



Substantiating the mechanisms of electronic and phonon friction in the conjugation of materials of samples (parts) by the methods of solid state physics

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Received: 20 February 2024; Revised 10 March 2024; Accept 16 March 2024

Abstract

The article elucidates the essence of the mechanisms of electronic and phonon friction in the coupling of samples (parts) using the methods of solid state physics.

It is shown that in the triboconjugation of samples made of metallic materials, the flow of fluctuation-electromagnetic and electron-phonon processes should be distinguished. Fluctuation-electromagnetic interactions have long-range effects, and electron-phonon interactions have short-range effects. Based on Lifshitz's fluctuation-electromagnetic theory, the force of friction in moving couplings of metal samples is substantiated, taking into account the frequency ratio in the atomic absorption spectrum and the plasma frequency. A formula for estimating the friction force was obtained, taking into account the dielectric function and the Clausius-Mossotti formula.

The electronic friction force was estimated using the "jelly" model and the generation of electron-hole pairs in the quantum perturbation theory of solid-state physics.

The mechanism of electronic friction was discovered based on the phenomenological theory of braking losses of slow ions in solids. The scheme of the model of the electronic friction mechanism is close to the Persson model, which connects the braking force with the electron scattering process. A refined formula for estimating the electronic friction force is proposed.

The strength of phonon friction is justified on the basis of structural effects that can be induced by the mechanism of breaking adhesive bonds, and perturbation theory. A formula was obtained for estimating the force of phonon friction, taking into account the frequency of phonons, the inverse decay time and the function of the two-dimensional Fourier image of the force of interaction between the atoms of the conjugated surface of the triboelement.

Cases of static and dynamic phonon friction are considered.

Electronic and phonon frictional forces are considered at the nanolevel. The Debye low-temperature approximation and refinement of the expressions for estimating the electronic and phonon friction forces are given, taking into account the type of interatomic potential.

Key words: fluctuation-electromagnetic interaction, electronic friction, phonon friction, perturbation theory, friction force, nanolevel, triboconjugation of samples.

Introduction

The energy of translational movement of tribocouples of samples (parts) is dissipated due to various dynamic mechanisms. Among the most important mechanisms of this type are the processes of fluctuation-electromagnetic interaction and excitation of electrons and phonons [1-3]. Fluctuation-electromagnetic and electron-phonon processes in the friction zone have their own specificity. Effects caused by short-lived excitations of the electron plasma and the formation of a set of electron-hole pairs can be attributed to the latter processes. While the fluctuation-electromagnetic interactions can be considered as long-range effects. This interpretation differs from that used in the work of Tomassoni and Widom [4]. Electronic processes at work in a broader sense are combined with fluctuation-electromagnetic interactions.



It is known from solid state physics [3] that the self-consistent quantum theory takes into account all possible types of excitations in the materials of parts in a single way. At that time, the development of such a theory, the final version of such a theory still needs further development, and possible types of excitations can be considered as subsystems with their own mechanisms. The specification of individual mechanisms is essential for a deeper understanding of the processes occurring in the surface layers of tribocoupled materials of samples (parts).

Literature review

The processes of single-particle excitations are forbidden by the laws of energy-momentum conservation in the absence of damping phonon and plasmon modes [5,6]. In the surface layers of parts materials, in the process of friction and wear, single acoustic phonons are generated by moving atoms, the speed of which is $v > v_s$, where v_s – is the speed of sound. At the same time, phonons are emitted in the cherenkov cone $\cos \theta = v_s / v$. In the presence of finite damping, particles can lose energy for the excitation of quasi-particles at arbitrarily low speeds of their movement [7,8].

