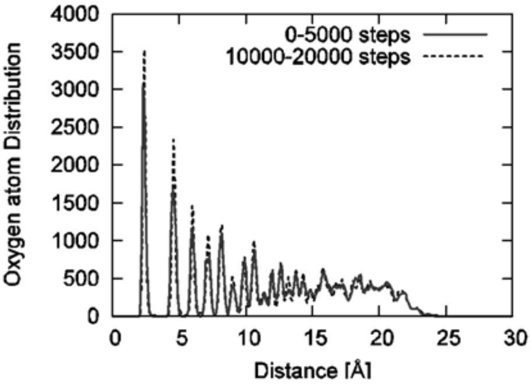

Fig. 2 Oxide atom distributions as a function of distance from a center of a $Ce_{0.6}La_{0.4}O_{1.8}$ cluster. The solid and dashed line plots the time average of that from 0 to 5,000 and from 10,000 to 20,000 steps, respectively. Here, one step corresponds to 2 femto second.

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Atomistic insights into the running-in, lubrication, and failure of hydrogenated diamond-like carbon coatings

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The tribological performance of hydrogenated diamond-like carbon (DLC) coatings is studied by molecular dynamics simulations employing a screened reactive bond-order potential that has been adjusted to reliably describe bond-breaking under shear. Two types of DLC films are grown by CH_2 deposition on an amorphous sub- strate with 45 and 60 eV impact energy resulting in 45 and 30% H content as well as 50 and 30% sp^3 hybridization of the final films, respectively. By combining two equivalent realizations for both impact energies, a hydrogen-depleted and a hydrogen-rich tribo-contact is formed and studied for a realistic sliding speed of 20 m s^{-1} and loads of 1 and 5 GPa. While the hydrogen-rich system shows a pronounced drop of the friction coefficient for both loads, the hydrogen-depleted system exhibits such kind of running-in for 1 GPa, only. Chemical passivation of the DLC/DLC interface explains this running-in behavior. Fluctuations in the friction coefficient occurring at the higher load can be traced back to a cold welding of the DLC/DLC tribo-sur- faces, leading to the formation of a transfer film (trans- ferred from one DLC partner to the other) and the establishment of a new tribo-interface with a low friction coefficient. The presence of a hexadecane lubricant leads to low friction coefficients without any running-in for low loads. At 10 GPa load, the lubricant starts to degenerate resulting in enhanced friction.

Reference:
L. Pastewka, S. Moseler, M. Moseler,
Tribol. Lett., in print, doi:10.1007/s11249-009-9566-8

Molecular dynamics simulation of gold solid film lubrication

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The lubrication mechanisms in ultrathin solid gold films confined between two rough nickel surfaces have been investigated employing classical molecular dynamics with a second moment tight-binding potential. Three types of nickel surfaces are considered: Ni(111), Ni(001) single- and a Ni(001)-(111) bicrystal. In all three systems, gold layers that have been quenched from the melt organise in (111) layers parallel to the nickel interfaces. The relative sliding of the two single crystal nickel tribopartners requires a shear stress of around 170 MPa – a value that is almost one order of magnitude lower than the ideal plastic shear stress of single crystal bulk gold. This reduced stress can be explained by a misfit dislocation mechanism in a single plane close to the Ni/Au interface. In the case of the Ni(001)-(111) bicrystal, the nickel grain boundaries induce grain boundaries in the quenched gold film which vanish during sliding. During subsequent sliding the nickel grain boundaries act as nucleation centres for dislocation loops leading to an increased shear stress of 490 MPa. The same is observed for an embedded hydrocarbon impurity. Also here dislocation loops are emitted on (111) planes that are tilted with respect to the sliding plane.

Describing bond-breaking processes by reactive potentials: Importance of an environment-dependent interaction range

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First nearest-neighbor models are routinely used for atomistic modeling of covalent materials. Neighbors are usually determined by looking for atoms within a fixed interaction range. While these models provide a faithful description of material properties near equilibrium, the limited interaction range introduces problems in heterogeneous environments and when bond-breaking processes are of concern. We demonstrate that the reliability of reactive bond-order potentials is substantially improved by using an environment-dependent first nearest-neighbor definition. In particular, this approach corrects the maximum forces required for bond-breaking. We are hence faithful that this interatomic potential can be used for a proper description of tribological processes.

Reference:
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Phys. Rev. B 78, 161402(R) (2008)

Large-scale molecular-dynamics simulations of the tribology of nanoscale metallic asperities

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Molecular dynamics simulations of the tribology of nanoscale gold contacts are reported. The formation of a neck upon bringing two asperities into contact, and its subsequent deformation and fracture upon shearing, are investigated, bearing special interest on the mechanisms of material flow underlying these processes. The influence of the presence of a liquid lubricant is also explored. The setup of large-scale simulations (hundreds of thousands atoms) allows us to make one step further, with respect to earlier works, towards connection with recent experimental works.

Heat transfer between elastic solids with randomly rough surfaces

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We study the heat transfer between elastic solids with randomly rough surfaces. We include both the heat transfer from the area of real contact, and the heat transfer between the surfaces in the non-contact regions. We apply a recently developed contact mechanics theory, which accounts for the hierarchical nature of the contact between solids with roughness on many different length scales. For elastic contact, at the highest (atomic) resolution the area of real contact typically consists of atomic (nanometer) sized regions, and we discuss the implications of this for the heat transfer. For solids with very smooth surfaces, as is typical in many modern engineering applications, the interfacial separation in the non-contact regions will be very small, and for this case we show the importance of the radiative heat transfer associated with the evanescent electromagnetic waves which exist outside of all bodies.

