Thermodynamic substantiation of the conditions of metal adhesion in dry friction

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Abstract. From the standpoint of thermodynamics, the conditions for the occurrence of adhesion and seizure in dry friction are considered. The setting of metals by friction is considered as a process of formation of a new phase in the form of points of adhesion. Dependences for the calculated estimation of the formation conditions of thermodynamically stable adhesion points are obtained

One of the important tasks in the design of various machines and mechanisms is to ensure the required wear resistance of their parts. A decrease in the coefficient of friction reduces energy dissipation and increases the energy efficiency of friction pairs. For these reasons, much attention is paid to the study of the nature and mechanisms of dry friction [1-4]. Most of the works are devoted to the study of the nature of sliding friction forces, factors that affect the coefficient of friction and wear rate. It is experimentally established that the force and coefficient of friction increase with an increase in the speed of relative movement of the contacting surfaces, as well as with an increase in the normal load. When certain values of these parameters are reached, the surfaces are set, which is characterized by a sharp increase in the friction force, the onset of intense wear, jamming and failure of the friction pair. However, the conditions for adhesion are not well understood at present. In the presented article, a mechanism and a computational model for assessing the conditions of the adhesion moment moment during dry friction are proposed.

We take into account that the phenomenon of adhesion is the process of establishment of interatomic bonds between the contacting surfaces. It brings the process of adhesion in friction with the welding process of pressure and makes it possible to use the energy hypothesis A.P. Semenov. According to this hypothesis, for the adhesion (formation of a metal bond) it is necessary that the energy of the surface atoms involved in the interaction rise above a certain level for a given metal. It is referred to as the energy threshold of adhesion $E_a$ [5].

It is known that the energy $U$ of surface atoms is different and can be represented as [6,7]

$$U = U_D + U_T + U_M,$$

where $U_D$ – is the mechanical energy of elastic distortion in the region of influence of a defect in the crystal lattice; $U_T$ – thermal energy; $U_M$ – mechanical energy of elastic compression of contacted volumes of metal under normal load.
Under friction, the formation and movement of crystal lattice defects occurs as a result of elastic-plastic deformation of micro protrusions. Thermal energy is released during the friction process. In Figure 1 shows the distribution of energy fields around a point surface defect. Adhesion is possible in the area where $U>E_A$. This area is bounded by a radius $R_U$.

![Figure 1. Scheme of distribution of energy fields around the crystal lattice defect.](image)

Considering the edge dislocation as a surface defect in [7], a dependence for the calculated estimation is obtained:

$$R_U = \left(\frac{a}{2(1-\mu)}\right) \tan \left[0.5 \arccos \left(\frac{4\pi^2 (k(T_m-T))}{Gb^2} - 1\right)\right],$$

where $b$ – is the Burgers vector of the edge dislocation; $a$ – interatomic distance; $G$ – shear modulus; $\mu$– Poisson's ratio; $k$ – Boltzmann constant; $T_m, T$ - melting point and current temperature of metal. The influence $U_M$ in formula (1) is neglected due to its small contribution to the overall energy balance $U$.

The occurrence of the adhesion point by the radius of seizure leads $R_U$ to the disappearance of free surfaces in these zones. Considering the free surface and near-surface layers of metal as a separate phase [8], we come to the conclusion that the adhesion process can be considered as a phase transition. As a result of this phase transition in the adhesion zones, the “surface” phase disappears and the “bulk” phase appears, which is characteristic of deep layers of metal.

On the other hand, the appearance of a thermodynamically stable phase is possible if this process is accompanied by a decrease in the free energy of the system. The decrease in the free energy $\Delta F_s$ of a system from two contacting volumes of the metal during the formation of one adhesion center is:

$$\Delta F_s = S_t \left(2f_s - f_{ib}\right),$$

where $f_s, f_{ib}$ are the specific free energy of the surface and the intergranular boundary, $S_t$ the area of the adhesion point.