Elementary excitations of quasiparticles are always accompanied by the final stages of energy dissipation in the triboconjugation of samples (parts) as a tribosystem in sliding processes. In the mode of contact mode of AFM [9-12], the proportionality of the speed of movement of quasi-particles to the dissipative (viscous) interaction forces of the conjugate surfaces of the samples (parts), which are relatively weak, is observed. In the contact mode, the total work produced by these forces does not exceed the value of $2 \cdot 10^{-22}$ J, while the work of adhesive friction forces is three to four orders of magnitude greater [13-16]. However, this estimate is based on an average velocity of the order of 1 m/s. At the same time, micro-slip occurs in 10^{-12} s, so the work of these forces should be increased by two orders of magnitude. In this case, the viscous force can be comparable to the force of static friction. At that time, dynamic friction plays a significant role in the processes of friction and wear in the tribosystem of parts samples.

A moving fluctuating dipole in the triboconjugates of sample materials (parts) induces electric currents on the friction surface. In this case, Joule damping is the final result of the friction process. In fluctuation-electromagnetic friction forces, accurate ideas about a number of main factors, such as their dependence on speed, distance to the surface, temperature, etc., have not yet been formed. The most general approach to solving the problems of fluctuation-electromagnetic friction is given by the fluctuation-electromagnetic theory of Lifshitz [17, 18].

Purpose

The purpose of the work is to find out the mechanisms of electronic and phonon friction in the coupling of sample materials (parts) based on the fluctuation-electromagnetic theory.

To realize the goal, the following tasks were performed:

1. Justification of the mechanism of fluctuation-electromagnetic friction in the couplings of metal samples (parts).
2. Elucidation of the mechanisms and contribution of electronic and phonon friction in the coupling of metal samples (parts).

Results

If a neutral atom in the material of the sample (part) has a speed v and moves parallel to the surface at a distance z from it, which exceeds the typical atomic dimensions, then a lateral (frictional) force proportional to the speed of movement acts on it. Taking into account the fluctuation-electromagnetic theory in solid-state physics, we can write:

$$F_{fr}^{fet} = \frac{3\hbar v}{8\pi z^5} \int_0^\infty d\omega \left\{ 2 \left[x''(\omega) \frac{d\Delta''(\omega)}{d\omega} - \Delta''(\omega) \frac{dx''(\omega)}{d\omega} \right] + \right. \\ \left. + \omega \left[x''(\omega) \frac{d^2\Delta''(\omega)}{d\omega^2} - \Delta''(\omega) \frac{d^2x''(\omega)}{d\omega^2} \right] \right\} \coth \left(\frac{\omega\hbar}{2k_B T} \right), \quad (1)$$

where ω – is the frequency of the absorption spectrum of the atom of the sample material (details); $x(\omega)$ – atomic polarizability; $\varepsilon(\omega)$ – dielectric function of the part material; k_B, \hbar, T – Boltzmann constant, Planck constant and thermodynamic temperature; $\Delta(\omega)$ – is a complex function depending on the dielectric function, which is equal to:

$$\Delta(\omega) = \frac{\varepsilon(\omega) - 1}{\varepsilon(\omega) + 1}. \quad (2)$$

Values with two dashes in formula (1) correspond to the imaginary numbers of the corresponding functions: $x''(\omega)$, $\Delta''(\omega)$. For the normal movement of a neutral particle to the conjugate surfaces of samples (parts), a formula similar to (1) has not yet been obtained.

The analysis of formula (1) shows that at $T = 0$ the force of friction is not equal to zero. This is a physical consequence of the existence of zero fluctuation of the electromagnetic field in materials. If we assume that $T \Rightarrow 0$, then formula (1) takes on a simpler form:

$$F_{fr}^{fet} = \frac{3\hbar v}{4\pi z^5} \int_0^\infty d\omega x''(\omega) \frac{d\Delta''(\omega)}{d\omega}. \quad (3)$$