Nanotribology of lubricated carbon-based nanocoatings

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Nanocoatings have the potential to improve the surface properties of various materials. They are of extreme importance for surfaces in sliding lubricated contact such as highly stressed automotive engine parts. Here, nanocoatings have to be optimized with respect to low friction properties and a high wear resistance to enhance the energetic and environmental efficiency. An additional variation of the tribological characteristics arises due to the presence of the fuel as the lubricant.
The present study employs atomic-scale simulations in order to assist the manufacturing and optimization of functional nanocoatings. Our investigations focus on two basic functional film species - tetrahedral amorphous carbon (ta-C) and transition metal enriched carbon (TM:C) coatings. These films are modeled and studied with the help of bond-order potentials such as the reactive empirical bond-order (REBO) potential [1] for carbon-carbon interaction and the Shibuta potential [2] for TM-carbon interaction. Our simulations also incorporate an adaptive cutoff scheme, which is able to enhance the REBO potential characteristics [3]. Since the tribological properties of lubricated engine parts depend not only on the properties of the nanocoatings but also on the lubricant, the hydrocarbon dodecan is selected as a representative of the fuel in the automotive engines. Preliminary results on the ta-C film morphology and its tribological properties such as friction coefficients with and without lubrication are presented.

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[2] Y. Shibuta et al., Chem. Phys. Lett. 472 (2009) 200
[3] L. Pastewka et al., Phys. Rev. B 78 (2008) 161402

Onset of frictional slip by domain nucleation in adsorbed layers

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It has been known for centuries that a body in contact with a substrate will start to slide when the lateral force exceeds the static friction force. Yet the microscopic mechanisms ruling the crossover from static to dynamic friction are still the object of active research. Here, we analyze the onset of slip of a xenon (Xe) monolayer sliding on a copper (Cu) substrate. We consider thermal activated creep under a small external lateral force and observe that slip proceeds by the nucleation and growth of domains in the commensurate interface between the film and the substrate. We measure the activation energy for the nucleation process considering its dependence on the external force, the substrate corrugation and particle interactions in the film. To understand the results, we use the classical theory of nucleation and compute analytically the energy of a domain wall which turns out to be in excellent agreement with numerical results. We discuss the relevance of our results to understand experiments on the sliding of adsorbed monolayers.

Surface chemistry and nanotribological properties of diamond surfaces

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We applied *ab initio* calculations to derive the potential energy surface (PES) describing the interaction of two diamond surfaces during their relative displacement. The shape of the PES deeply influences the frictional behavior of the system. Diamond presents remarkably low friction and wear, particularly in humid environments. We analyzed the effects of the surface chemical composition, structure and orientation on the shear strength (friction force per unit area) of diamond interfaces. We also provide a full microscopic description of the interaction of water with diamond (001) surfaces. We performed calculations within the framework of density functional theory including long-range van der Waals interactions. We considered both native and hydrogenated surfaces. We calculated the structure and the energetics for molecular and dissociative adsorption, and in the case of exothermic processes, we determined the energy barriers for dissociation. Our results allow prediction of the formation of water islands on native surfaces that grow along and perpendicularly to dimer rows. Moreover, they highlight the role played by the water coverage in determining the adsorption mode (physisorption or dissociation), suggesting an explanation for experimental results on similar Si(001) surfaces. Finally, we provide an understanding on the mechanism of carbon dangling bond passivation by water which is the key factor in determining the excellent tribological performances of diamond in humid environments as measured in experiments.

Connecting atomistic and continuum models of contact area, stiffness and friction in single and multi-asperity contacts

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Dept. Physics and Astronomy, Johns Hopkins University

B. Luan
IBM Physical Sciences Division

The real area of intimate contact between surfaces plays a central role in continuum theory, but the meaning of contact is unclear at atomic scales. The first part of the talk will describe the effect of atomic scale roughness, thermal fluctuations and adsorbed layers on different definitions of contact between atomically and macroscopically rough surfaces.[1-3] Thermal fluctuations play an important role at typical experimental temperatures. At low loads, the number of atoms feeling a repulsive force at any instant rises linearly with load. Atoms fluctuate in and out of contact, and spend less than half their time in contact until the mean repulsive contribution to the pressure is comparable to the ideal hardness. A simple mean-field model provides a quantitative explanation for this behavior and explains why the distribution of instantaneous forces has a nearly universal exponential form. Multiscale methods are used to examine contact and friction for surfaces with roughness on a wide range of length scales. The contact area, stiffness and friction tend to rise linearly with load, even at zero temperature, but the slope depends on atomistic details that are not included in continuum models.

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3. S. Cheng and M. O. Robbins, arXiv:1004.1202

Nanotribological Studies on Carbonic Interfaces Formed by Graphene, Fullerene and Carbon Nanotube

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1. Introduction

Control of friction is one of the most practical problems in our daily life, which covers almost all the areas from basic science such as physics, chemistry and biology, to industrial technology such as mechanical and material engineerings and energy problems. Recently carbon materials have been tried to used as electronic, optical and mechanical devices. In this talk we discuss our recent simulation studies on nanotribology at carbonic interfaces formed by graphene, fullerene and carbon nanotube.

