ENTROPY-BASED METHOD FOR ASSESSING THE DESTRUCTION OF SURFACE LAYERS OF MATERIALS UNDER FRICTIONAL INTERACTION

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Abstract: The process of frictional interaction is characterized by intense plastic deformation of the surface layers that precedes their destruction. This plastic deformation occurs within a thin surface layer and is accompanied by extremely high rates of deformation and diffusion-several orders of magnitude higher than those observed during bulk deformation. Due to the repeated interaction of asperities on the actual contact spots of the rubbing surfaces, the absorbed mechanical energy is relatively uniformly distributed over the surface. Typically, during friction, two bodies remain in contact and move relative to each other. This process is generally accompanied by physico-chemical interactions with the surrounding environment. To simplify the model of friction and wear, this study considers the destruction of surface layers caused by fixed abrasive particles, where the process is not complicated by external physico-chemical interactions. Under such conditions, the surface layers enter a highly nonequilibrium state, forming a so-called “third body,” whose structure and properties differ significantly from those of the original material.

Keywords: wear resistance, friction, entropy, abrasive wear, surface layers, thermodynamics, deformation energy

Introduction

In the crystal lattice of metallic materials subjected to deformation, various defects such as vacancies and dislocations are formed, which increase the structural disorder of the material [1,2]. In undeformed metals, the average dislocation density is approximately 10^6–10^8 cm^{-2}, whereas in work-hardened metals it increases up to 10^{11}–10^{12} cm^{-2}.

Methods

During friction, two bodies remain in contact and move relative to each other. In this case, one of the bodies (the abrasive) wears so slowly that its wear can be neglected. Therefore, the thermodynamic system can be represented by a single body that undergoes wear and receives energy from another, non-wearing body (Fig. 1) [2,3]. This forms the basis of the entropy- based model of abrasive wear.

Fig. 1. Schematic representation of entropy flows in an open thermodynamic system under frictional interaction

It is assumed that the mechanical energy introduced into the system during the relative motion of the bodies dissipates through the mechanism of plastic deformation, and the amount of dissipated energy is equal to the mechanical energy supplied. The energy that continuously feeds the system and dissipates within the surface layers during friction-induced plastic deformation is divided into two components: the energy that causes structural changes in the material, and the energy that does not result in such changes.

The thermodynamic state of the system is determined by the flow of crystalline structure defects (vacancies, dislocations, etc.) both within and beyond the system boundaries. These defects are introduced into the system as a result of plastic deformation and leave the system through defect annihilation and mass exchange (wear products) with the external environment (Fig. 1).

To determine the entropy balance of the friction pair, the components of the energy balance for the steady-state wear process were used. According to [4,7], the energy balance of the friction and wear process can be expressed as follows:

$W = Q + \Delta U + E\sigma + Evp,$ (1)

where W is the friction work;

Q - is the thermal effect of friction;

ΔU - is the change in the internal energy of the surface layers and the wear products;

Eσ - is the energy of destruction;

Evp - is the energy of secondary processes.

Experimental studies [5] have shown that the components of the energy balance associated with the formation of new surfaces (Eσ) and with secondary processes (Evp)-such as triboluminescence, tribo-emission, acoustic noise, and other phenomena-are negligibly small and therefore can be disregarded.

Accordingly, from Eq. (1) we obtain

$W = Q + \Delta U,$ (2)

where W is the friction work; Q- is the thermal effect of friction; ΔU

-is the change in internal energy.

When considering the processes of friction and wear from the standpoint of the thermodynamics of irreversible processes, it should be noted that a friction pair represents a typical example of an open thermodynamic system. Such a system exchanges both heat (the thermal effect of friction) and matter (wear products and physico-chemical interactions with the environment) with its surroundings. For systems of this type, the total entropy change dS can be divided into two components: the entropy production diS, caused by internal transformations within the system, and the entropy flux deS, resulting from interactions with the external environment [6].

$dS = d_iS + d_eS$

The total change in entropy dS can be represented as the sum of two terms, diS and deS, each having a distinct physical meaning.

The entropy production diS in irreversible transformations within the system is always non-negative (diS > 0). A specific feature of the second law of thermodynamics is that the term diS, which describes entropy production, is always positive and serves as a quantitative measure of irreversible changes occurring inside the system.