Based on solid-state physics, the strongest line in the absorption spectrum of an atom is the frequency ω_0 . Then, considering the attenuation coefficient equal to zero, for the imaginary part of the part of the polarizability function, we will have the expression:

$$x''(\omega) = \frac{\pi e^2 f_{0tr}}{2m_e \omega_0} \delta(\omega - \omega_0), \quad (4)$$

where e, m_e, f_{0tr} – are the charge and mass of the electron, as well as the strength of the transition oscillator. Substituting (4) into (3), we use the standard approximation of the Drude-Lorentz model for the dielectric constant of the metal (sample material (parts)), we get:

$$F_{fr}^{fet} = \frac{3\hbar e^2 f_0 \tau^2 v}{4m_e z^5} \frac{y^2 (12x^4 - 4x^2 y^2 + 4x^2 - y^4)}{x(4x^4 - 4x^2 y^2 + 4x^2 + y^4)^2}, \quad (5)$$

where $x = \omega_0 \tau$, $y = \omega_p \tau$, ω_p and τ – plasma frequency and relaxation time of metal electrons. Analyzing formula (5), it can be seen that the sign of the force F_{fr} depends on the ratio of the frequency in the absorption spectrum of the atom and the plasma frequency. When their ratio is $\omega_p \geq \sqrt{2}\omega_0$, the force F_{fr} is a braking force. For the typical metals from which the samples (parts) are made, the specified parameters acquire the following values: $\tau = 10^{-4} - 10^{-5}$ s, $\omega_p = 5 - 15$ eV. This condition is almost always fulfilled. At that time, the reverse situation is also possible for the high-frequency absorption lines of the atom: the lateral force F_{fr} can become accelerating. However, it should be noted that the absolute values of the integral of the overlap of the absorption spectra of atoms depend on the values of x, y in formula (4). Therefore, for a correct assessment of the total frictional force F_{fr} , a detailed consideration of the absorption spectrum of the atom in a narrow range of frequencies around the value of $\omega_p / \sqrt{2}$.

The lateral force of friction acting in the moving tribosystem of conjugation of samples (parts) in the additive approximation [19] can be obtained from formula (1). To do this, the function $\alpha(\omega)$ is represented by the dielectric function $\varepsilon_1(\omega)$ of the material of the moving sample (parts) using the Clausius-Mossotti formula and integrating it over the volume of the surface layer of the friction zone. As a result, we get the formula:

$$F_{fr}^{fet} = -\frac{3}{64\pi} \frac{\hbar R v}{h^3} J(\varepsilon_1(\omega), \varepsilon(\omega)), \quad (6)$$

where R – is the radius of curvature of the moving sample surface in the contact zone with the conjugated sample (part); $J(\varepsilon_1(\omega), \varepsilon(\omega))$ – is the frequency integral, which coincides with the similar integral in formula (1) when replacing the expression of the polarizability of the atom with the expression:

$$\Delta''(\omega) = \text{Im}\{[\varepsilon_1(\omega) - 1]/[\varepsilon_1(\omega) + 2]\}, \quad (7)$$

It follows from formula (6) that the temperature dependence of the friction force becomes significant under the condition:

$$\omega \hbar \leq 2k_B T, \text{ when } \coth x \rightarrow x^{-1}, \quad (8)$$

At room temperature we have: $2k_B T \approx 0,05 eB$. This indicates that the main contribution to the materials of the samples (parts) is given by low-frequency absorption processes. This is similar to dipole relaxations in dielectrics and infrared absorption in ionic and conducting crystals.

Estimates of friction force values according to formula (6) were made for combinations of different types of materials. If $R = 10 - 20$ nm, $v = 1$ m/s, $z = 0,2 - 0,3$ nm, then at room temperature we obtain the following friction

forces in the range of 0.1-10 nN . Such forces can make a significant contribution to the damping coefficients of lateral oscillations at a Q-factor of the order of 10^4 - 10^5 .