2. Method

We have developed the molecular- mechanics and dynamics simulators describing the elementary process of atomic-scale friction at the carbonic interface comprised of graphene, fullerene, and carbon nanotube.

3. Results

3.1 Superlubricity at C_{60}/graphene interface The graphene/C_{60}/graphene interface exhibits characteristic superlubricity and periodic anisotropy depending on the scan direction, the mechanism of which is ascribed to the C_{60} rotation and the elastic contact of the C_{60} with the graphene [1,2].

3.2 Wear at graphene/graphene interface Atomic-scale wear appeared in friction force microscopy (FFM) is studied [3]. As FFM tip is pushed toward the graphite surface, the graphene sheet is attached to the FFM tip under a loading force larger than a critical value. The plastic deformation occurs after the scan. Thus the transition from the nanotip state to the graphene-tip state occurs.

3.3 Peeling at CNT/graphene and graphene/graphene interfaces During the adhesion and peeling processes of the carbon nanotube (CNT)[4] and graphene [5], we numerically clarified the characteristic transition from the line- to the point-contacts of the CNT and that from the surface- to the line-contacts of the graphene, which reproduces well the experimental features.

4. Conclusion

We have developed the nanotribological simulator of the carbonic interfaces and studied atomic-scale friction for various mechanical phenomema of superlubricity, wear, adhesion and peeling. I would like to acknowledge Prof. K. Miura, Aichi Univ. of Educ. and Mr. N. Itamura, Seikei Univ., for collaborations.

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Superlubricity of C_{60} and C_{70} Bearings

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1. Introduction

The realization of a novel lubric system, making it possible for nano- and micromachines to move easily, have been strongly desired. Such a lubricant can also contribute to move variety of macroscopic objects. We have recently developed graphite/C_{60}/graphite system [1] and C_{60} intercalated graphite films consist of altenating close-packed fullerene monolayers and graphite layers [2], which are expected to provide an exciting breakthrough in industrial development.

2. Method

In this talk, the mechanism of superlubricity of graphite/C_{60}/graphite interface is numerically studied using molecular mechanics [3-5]. As a model of the graphite/C_{60}/graphite interface, the close-packed C_{60} monolayer inserted between two rigid graphite sheets is used. The periodic boundary condition within the (0001) plane is applied to the 1×1 unit cell. For each graphite interlayer distance the metastable structure of the graphite/C_{60}/graphite interface is calculated by minimizing the total energy using the structural optimization, Polak-Rebiere-type conjugate gradient (CG) method.

3. Results

First the simulated interlayer distances of about 1.3 nm [3,4] are in good agreement with previous experimental results [1,2]. Next the frictional feature along the [1010] direction of the graphite/C_{60}/graphite interface is investigated and compared with that of the graphite/graphite/graphite interface.

The friction coefficient of the graphite/C_{60}/graphite interface decreases to about 30% of that of the graphite/graphite/graphite interface. It is clarified that the three-dimensional degree of freedom of intercalated C_{60} motion is one of the origins of the superlubricity of the graphite/C_{60}/graphite interface along the [1010] direction [4,5]. We will also report anisotropy of superlubricity and C_{70} molecular bearings.

4. Conclusion

In this talk, the superlubricity of the fullerene intercalated graphite is numerically investigated. The friction coefficient of the graphite/C_{60}/graphite interface decreases to about 30% of that of the graphite/graphite/graphite interface. It is clarified that the three-dimensional degree of freedom of intercalated C_{60} motion and effect of elastic deformation of C_{60}.molecule mainly contribute to the superlubricity of the graphite/C_{60}/graphite interface.

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Trends of Micro-scale Simulations in Tribology in Japan

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ABSTRACT

The use of computational simulations to investigate complicated phenomena has become increasingly common because of advances in computers and theoretical formulation and because of improvements in the algorithmic implementation theoretical formulation. While these simulations are effective for solving many industry-related problems, there is still room for improvement in the application of simulation technologies to product design. The main problem is the lack of precision in simulations of complicated phenomena. This is particularly evident in tribology, where the experimental approach plays a central role in the study of friction, lubrication, and wear.

Micro-scale phenomena have been actively studied actively in Japan, and this report reviews developments in the application of simulation technologies to micro-scale tribological phenomena in Japan and describes possible future methodology.

First described here is the development of the molecular dynamics technique for simulating interface diffusion, which is the dominant factor in the mechanical failure of thin-film devices. The technique has been used to investigate the adhesion strength of interconnect films and to find effective methods for suppressing interface diffusion and stabilizing interfaces. Then described is a molecular dynamics simulation of the wear and friction that occur when a pin slide over a thin film. Finally described,as another approach, is the behavior of a lubricant between two solid surfaces that is simulated using a particle method based on continuum dynamics or molecular dynamics.

1. Introduction

The progress of computational engineering, based on modeling technology and numerical computation technology, has been stimulated by developments in visualization technology, optimization technology, and the knowledge database (Figure 1). Simulation technology has been shown to be effective for solving many industry-related problems, but its application to product design is problematic for several reasons. One is the shortening of design turn-around-times. Product life cycles becoming shorter and computational resources are limited, so efficient design methods that shorten the design lead-time are needed. Another problem is the lack of analysis precision for complicated phenomena such like tribological phenomena.