The entropy flux deS characterizes the exchange of entropy between the system and its surroundings—either as an inflow of entropy from external sources into the system or as an outflow in the opposite direction. For open systems, i.e., systems that can exchange both heat and matter with the environment, deS contains components associated with heat transfer and with the transfer of matter. The change in entropy deS due to inflow and outflow processes may be either positive or negative.

The frictional work W determines the flow of defects entering the system during plastic deformation. As a result, entropy diS is generated within the system.

diS= W / Tf ,

where Tf is the temperature in the friction zone.

The process of abrasive wear is characterized by significant plastic deformation of the surface layers, which precedes their destruction (wear). As a result of plastic deformation, defects in the crystal structure—such as vacancies, dislocations, and others—are generated, increasing the structural disorder of metals. According to [7], under severe deformation, crystallites are fragmented into subgrains and blocks as small as 10 nm or less, misoriented with respect to each other by angles of about 30–35°. At the boundaries of these blocks, lattice distortions become so large that the state of the material approaches an amorphous one. These blocks are elastically distorted and contain a high concentration of crystal lattice defects.

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The dislocation density may reach 10^{11}–10^{12} cm^{-2}, and under such conditions, the material exhibits properties more characteristic of an amorphous rather than a crystalline state, which indicates the achievement of maximum structural disorder [8]. As is well known, entropy is the measure of chaos and disorder in nature [9]. Therefore, the processes of plastic deformation and material destruction during abrasive wear can be evaluated in terms of entropy change.

Plastic deformation is accompanied by two simultaneous and opposing processes: hardening and softening. A small portion of the crystal lattice defects associated with hardening remains (accumulates) in the material as the stored deformation energy ΔUe. This energy alters the internal structure of the material, increasing its structural disorder. The configurational entropy dikS associated with these structural changes can be expressed as follows:

dikS = ΔUe / Tf

Softening is associated with the annihilation of most structural defects and the conversion of their energy into heat Q. The heat released during the process of plastic deformation increases the temperature of the surface layers of the material by ΔUT and is subsequently dissipated into the surrounding environment through heat exchange QT.

Q = ΔUT + QT (6)

The heat ΔUT increases the vibrational energy of atomic motion,
resulting in an increase in vibrational entropy.ΔUT
where ΔV is the volume; ρ is the material density; c is the specific

heat capacity; and T is the ambient temperature.

Both the configurational entropy dikS and the vibrational entropy di_vS quantitatively reflect the irreversible changes occurring in the surface layers of the material, indicating the degree of their structural disorder and degradation.

$dipS = dik\,S + di\text{в}\,S = \Delta U / Tf$

and can serve as a measure of the rate of this destruction.

The entropy flux deS determines the exchange of entropy between the system and its surroundings, either through the transfer of entropy from external sources into the system or in the opposite direction. A friction pair represents an open thermodynamic system that exchanges not only heat QT but also matter with the environment-specifically, wear products ΔVi and chemical interaction products-whose flux is also directed into the surroundings.

For such systems, the entropy flux includes components associated with heat transfer (deqS), mass transfer (devS), and the chemical interaction of the tribosystem with the environment (deμS). The heat QT leaves the system without altering its structure, and the corresponding entropy flux deqS is expressed as follows:

$deqS = -\,QT / Tf$

According to the developed concepts of surface layer destruction in friction pairs, the material of the wear products is characterized by a limiting (critical) degree of structural disorder, that is, by the critical entropy density s*. The state of maximum disorder is essentially an amorphous state [9]. However, since the initial state of the friction pair material is characterized by the initial levels of configurational entropy density Sok and vibrational entropy density S_{ov}, the expression for the increment of entropy density Δsip during the wear process can be written as follows:

$\Delta sip = s^* - Sok - S_{ov}$

Then the entropy flux of matter devS is given by: $devS = -\,\Delta sip \cdot \Delta V\text{и} = -\,(s^* - sok - so\text{в}) \cdot \Delta V\text{и}$,

where ΔVi is the volume of the wear products.

The entropy flux associated with the chemical interaction of the tribosystem with the surrounding environment, deμS, is given by:

$de\mu S = -\,i\;i\;\Sigma\mu\,\Delta N$, (3)

where μ_i is the chemical potential of the i-th component, and ΔN_i is the number of particles of that component of the substance. The total entropy flux is expressed as:

$de\,S = deq\,S + dev\,S + de\mu S = -\,QT / Tf - \Delta sip\,\Delta V\text{и} - i\;i\;\Sigma\mu\,\Delta N$

Based on the developed entropy-based approach [9], an analytical relationship has been derived for assessing the rate of abrasive wear under steady-state friction conditions. In the case of abrasive wear, the chemical interaction between the material of the friction surfaces and the surrounding environment can be neglected; that is, it can be assumed that $\Sigma\,\mu_i\,\Delta N_i = 0$.