The value of the factor due to the force of dynamic friction can be estimated by the formula:

$$Q = k_1 v / 2\Omega_1 F, \quad (9)$$

where k_1 – rigidity; Ω_1 – the frequency of the material of the samples (parts), which is an order of magnitude higher than the frequency of normal oscillations. At a stiffness of 100 N/m, a frequency of 10^6 - 10^7 Hz, a speed of 1 m/s and for a force of 1-10 pN, the Q factor is equal to: $Q = 5 \cdot 10^5 - 5 \cdot 10^7$.

The measurement of the Q-factor shift due to electromagnetic coupling with the surface is a real experimental task.

Electronic friction is a component of fluctuating electromagnetic friction. The mechanism of electronic friction associated with the generation of electron-hole pairs. It was first analyzed by Persson in connection with the problem of damping of lateral vibrations of films adsorbed on a metal substrate [8, 9]. At the same time, the connection between the force of friction, which occurs during the scattering of conduction electrons on the oscillating atoms of the adsorbate, and the change in the resistance of the sample material (parts) was used. If the return time of the damping of the lateral oscillations of the adsorbate atom is denoted by $1/\tau_s$:

$$F_{fr}^e = M_a n_s v / m_e n_e d \tau_s, \quad (10)$$

where M_a and n_s – mass and surface density of film atoms on the surface of the sample (details); m_e , n_e and d – are mass, conduction electron density and film thickness. The coefficient is proportional to the speed and can be considered as the inverse relaxation time $\gamma_s = 1/\varepsilon_s$ associated with an additional electron scattering mechanism. As a result, the specific resistance of the surface layer of the sample material (parts) increases by the amount:

$$\Delta\rho_e = m_e / n_e e^2 \tau_e = M_a n_s / n_e^2 c^2 \tau_s, \quad (11)$$

and the desired decay time τ_s is equal to:

$$\tau_s = \frac{M_a n_s}{n_e^2 e^2 d \Delta\rho_e}, \quad (12)$$

This theory provides acceptable estimates of the damping time of the lateral movement of atoms (molecules) in the surface layers of sample materials (parts) in the case of physical and chemical adsorption. At that time, it was based on a very simplified model that did not take into account the structure of the surface layer and the nature of the distribution of electrons near its surface.

In the quantum theory of perturbations [20], braking losses of material atoms of samples (parts) upon excitation of electrons are considered. A "jelly" model with a sharp potential jump at its spatial boundaries is proposed for conduction electrons. Assuming that the braking force does not change for heavy atoms with a mass of M_a , then the damping time of their lateral motion is equal to:

$$\Delta t_e = \frac{M_a v}{F_{fr}} = \frac{2\pi M_a}{27\hbar r_B^2 k_F^4}, \quad (13)$$

where k_F – is the Fermi vector of electrons (metal) of the sample material (parts); r_B – is the Boriv radius. The estimate according to formula (13) shows that the decay time of atoms of the order $(1,1\dots1,5) \cdot 10^{-11}$ s. The damping time of the lateral movement of atoms in the sample material (parts) can be reduced with the help of the following factors:

1. Energy losses of atoms with a large nuclear charge should be greater, since the effective charge of heavy atoms is greater than unity.
2. For surface layers of material (films) with a regular N-fold periodic structure, where N – is the number of atoms in the surface layer (film).

The considered theory gives too large values of the electronic friction force and small damping times of the motion of atoms in the surface layers and in adsorbed films.

Another approach to the detection of electronic friction mechanisms is based on the phenomenological theory of braking losses of slow ions in solids: energy losses appear as a result of the hypothetical exchange of electrons belonging to moving atoms. In the triboconjugation of samples (parts), there is an exchange of electrons between their atoms on friction surfaces in the tribosystem. At the same time, each electron of the triboelement that crosses the surface of equal potential of the tribosystem "element 1 - element 2" loses the momentum of relative motion $m_e v$. In fact, this scheme is close to Persson's model, which relates the braking force to the electron scattering process. According to this theory, the energy loss by a neutral atom of triboelement 1 with a nuclear

charge Z_1 and speed v flying at a distance b from an atom of the conjugate surface of triboelement 2 with a nuclear charge Z_2 is equal to:

$$\Delta E = \frac{m_e e^2}{\hbar} \frac{0,35(Z_1 + Z_2)^{5/3}}{\left[1 + 0,16(Z_1 + Z_2)^{1/3} b / r_B\right]^5} v, \quad (14)$$