Friction and wear arise when two substances slide face to face in opposing directions, but the origins of friction force and wear are unclear. One approach to elucidating their mechanisms is the microscopic approach, which views objects at atomic- or molecular-level resolution. It is represented experimentaly by imaging techniques like STM (scanning tunneling microscopy) and AFM (atomic force microscop) and is presented theoretically by simulations based on molecular dynamics (MD) or molecular orbital (MO) calculation and particle dynamics.

A hierarchical viewpoint has become important in the use of simulation during the development of industrial products [1], and this report reviews recent developments in the application of simulation technologies to phenomena at various scales (Figure 2) during the understanding of tribological phenomena in Japan. It also mentions a possible future methodology.

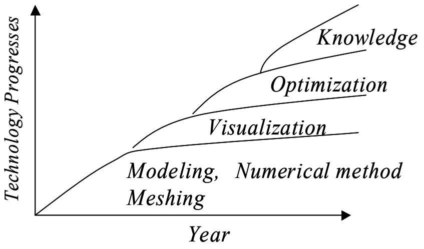


Fig. 1 Progress in simulation technology [1].

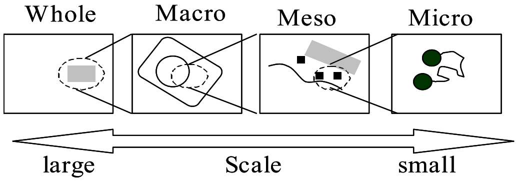
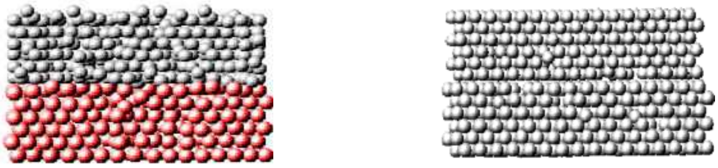


Fig. 2 Various scales in a hierarchy for products and phenomena [1].

2. Molecular-scale simulation in interface [2] [3]

A molecular-dynamics technique for simulating interface diffusion, a dominant factor in the mechanical failure of thin-film devices, has been used not only to find effective methods for suppressing interface diffusion and stabilizing interfaces [2] but also to identify. Barrier-underlayer materials effective for improving the adhesion strength of interconnect films. As shown in Figure 3, ruthenium was found to be an effective underlayer material for improving the adhesion of Cu interconnects. On the other hand, *ab- initio* first-principles simulation can be used to calculate to not only dynamic properties of matter but also an electromagnetism characteristic [3].



Cu/TiN

Cu/Ru

Fig. 3 Atomic configuration at a thin-film interface [2].

3. **Atomic-Scale Modeling of Friction** [4] [5] [6] [7] [8]

The origin of friction at the site of contact between two solids surfaces in relative motion has long been a concern of scientists. Friction can occur without yielding wear if the deformation at the interface remains within the elastic limit. On the other hand, a superlubric state was found in a molecular dynamic simulation study of the incommensurate Frenkel-Kontorova model [4, 5]. Several MD simulations of atomic planes sliding in the absence of external force were studied [6].

The mechanism of the superlubricity of fullerene bearings was studied numerically using molecular mechanics simulations [7]. The study, investigating the superlubricity along the $[10\bar{1}0]$ direction of the graphite/C60/graphite interface, clarified that in a system with a C60 bearing the friction coefficient and lateral stiffness along the $[10\bar{1}0]$ direction were lower than those in a system with a graphite bearing because of the C60 rotation and the elastic contact at the C60/graphite interface. The superlubricity of the C60-bearing system was also found to show marked anisotropy with a 60° periodicity. In the model of the C60-bearing system shown in Figure 4 [8], the close-packed structure of the C60 molecules is used and only the intercalated C60 molecule and graphene sheet sandwiched by the upper and lower rigid grapheme sheets are assumed to relax. Within the (0001) plane the periodic boundary condition is applied to the 1×1 unit cell of the C60 bearing system, and the Tersoff and the modified Lennard-Jones potential vdW *V* are used as the covalent bonding and non-bonding energies, respectively. For the mean loading force $<F_Z>= 0.27$ nN, the mean lateral force $<F_L>$ of the upper grapheme sheet is plotted as a function of the scan angle θ in Figure 5. Here, θ=-30, 30, and 90° are equivalent to the commensurate $[10\bar{1}0]$ direction among the intercalated C60 molecule (graphene sheet) and the upper and lower graphene sheets. Similarly, θ=0 and 60°_are equivalent to the commensurate $[12\bar{3}0]$ direction.

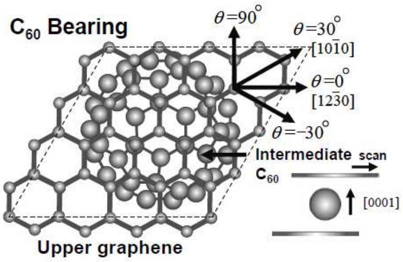


Fig. 4 Model of the C-60 bearing system (graphite/C60/graphite interface) [8].

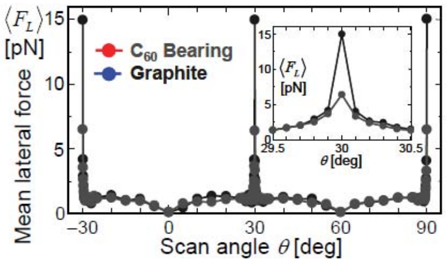


Fig. 5 Mean lateral force as a function of the scan angle [7].

