

MODELS OF FRICTION AND WEAR OF DLC FILMS

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ABSTRACT

Wear and friction of DLC (diamond-like carbon) covered counterparts are under consideration. Experiments showed that abrasion is the leading wear mechanism at the beginning of the wear process. However, the ability of the surface to wear away the counterpart reduces very rapidly, often as a power law function of the cycle numbers. This phenomenon was explained assuming that the initial abrasiveness of a coating is determined by the number of the nano-sharp asperities that were in contact with the counterpart, i.e. by the number of the sharp asperities within the nominal region of contact. On this basis, a model of abrasive wear was developed, using the concept of statistical self-similarity of distribution of the nano-sharp asperities within the current contact region. After the sharp asperities were blunted or removed from the contact region, the wear is related either to phase transformations or to chemical mechanisms. Recent experimental studies of dry sliding between two hydrogenated DLC coated counterparts in low oxygen environment showed that adsorbates have considerable influence on friction and the friction coefficient increases with the increasing of the time interval between contacts. The observed friction phenomena are assumed caused by a reaction between the adsorbate and carbon atoms of the coatings, and when the slider passes a point on the track, it removes mechanically some adsorbate from the surface. The mechanical action leads to re-exposure of the surface to gases in the environment. We assume that there is a transient short-life high temperature field at the vicinities of contacting protuberances that may cause various transformations of the surface. We

suppose that first an adsorbate molecule becomes physically adsorbed to the surface and then chemisorption may occur between the carbon atoms of the coating and the 'sticky' oxygen atoms. The atoms or molecules of adsorbate interact with the counterpart. Our modeling established a direct connection between this kind of molecular friction and gradual wear. Using the new adsorption-desorption model, the numerical analyses of the friction coefficient were compared with experimental DLC friction results.

INTRODUCTION

Carbon-containing thin films such as DLC and boron carbide have the ability to enhance the fatigue resistance of heavily loaded steel components [1]. This is because these coatings can polish away asperities on the counterparts [2]. In recent studies of the kinetics of abrasive polishing of steel balls by the DLC and B₄C coatings, it was found that during repeated passes of a ball over the same region of a surface the abrasion rate drops significantly with every pass of the ball, coinciding with the loss of relatively sharp nanometer-scale DLC asperities, even as the micrometer scale structure is unchanged [3-5]. When there are no sharp asperities anymore gradual wear is observed. Often smooth DLC coatings show super low coefficient of friction (COF) [6, 7].

ABRASIVE WEAR

Assuming self-similar changes of the distribution function characterizing the statistical properties of patterns of scattered surface sharp asperities [1, 5], one can obtain that the average

distances $l(t)$ among sharp asperities and their number $N(t)$ are the power-law functions of the number of cycles n $l(n) = l(n_1)(n/n_1)^\alpha$, $\alpha > 0$ and hence, both the total amount of material removed from the central part of the slider and the abrasiveness $\overline{A(n)}$ are also the power-law functions $\overline{A(n)} \approx \overline{A(1)}n^{1-4\alpha}$. This explains the experimentally observed relations [4]. We have also explained wear and abrasiveness of hard carbon-containing coatings under variation of the load [8].

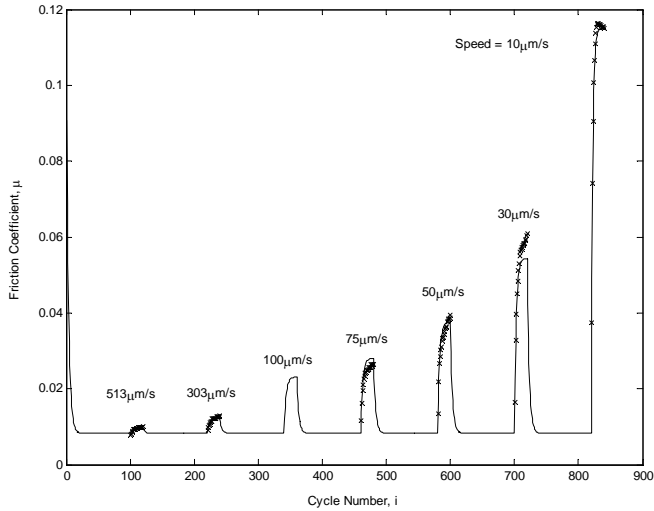


Figure 1. Friction coefficient as a function of sliding speed and cycle numbers. Data points (x) are the reciprocating pin-on-disk experimental data (from Heimberg et al. [9]) for DLC on DLC contact. Solid lines represent data obtained using numerical simulation of the friction coefficient based on the integral of the Elovich equation (1).

FRICITION AND GRADUAL WEAR

Ab initio calculations of the bond dissociation energies (BDE) between atoms were performed using Gaussian98 at the Møller-Plesset level of model chemistry. It was found that the BDE is 523kJ/mol, 1447kJ/mol, and 295kJ/mol for C-C, C-O and C-H bonds respectively. It is concluded that carbon wear particles will not be formed during gradual degradation since the coating carbon molecules are dissolved within the environment gases as CO or CO₂. The COF (μ) is considered as the following sum $\mu = \mu_c + \mu_{mol,1}$, where, $\mu_{mol,1}$ is the part of the COF caused by the breaking of interatomic bonds between the adsorbate and a surface, and $\mu_c = \mu_{mech} + \mu_{mol,2}$ is the part caused by mechanical effects and by all other molecular effects, in particular by the lattice oscillation mechanism. To describe the adsorption/desorption processes of the active gases, we assume that the Elovich equation describes the adsorption process $d\theta/dt = Be^{-\alpha\theta}$, where α and B are constants during an experiment, and θ is the fractional part (the relative

amount) of solute adsorbed at time t . The coverage $\theta(k,i)$ at point k during the cycle i increases in value continuously due to adsorption and decreases abruptly (the jump $[\theta(k,i)]^\pm$) when the disk passes the point. The jump is proportional to the coverage and probability (p) of the adsorbate removal. The average COF is:

$$\mu(i) = \mu_c + \frac{c}{n_m} \sum_{k=1}^{n_m} [\theta(k,i)]^\pm \quad (1)$$

This model allows us to describe recent experimental studies of dry sliding between two hydrogenated DLC coated counterparts in low oxygen atmosphere [9]. The numerical results showed that for a wide range of pin speeds the model compares well with the experiments (see Fig. 1.). The models [10, 11] help to explain how microscopic processes, such as the breaking and forming of interatomic bonds, may affect macroscopic phenomena, such as friction and wear.

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