Assuming that the material of the sample (parts) has a uniform distribution of atoms with a density n_a , and the moving atom is at a distance z from the surface. After integrating (14) over all possible aiming parameters of atomic motion, we have:

$$F_{fr}^e(z) = \frac{dE(z)}{dz} = -0,7(Z_1 + Z_2)^{5/3} \frac{m_e e^2}{\hbar} n_a v \times \int_z^\infty \frac{b \arccos(z/b) db}{\left[1 + 0,16(Z_1 + Z_2)^{1/3} b / r_B\right]^5}, \quad (15)$$

The specified theory makes it possible to obtain an expression for the braking force acting on a moving triboelement, using the "jelly" model and the locally flat approximation for the distribution of electrons within the homogeneous contact of the materials of the conjugated surfaces of the samples (parts):

$$F_{fr}^e \approx \frac{3\pi}{10} (3\pi^2)^{1/3} \hbar v n_e^{4/3} \frac{(R + h/2)^2}{b^2 R^2} (1 + bR) \exp(-b\bar{h}), \quad (16)$$

where \bar{h} – is the average distance between the conjugate surfaces of triboelements; n_e – is the electron density in the surface layer of the material.

For electrically conductive materials of triboelements in the case of "Al-Al" contact, $b \approx 1,19 \text{HM}^{-1}$, at $R=20 \text{ nm}$, $h = 0,2 \text{ nm}$, $v = 1 \text{ m/s}$ we obtain $F_{fr} \approx 0,67 \text{pH}$ by expression (16). The role of this mechanism in the case of contact of non-conductive materials is insignificant.

Phonon friction is also a component of fluctuating electromagnetic friction. There is still no generally accepted point of view about dynamic phonon friction either. This is partly due to the fact that the corresponding mechanism is manifested on the basis of structural effects that can be induced by the mechanism of breaking adhesive bonds.

Using perturbation theory, it is possible to obtain a formula for estimating the braking force (phonon friction) of a single adsorption atom (film) of the surface layer of the material of the samples (parts):

$$F_{fr}^f = \frac{1}{M} \sum_k \frac{\gamma k_x^2 |f(\vec{k})|^2 v_a}{\left[\Omega_0(\vec{k})^2 - k_x^2 v_a^2\right]^2 + \gamma k_x^2 v_a^2}, \quad (17)$$

where $\Omega_0(\vec{k})$ – is the phonon frequency; γ – reverse decay time; k_x – projection of the wave vector \vec{k} on the direction of movement; v_a and M_a – are the speed and mass of the atom in the surface layer (film) of the material of the samples (parts); $f(\vec{k})$ – is a two-dimensional Fourier image of the force of interaction of atoms with the conjugated surface of the triboelement. If the force F_{fr}^f – is periodic, then the function $f(k)$ is proportional $\delta_{\kappa,G}$, where G – is a two-dimensional vector of the inverse lattice. For the case, $\gamma \rightarrow 0$ formula (17) takes the form:

$$F_{fr}^f = \frac{\pi}{M} \sum_k k_x |f(\vec{k})|^2 \delta(\Omega_0(\vec{k}) - k_x v_a), \quad (18)$$

The equality follows from formula (18):

$$\Omega_0(\vec{k}) = k_x v, \quad (19)$$

which determines the condition of phonon generation in the triboconjugated materials of the samples. At the same time, it is obvious that this equality cannot be fulfilled at speeds lower than the speed of sound. At that time, $\gamma \neq 0$ the more general formula (17) gives the finite force of phonon friction. The value of phonon friction is a small value proportional to the expression $\gamma v_a / \Omega_0^4(G)$, at $v_a \rightarrow 0$.