4. Atomic-Scale Modeling of Wear [9] [10]

Molecular simulation played a role in the understanding of wear [9, 10]. Molecular dynamics simulation was used to investigate wear models of frictional sliding between a pin and a thin carbon film containing nitrogen [9]. In this simulation was developed the advanced Tersoff interatomic potential describing nonequilibrium atomic structures produced by the addition of nitrogen. A genetic algorithm is used to optimize many potential parameters that are fitted to the first-principles cohesive energies of various systems under stress. This optimization algorithm converges towards a set of potential parameters that well describe not only crystals but also amorphous systems. Micro-tribological MD simulations of the abrasive wear state of carbon films into which nitride was injected were used to examine the ways in which the dynamics properties of wear atoms were influenced by the nitride content and the nitride distribution.

In this model (Figure 6), a pin is pushed to the film and the wear occurring when it rubs the surface is simulated. These simulations show that wear is minimized when about 20 to 30 percent nitrogen is added (figure 7), and the simulation results qualitatively correspond with experimental results.

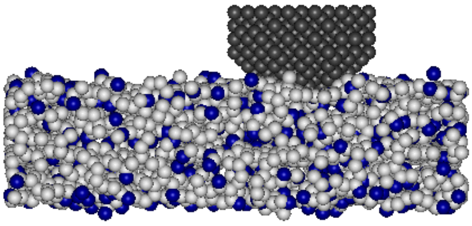


Fig. 6 Simulation model (N content=20%) [9].

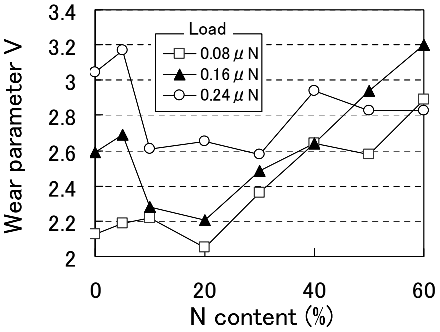


Fig. 7 Wear parameter as a function of N content [9].

5. Lubrication simulation [11] [12] [13] [14]

Lubricants play key roles in several kinds of machine systems. They have generally been fitted into the machine design, but sometimes their properties govern the machine design [11, 12, 13]. For monolayer perfluoropolyether (PFPE) films coated on a solid substrate, their behavior with respect to the approach and separation movement of another solid surface was simulated using molecular dynamics [11]. The presence of polar end groups caused contact to Zdol films and separation from Zdol films to occur at shorter solid-solid distances than contact to and separation from Z films. Liquid transfer to the solid surface was also less noticeable for Zdol than for Z. On the other hand, Zdol films exhibited stronger than Z films.

Figure 8 illustrates the simulation model. These polymers were described by a coarse-grained bead-spring model in which each polymer contained 10 spherical beads connected by springs. The lubricants used were PFPE Z, which are linear chain copolymers with identical backbones but different end groups. Figure 9 show the side-view snapshots of PFPE Z and Zdol films.

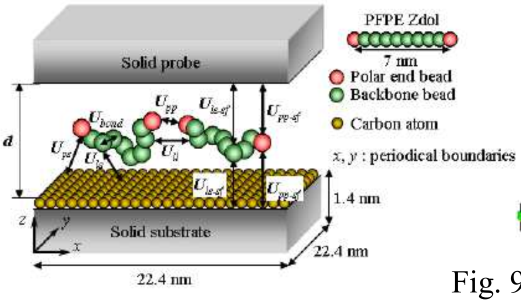


Fig. 8 Simulation model [11].

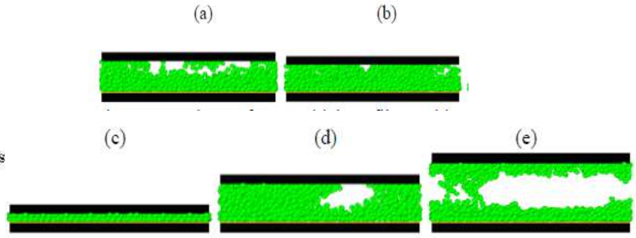


Fig. 9 Snapshots of 2-nm-thick Z films with respect to the relative displacement of two solid surfaces [11].

A classical molecular dynamics (MD) method cannot simulate the tribochemical reaction dynamics because it does not consider the electrons in nature. Although the first-principles - based MD method has recently been used for understanding the chemical reaction dynamics of several molecules in the tribology field, it cannot be used to simulate the tribochemical reaction dynamics of a large complex system including solid surfaces and interfaces because the computational cost is too high. A new quantum chemical MD tribochemical simulator based on a hybrid tight-binding quantum chemical/classical MD method, however, has been developed recently [12]. In this simulator the central part of the chemical reaction dynamics is calculated by the tight-binding quantum chemical MD method and the remaining part is calculated by the classical MD method. It can therefore be used to study the tribochemical reaction dynamics of systems too complex system to be studied, using the conventional classical MD or the first-principles MD methods. The dynamic behavior of the molecule in the heated oil phase was studied. As shown in Figure 10(*a*), the simulation model consisted of one MoDTC molecule and 22 molecules of poly-alpha-olefin (PAO4). A classical MD calculation was first performed for the constructed model, and subsequent calculations by the quantum chemical MD tribochemical simulator were carried out for four different snapshots obtained by classical MD. Four diatomic interactions in the MoDTC molecule were focused on: the MoA–SA, CA–SB, CA–OA, and MoA–OA interactions shown in figure 10(*b*). The structural changes of the MoDTC molecule during the simulation were observed (Figure 11).