As a criterion for evaluating the wear resistance of a material, the critical entropy density (s*) is proposed. The value of this parameter for a given material depends solely on its physico-chemical nature.

$S(t) = Sok + Sov + \Delta Sip \leq S^* = const$,   (4)

where s(t) is the entropy density of the material at time t; Sok - is the initial configurational entropy density associated with defects in the original structure of the material; Sov - is the initial vibrational entropy density associated with the ambient temperature; ΔSip - is the increment of entropy density at time t; S* - is the critical entropy density of the material.

The critical entropy density s* represents the total entropy accumulated per unit volume of the material at the moment of failure. It characterizes the critical degree of structural disorder in the friction surface material. The entropy increment Δsip during the process of abrasive wear occurs both as a result of the formation of various crystal structure defects (vacancies, dislocations, etc.) and due to an increase in the temperature of the deformed material volumes.

For the reference point (S = 0), the entropy density of a defect-free material at absolute zero temperature (T_0 = 0 K) is taken. However, the initial (pre-wear) state of the material is characterized by an initial vibrational entropy density Sov, which depends on the ambient temperature T. The value of the initial vibrational entropy density Sov is assumed to be equal to the standard entropy of the material at 298.15 K.

Sov=$S0$ $_{298}$

In the initial structure of real metals and alloys, there are always defects in the crystal lattice, the degree of disorder of which is measured by the initial configurational entropy density Sok. The value of this parameter, at the standard temperature of 298.15 K, is determined as follows:Sok

= ueo ,   (5)

298where e_{ou} is the initial level of the material’s stored (latent) energy

density in its original state [8].ueo

= $u * (\sigma T)2$

$So$where u* - is the critical density of internal energy;

σT - is the yield strength;

S_0* - is the true shear resistance of the material.

The strength criterion above, in its appearance, resembles the criterion for structural failure under wear [10]. However, a significant difference of the proposed failure criterion is that the critical entropy density is reached not due to the entire contribution of the system’s entropy production diS, but only due to that portion dipS which is associated with

changes in the surface layer, i.e., with variations of the configurational entropy diS and the vibrational entropy di$_v$S of the material.

Let us compose the entropy balance equation for the steady-state process of abrasive wear, treating the friction pair as an open thermodynamic system.

The steady state in which the system resides is a non-equilibrium state in which dissipative processes proceed at zero rates. The quantities that describe the system (temperature T, specific load P, sliding velocity V) n the steady state cease to depend on time. In this state the entropy of the system is also time-invariant, i.e., the time derivative of the system entropy is zero ($dS = 0$) [11]. Therefore, from (2) we obtain

$- d_i S = d_e S$, (7)

The heat flux QT and the mass flux ΔVi that leave the system and determine the negative entropy flux deS are compensated by the entropy production −diS. A negative entropy flux means that, during friction, the system supplies entropy to the external world by exchanging heat and matter with it. Consequently, in the steady state the system continuously increases the entropy of the surroundings. Using Eqs. (2), (4), (5), (6) and (7), and taking into account that for abrasive wear $\Sigma \mu_i \Delta N_i = 0$, we obtain the following relation.$\boldsymbol{\Delta} V$

$= \mathrm{d}\, ipS = \mathrm{d}\, ipS = \mathsf{s} fPVt$

, (8)u $\boldsymbol{\Delta} SipSo{-}Sob{-}Sok$

$Tf(So{-}Sob{-}Sok)$where δ is the relative value of the stored deformation energy; f is the coefficient of friction; P is the normal load; V is the sliding velocity; t is the wear time; Δsi_v is the change in vibrational entropy density during the wear process.

The strength condition (3) and the analytical equation (6) for evaluating abrasive wear under steady-state friction conditions, obtained using the entropy-based approach, differ from the corresponding dependencies derived from the energy-based approach-where the internal energy of the material u* is used as the wear criterion-by a factor of 1 / Tf.

Conclusion

The presented thermodynamic approach to assessing material degradation under abrasive wear conditions makes it possible to analytically relate wear resistance to thermodynamic (entropic) parameters that reflect the physical nature of the phenomena occurring in the deformed and damaged layers of the friction pair.

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