To obtain a realistic estimate of the braking time by a surface layer or an adsorbed film that forms a structure incommensurate with the adsorbate. Triboelement materials must be partially disordered. This breaks the translational symmetry and greatly increases the strength of the phonon friction, or uses an exaggerated phonon decay time (10^{-3} s). In the latter case, it follows from formula (18) that the force of phonon friction is equal to:

$$F_{fr}^f = \frac{\pi^2 N}{GM v_s^2} |f(G)|^2, \quad (20)$$

where N – is the number of atoms of the surface layer of the material of the sample (parts) or film; v_s – speed of sound; G – is the minimum vector of the inverted lattice.

In this case, the force of phonon friction does not depend on the speed. Obviously, its value largely depends on the parameters N , v_s , $f(G)$. The results of the study indicate that the assessment of the role of this mechanism of phonon friction requires additional analysis and justification. The speed of phonons in small-sized films is closer to 100 m/s than to 1000 m/s [7,8], and the value of the Fourier factor $f(G)$ should significantly depend on the distance z between the film and the surface, decreasing with increasing z .

Dynamic phonon friction also occurs during the movement of individual atoms, and the corresponding forces of phonon friction can be estimated within the framework of quantum perturbation theory. At the same time, the most significant role is played by the scattering processes of surface phonons in the film or surface layers of the material of the samples (parts). For the high-temperature phonon acoustic spectrum corresponding to the thermodynamic temperature T and the condition $v/v_s < 1$, the force of phonon friction is equal to:

$$F_{fr}^f = \frac{S(k_B T)^2}{(\hbar v_s)^3} |U_G(z)|^2 \frac{v}{v_s}, \quad (21)$$

where $U_G(z)$ – is the two-dimensional Fourier factor of the interaction potential of the atom with the surface of the sample material (details); S – is the area of the unit cell. The dependence on the distance z is determined by a specific type of Fourier factor $U_G(z)$, and the quadratic dependence on the thermodynamic temperature is due to the two-dimensional phonon spectrum of the surface of the sample material (details).

Note that the estimate of the phonon friction force uses the interatomic potential of the form:

$$v(r) = -C_0 r^{-6} \left(1 - 0,5(r_0/r)^6\right), \quad (22)$$

where $C_0 = 3,75 \cdot 10^{-78} \text{ J} \cdot \text{m}^6$, $r_0 = 3,8 \cdot 10^{-10} \text{ m}$. Calculations show that the phonon friction mechanism provides the observed retardation time of the order of 1 ns if the atom is actually adsorbed at a distance of 0,3-0,35 nm from the surface.

Phonon friction is considered at the nanolevel. At the same time, the presence of a vacuum gap (of atomic size) between the triboelements does not prevent the passage of phonons, which carry out momentum transfer, and is taken into account due to the change in the speed of sound. In the Debye low-temperature approximation, the force of phonon friction is equal to:

$$F_{fr}^f = \frac{\pi^3}{45} \left(\frac{k_B T}{v_s \hbar}\right)^4 R^2 \hbar v \frac{v_t}{v_s}, \quad (23)$$

where v_t and v_s – are sound speeds through tribocontact and in volumes of material. At $R = 20 \text{ nm}$, $v = 1 \text{ m/s}$, $v_s = 6600 \text{ m/s}$ (silicon), $v_t/v_s \approx 0,1-0,01$, $T = 300 \text{ K}$, the estimate for the friction force gives a value of $F_{fr}^f = 0,5-5 \text{ pN}$, comparable with those to which other mechanisms of dynamic friction lead.

The tangential stress τ_s applied to the intermediate layer of atoms (molecules) located between the triboelements is a function of the sliding speed $\tau_s = \tau_s(v)$. At the same time, the adsorption film can be in both a solid and a liquid state, alternately "oscillating" between triboelements during the movement of the upper one in the "sticking-sliding" mode, and the thermodynamics of the corresponding phase transition is characterized by a phase diagram in the "temperature-degree of coating" variables.