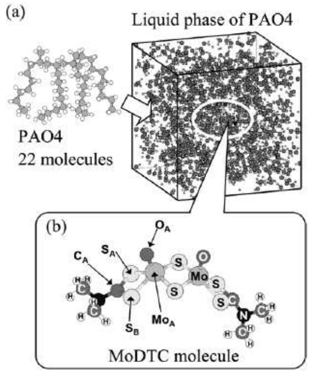


Fig. 10 (a) Calculation model used for the study of dynamic behavior of MoDTC molecules in PAO4 and (*b*) structure of MoDTC molecule in the oil phase [14].

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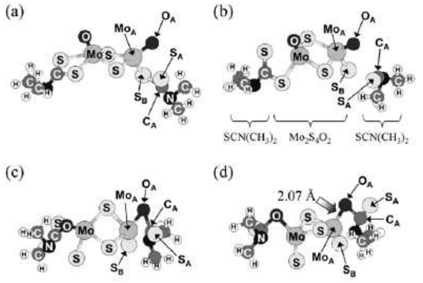

Fig. 11 Structures of MoDTC molecule in PAO4 at simulation times of (*a*) 100 fs, (*b*) 200 fs, (*c*) 400 fs, and (*d*) 500 fs [14].

6. Meso-scale simulation (particle dynamics simulation) [15] [16] [17]

Simulation range is limited in MD and MO methods, but particle-based methods can applied to a wide range of interface phenomenon. The moving-particle semi-implicit method (MPS) has been very popular in Japan [18].

Particle-based numerical simulation was used to investigate the dynamic behavior of the meniscus bridge [15]. The numerically simulated growth process of a meniscus bridge agrees qualitatively with experimental snapshots, but the simulation finishes growth much faster than the growth observed experimentally. This simulation used the static contact angle model, which causes an unnatural curve at the beginning of the growth. It is found that the contact angle plays an important role in the dynamic process of the meniscus bridge formation. As shown in figure 12, after the droplet contacts the upper wall (0 ms) the top of the droplet starts to spread and form the liquid bridge. This value corresponds to the contact angle from the experimental snapshot of the droplet on the optically flat glass (BK7).

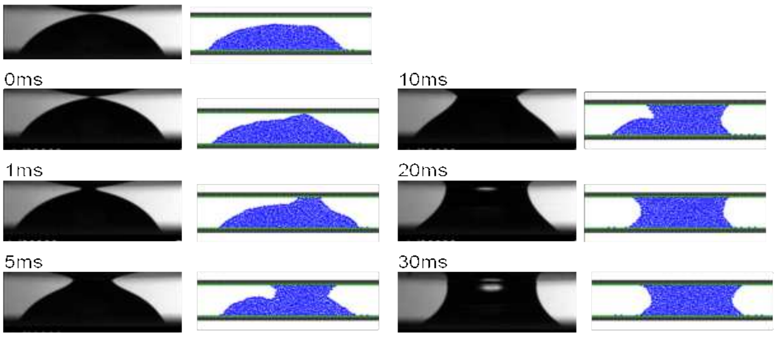

Fig. 12 Snapshots of experimental and simulation results [15].

Lubricant behavior within the head-disc clearance was simulated using a particle method based on continuum dynamics [16]. The results obtained when lubricant behavior was simulated for various sets of surface tension and viscous stress showed that the viscosity of the bulk condition depends more on viscous stress than surface tension. A few droplets were ejected when the lubricant reached the tail of the slider, where the viscous stress was 10^{-4} of bulk condition. Eventually, the lubricant on the bottom of slider surface moved onto its sidewall. The initial lubricant bridge was deformed by viscous stress, where viscous stress was 10^{-2} of the bulk condition (Figure13). There is no spread of lubricant on the slider surface. Eventually, part of the bridge was left on the slider.

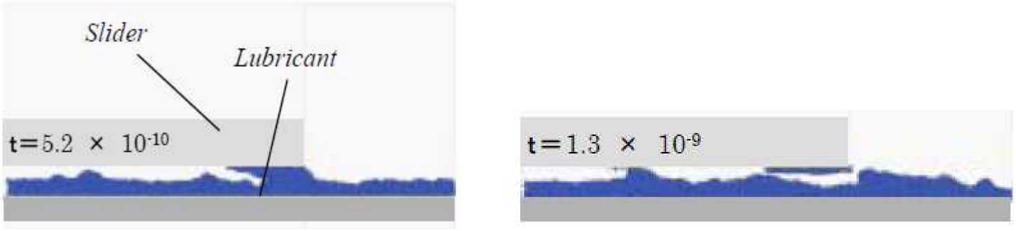

Fig. 13 Lubricant behavior in clearance between slider and disc[16].

7. Future methodology

In various kinds of product areas the demands are so severe that it is hard to make a good product by using only a traditional way of thinking we need a new approach to the elucidation of tribological phenomena: a multi-scale and multi-physics approach. The most important point for tribological simulation is the development of a high-accuracy model for the physical system of interest. The mathematical description of the model is given by physical laws, boundary conditions, and initial conditions and may be expressed as algorithms which can be carried out by numerical procedures. In addition, in the concept of the true-contact-area model, the effective area of true contact is determined from surface geometry and material properties when the distance between two surfaces is given. We thus need a simulation model composed of the following parts:

(1) a contact model to determine the true contact area and the contact load from the distance between two surfaces, the surface profile, and micro-scale material properties;
(2) a thin film lubrication model to define film thickness behavior, fluid film pressure, and the load balance supported by the fluid pressure;
(3) a validation method comparing simulation results and experimental results;
(4) a statistical model that express the uncertainty of the actual phenomena and the simplicity of the simulation model.

Some viewpoints are important to elucidating a complicated phenomenon in this simulation model. Several approaches seem necessary for a tribological simulation to be used in product design. First, a data-base of the standard contact model that expresses the actual surfaces to a certain degree of precision is very useful. Second, also useful is the technology with which a standard model based on experimental data is identified. Furthermore, quantification of the precision of each simulation model is also important. Third, also necessary is data-base comparing experimental results with a simulation-model data. That is, verification and validation of simulation results are valuable. We'll also need way to interpret analysis results in consideration of various knowledge databases. Finally, we have to pay attention to the analysis of robustness, unevenness, and variation. Key technologies are optimization, knowledge technology, statistical methods, and data mining. They are intellectual design approaches to elucidating complicated phenomenon in tribology.

We think that an intellectual design system can be carried out when multi-scale simulation technology, with which a simulation model of each scale is connected, cooperates with the "envisioning" approaches such as exploration technology and the knowledge technology. As a result, not only high reliable but also value-added products will be produced.

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Nanoscale Wear in Materials Tribology

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The field of materials tribology has entered a phase of instrumentation and measurement that involves accessing and following the detailed chemical, structural, and physical interactions that govern friction and wear. At the "frontier of fundamental tribological research" is the development of new experimental methods that are capable of monitoring phenomena that occur within the life of a sliding contact. This talk will highlights *in situ* approaches as applied to materials tribology — *the study of contacting surfaces and interfaces in relative motion.* The findings are that very thin surface films of only a few nanometers in thickness are often responsible for the protection and performance of many modern tribological materials.

Multiscale Aspects of Tribology

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Severe material deformation processes as found in tribology or metal forming are accompanied by significant structural changes of the near-surface volume. In addition, due to cyclic creep also the bulk experiences mechanical interactions represented, e.g., by the formation of dislocations and of shear bands. As a result, these effects have multi-scale properties and run on different time scales. Consequently, a forecast that targets lifetime aspects is hardly possible or prone to large errors.

In order to determine the material properties, sophisticated characterization methods have to be applied. Since mainly near-surface material properties are of concern, reliable methods must be used to distinguish between artefacts and real features of the material.

This contribution focuses on the testing and understanding of fine grained and nanocrystalline materials, their formation and characterization.

Tribology at the Nanoscale: Insights from Atomistic Simulations

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Understanding the mechanisms associated with nanometer-scale tribology and wear is critical to controlling these behaviors. Here, these mechanisms are discussed for nanostructured and molecular systems.

First, classical, reactive molecular dynamics (MD) simulations are used to examine the tribological responses of onion-like carbon (OLC) fullerenes with and without a residual diamond core placed between sliding diamond-like carbon surfaces. The simulations predict that there is no discernable difference due to the presence of the diamond core. However, the frictional behavior of these systems is predicted to be highly dependent on the interactions that take place between the fullerenes and the surfaces. Without the formation of bonds with the substrates, the OLC fullerenes are able to roll and thus have extremely low frictional forces. As bonds begin to form between the fullerenes and the surfaces, the OLC fullerenes begin to slide which causes a significant increase in the observed friction.

Second, the molecular responses of small, fluorocarbon molecules trapped between self-mated and aligned polytetrafluoroethylene (PTFE)-PTFE surfaces are also considered. Two fluorocarbon molecular classes are considered: C_2F_6 and C_8F_{18}, and the effects of film thickness for each class are compared. The simulations predict that the systems with thicker lubricating layers exhibited a friction coefficient that is significantly lower than those with thinner lubricating layers. They also predict that the smaller lubricating molecules enhance lubrication by rolling, while the larger molecules only slide. Interestingly, unlubricated PTFE-PTFE self-mated systems demonstrate low friction coefficients and molecular wear when the chains slide in a direction parallel to the chain align.

This work was supported by the National Science Foundation (grant CMMI-0742580) and an AFOSR-MURI (grant FA9550-04-1-0367).

Atomistic Simulations of Tribology at Sliding MoS_2 Surfaces

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Molybdenum disulphide (MoS_2) is the most commonly used solid lubricant coating in aerospace applications. In this work, we develop new empirical many-body potentials for Mo and S systems and examine nano-scale friction between sliding MoS_2 surfaces using classical molecular dynamics (MD) simulations. In particular, MD simulations of Mo cross-linked MoS_2 interfacial sliding at various loads, temperatures and sliding directions are carried out. The loads and friction forces are extracted to calculate the friction coefficient of the MoS_2 as a function of temperature, and the results are compared to experimental pin-on-disk measurements of MoS_2 coatings and AFM measurements on single crystal MoS_2 surfaces. The results from both the DFT calculations and the MD simulations help us to better understand the origins of lubricity on MoS_2.