If the film is in the liquid phase, then the sliding speed of the upper triboelement can be different from zero at arbitrarily small values of the shear stress. If the film has solidified, then $\tau_s \neq 0$ and $v = 0$. The lack of adhesion is therefore associated with the formation of a two-dimensional liquid layer. This is consistent with the results of experimental studies. If the film is in the solid phase and has a structure comparable to the substrate, then this structure is preserved until the tangential stress τ_s reaches a critical level τ_{0s} , at which the film passes into the liquid phase. When the tangential stress is reduced τ_s to values smaller than τ_{0s} This indicates that this model explains the hysteresis of the phonon friction forces in the triboconjugated materials of the samples.

To identify the conditions of the absence of phonon friction in tribosystems, a model of the dynamics of an isolated atomic chain is used. Since the phonon modes of a solid body of finite dimensions are separated from each other by a fairly wide interval, a situation may arise when the distance between the modes exceeds the natural width of the absorption frequency lines. In this case, the transition of translational motion into vibrational modes (and, finally, into thermal energy) is complicated, and the motion can be carried out without losses (absence of phonon friction) for a long period of time. For the acoustic boundary of a three-dimensional cubic sample, the corresponding condition has the form:

$$\frac{(v_s \pi / Na)^2}{\omega} \gg \gamma, \quad (24)$$

where $Na = L$ – is the size of the cubic sample; α – became a cage.

At $v_s = 10^5$ m/s, $L = 1$ cm this condition gives $\gamma\omega < 10^{11}$ c⁻², which can be the case for low-frequency acoustic modes.

In the far infrared region (<15 MeV), the attenuation constants were 0,2-1,1 MeV. In this case $\omega\gamma = 10^{24}-10^{25}$ s⁻². The half-width of the absorption lines was found to be in good agreement with the formula:

$$\gamma = \frac{M_{ad}\omega_0^2}{S_{ad}\rho v_s}, \quad (25)$$

where M_{ad} – is the mass of the adsorbate ; ω_0 – frequency of oscillations; S_{ad} – is the surface area occupied by the adsorbate ; ρ and v_s – is the mass density of the substrate and the speed of transverse phonons. Damping of the translational motion of molecules (atoms) in the direction normal to the surface can be satisfactorily explained by the phonon mechanism. This is observed under the condition:

- frequency of oscillations of molecules (atoms) is much less than the frequency of volume phonon modes;
- there are no even weak chemical interactions that can lead to the emergence of a dominant contribution of electronic excitations (electronic friction).

The presented theoretical reasoning is specific to samples (parts) made of metal materials. As for the theory of friction of polymers on a solid surface, a new approach is proposed, according to which the largest contribution to the friction force is related to the contribution of internal friction, due to the fluctuating character of the surface stresses acting on the polymer from the side of the microprotrusions of the solid surface. Another contribution is related to the strength of adhesion. At low sliding speeds, adhesion forces deform the polymer surface in such a way that it fills indentations in the surface relief. At very low relative speeds of movement of triboelements, the first mechanism dominates, since most polymer materials exhibit significant internal friction even at very low frequencies (about 0,1 s⁻¹).

Conclusions

1. It was found that the theoretical understanding of the mechanisms of electron-phonon friction at the nanolevel remains at a rather low level. There is no single quantum theory that self-consistently takes into account all types of elementary processes occurring in the materials of samples (parts) in the contact zone. There is no unified approach regarding the quantitative characteristics and relative role of electronic, electromagnetic, and phonon excitation mechanisms. Today there is no differentiation between them. At that time, there are two types of nanostructure friction: static, independent or weakly dependent on speed, and dynamic, proportional to speed. The microscopic theory of static friction is still phenomenological, and the mechanisms of dynamic friction are more detailed, but require further verification.