This work was supported by AFOSR-MURI grant FA9550-04-1-0367.

Polymer Brushes and Lubrication

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Nature lubricates with an aqueous solution of biomolecules—mostly glycoproteins. These consist of a proteinaceous backbone with sugar side chains. Glycoproteins attach to the surfaces to be lubricated via hydrophobic and other interactions, and expose sugar chains at the sliding surface. These sugars appear to play the role of maintaining a relatively immobile water layer, which holds the surfaces apart and provides a low-shear-strength interface.

Synthetic polymer brushes can be used in a similar, somewhat biomimetic, fashion, in order to lubricate sliding surfaces in a liquid that is a good solvent for the brushes. The brushes are resistant to compression due to osmotic pressure, and entropic forces also resist their interdigitation. In our laboratories, we have synthesized a number of graft copolymers, with structures resembling those of simple glycoproteins, and these have proven to be highly effective in the formation of polymer brushes on a variety of systems, with concomitantly impressive lubrication behavior, notably on soft surfaces in an aqueous environment.

Since the grafting density of the brush chains has a number of positive effects on the lubricating properties of the brush, it was also decided to also adopt a “grafting from” approach, whereby the polymer chains were actually synthesized on the surface, with the brush forming during synthesis. Such brushes have shown not only to produce very low friction, but also to show promising anti-wear properties.

Wear of Nanocrystalline Ceramics by Atomistic Simulations

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Ceramics show outstanding mechanical properties such as high strength and high hardness over a wide range of temperatures and are stable in harsh environments. However, the low fracture toughness of ceramics limits their practical utility for instance as wear-resistance coatings. There have been several reports of improving the fracture strength of ceramics by reducing the grain sizes to nanometer regime. At the same time it has been suggested that use of nanoscale tools leads to ductile machining by suppressing fracture in these small scale deformations. Choosing silicon carbide (SiC) as a model ceramic, we have performed large scale parallel molecular dynamics (MD) simulations of wear in nanocrystalline (nc) SiC to understand the toughening mechanisms in the presence of grain boundaries and the effect of grain size on plasticity in ceramics. Dislocation plasticity inside the grains, grain boundary sliding and grain boundary fracture have been identified as the deformation mechanisms active during wear in nc-SiC whereas separate simulations of wear performed on single crystal SiC show only dislocation plasticity. We have quantified the contribution of each of these mechanisms to strain relaxation inside the deformation zone as a function of grain size and the depth of cut. In order to determine the effect of pre-existing flaws on wear, we performed separate simulations of crack propagation in nc-SiC. We find that nc-SiC exhibits R-curve behavior and that the interplay between grain boundary sliding and inter-granular fracture is critical for control of wear in nc ceramics. Sliding at the grain boundaries can be controlled by dopants. To discuss the effect of doping on grain boundary sliding and overall mechanical response of the material, we will show results of large scale MD simulations of nanoindentation of ultrananocrystalline diamond (UNCD) with varying percentage of H atoms in the grain boundary regions.

Two-scale approach to the diffuse scattering of visible light from rough surfaces

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Experimental techniques applied to analyze rough surfaces are commonly optical ones, which e.g., by monitoring the diffusely scattered light, quantitatively access the roughness of these surfaces. Beyond the obvious technological interest, an ab initio (first-principles) investigation of the optical properties of rough surfaces is also challenging because it implies a suitable multiscale framework.

In the present contribution a two-scale approach to the diffuse light scattering from rough surfaces [1] is presented and applied, within which the macroscopic Maxwell equations are numerically solved for ab initio calculated layer-resolved permittivities in the case of an incident visible light propagating in form of a harmonic plane wave.

In fact, the ab initio inter- and intra-layer contributions to the complex optical conductivity tensor are firstly calculated based on the Luttinger formalism and by means of a contour integration within the spin-polarized relativistic screened Korringa-Kohn-Rostoker method. These contributions are then summed up to form the layer-resolved permittivities, which in turn uniquely characterize from an optical point of view the surfaced system of interest and yield together with the roughness of the surface the set-up of the next, macroscopic part of our two-scale scheme. On the latter length scale, a 2×2 matrix technique, which properly accounts for all possible reflections and optical interferences within a layered system, is extended to also account for the roughness of the surface layer.

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Multiresolution FEM-BEM contact mechanics

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The recently developed FEM-BEM scheme by the authors [1] completely exploits the main advantages of both finite element and boundary element methods by solving the elastic multi-asperity contact problem within BEM for which all influence coefficients are prior calculated applying FEM.

A multiresolution analysis (MRA) of tribological / engineering surfaces, on the other hand, allows one to unambiguously separate their form from their waviness and roughness at any level of resolution based on the lifting scheme, i.e., using second generation wavelets.

First, preliminary results on the stress distribution, contact area and interfacial separation, respectively, have already shown that combining our FEM-BEM scheme with the MRA, the so obtained multiresolution contact mechanics straightforwardly permits one to separately and fully controlled investigate the impact of waviness and roughness on each aforementioned quantity of interest at different levels of resolution.

In addition, in the present contribution, an attempt will be also made to relate the MRA provided purely mathematical decomposition of tribological / engineering surfaces to the various length scales detectable in their waviness and roughness.

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