2. Macroscopic contact mechanics provides an acceptable interpretation of experimental dependences such as "friction force – load force" and measurements of the area of elastic nanocontacts . At that time, a simple extrapolation of the mechanical properties of the materials of the conjugated samples (parts) to the nanostructural level can lead to significant errors. Parameters such as contact area, shear stress, and work of adhesion at the nano-level can undergo significant changes. It was also found that the existing contact models do not allow describing more complex effects related to the interphase atomic and electronic structure, chemical composition and microscopic mechanisms.

3. The method of molecular (atomic) dynamics when applied to nanoindentation and nanofriction generally gives a satisfactory description of the energy, structure and dynamics of contacts, as well as a number of other tribological effects. In the simulation, ultra- short time intervals, high speeds of nanoprobess and limited statistics of nanoparticles are forced to be used . Increasing the simulation time (or the number of particles) to realistic values is fundamentally impossible due to the huge costs of machine time and the accumulation of errors in the calculation of the kinetic energy of particles.

4. It was determined that all dynamic mechanisms of friction at the nanolevel , despite existing differences, lead to quantitatively close values of friction forces of about 1 pN at probe speeds of 1 m/s. The presence of specific, for different mechanisms, dependences of friction forces on the radius of the probe, temperature and other physical parameters of tribocontacts makes it possible to choose between the available models based on the measurement of damping decrements in the vibration mode. This creates a basis for the development of new methods for diagnosing the parameters of nanostructures by non-destructive methods.

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Аулін В.В., Тихий А.А., Кузик О.В., Гриньків А.В., Лисенко С.В., Жилова І.В. Обґрунтування механізмів електронного та фононного тертя в спряжених матеріалів зразків (деталей) методами фізики твердого тіла

В статті з'ясовано сутність механізмів електронного та фононного тертя в спряженнях зразків (деталей) методами фізики твердого тіла.

Показано, що в трибоспряженнях зразків з металевих матеріалів слід розрізняти протікання флуктуаційно-електромагнітних і електронно-фононних процесів. Флуктуаційно-електромагнітні взаємодії мають далекодіючі, а електронно-фононні – короткодійні ефекти. Виходячи з флуктуаційно-електромагнітної теорії Ліфшиця обґрунтовано силу тертя в рухомих спряженнях металевих зразків, враховуючи співвідношення частоти в спектрі поглинання атома і плазмової частоти. Отримано формулу для оцінки сили тертя, враховуючи діелектричну функцію і формулу Клаузіуса-Моссоті.

Оцінку сили електронного тертя проведено, використовуючи модель "желе" та генерацію електрон-діркових пар в квантовій теорії збурень фізики твердого тіла.

Виявлення механізму електронного тертя здійснено, виходячи з феноменологічної теорії гальмівних втрат повільних іонів в твердих тілах. Схема моделі механізму електронного тертя близька до моделі Персона, що зв'язує силу гальмування з процесом розсіювання електронів. Запропоновано уточнену формулу оцінки сили електронного тертя.

Силу фононного тертя обґрунтовано на основі структурних ефектів, які можуть індукуватися механізмом розриву адгезійних зв'язків, та теорії збурень. Отримано формулу для оцінки сили фононного тертя з урахуванням частоти фононів, зворотного часу затухання та функції двомірного Фур'є-образа сили взаємодії атомів спряженої поверхні трибоелемента.

Розглянуто випадки статичного та динамічного фононного тертя.

Електронна та фононна сили тертя розглядаються на нанорівні. Дано дебаєвське низькотемпературне наближення й уточнення виразів для оцінки електронної та фононної сил тертя з урахуванням виду міжатомного потенціалу.

Key words: флуктуаційно-електромагнітна взаємодія, електронне тертя, фононне тертя, теорія збурень, сила тертя, нанорівень, трибоспряження зразків