The formation of chemical bonds between surface atoms in the centers of adhesion indicates that they are close to the value of the crystal lattice period $a$. The absence of a chemical bond between the surface atoms outside this adhesion point suggests that the surface atoms of bodies are separated by a certain distance $m > a$. A change in the distance between the surface atoms of two bodies in a certain zone $l$ of the transition from the adhesion point to free surfaces should cause the appearance of elastic distortions of the crystal lattice, decreasing with distance from the boundary of the adhesion point (Figure 2).
Adhesion point
The area of distortion of the crystal lattice

Figure 2. Scheme of stresses around the adhesion point.

Since these stresses are localized in the area of violation of the ordered structure of the crystal lattice, they can be attributed to stresses of the third kind.

The increment of the free energy of the system due to the occurrence of the boundary of the adhesion point is

$$\Delta F_f = L_B f_B,$$  \hspace{1cm} (4)

where $L_B$ is the extent of the boundary of the adhesion point, $f_B$ is the free energy of the boundary of the adhesion point.

Taking into account (3) and (4), we obtain a thermodynamic condition for the formation of a stable adhesion point:

$$(S_s - 2 L_B f_B) + L_B f_B < 0,$$  \hspace{1cm} (5)

It follows from expression (5) that the resulting adhesion points are stable if the condition is met:

$$S_s > \frac{f_B}{2 f_s - f_B}.$$  \hspace{1cm} (6)

Based on (6) for the active center, the critical radius $R_{cr}$ sufficient for the formation of a thermodynamically stable adhesion point will be:

$$R_{cr} = \frac{2 f_B}{2 f_s - f_B},$$  \hspace{1cm} (7)

To estimate the value $f_B$, we present the boundary of the adhesion point as a ring prismatic dislocation with the Burgers vector $b_f$. With this in mind, in [6, 7] for the case of a compound of homogeneous metals, an expression for the calculated estimate of the critical radius $R_{cr}$ is obtained

$$R_{cr} = 1.25 \frac{G b_f^2}{\pi (1 - \mu) (2 f_s - f_B)},$$  \hspace{1cm} (8)

where $G$ – shear modulus; $\mu$– Poisson's ratio

The phenomenon of seizure begins when the inequality begins to be fulfilled

$$\frac{R_U}{R_{cr}} > 1.$$  \hspace{1cm} (9)
When \( \frac{R_u}{R_{cr}} < 1 \) formed, the centers of adhesion are thermodynamically unstable and randomly disintegrate, without leading to seizing.

Given (2) and (8), inequality (9) will take the form

\[
\frac{a\pi(2f_s - f_b)\tan 0.5\arccos \left(\frac{4\pi^2 \left( \frac{k(T_a - T)}{Gb} \right) - 1}{1.25} \right)}{2.5Gb_f^2} > 1, \tag{10}
\]

The dependence (10) is obtained for the case of ascertaining metals with similar properties. In friction pairs, metals with sharply different properties, such as steel and bronze, usually come into contact. This interaction case is reduced to the case of friction of homogeneous metals with some intermediate physical and mechanical properties. Thus, in the case of connecting homogeneous materials 1 and 2 (Figure 3), the distortion of the crystal lattices of the metals being welded will be symmetrical with respect to the contact surface and \( m_1 = m_2 = m \).

![Figure 3](image1.png)

**Figure 3.** Scheme of the location of free surfaces around the adhesion point when contacting homogeneous materials.

When materials with different elastic properties are in contact, for example, for the case \( E_2 > E_1 \) (where \( E_2 \) and \( E_1 \) are the modulus of elasticity of the metal friction pairs), distortions of the crystal lattices will not be symmetrical with respect to the contact plane (Figure 4).

![Figure 4](image2.png)

**Figure 4.** Scheme of the location of free surfaces around the adhesion point when contacting materials with different properties

Based on Hooke's law after a number of assumptions, an upper estimate of the value of the critical radius of the adhesion point between materials with different elastic modulus of metals was obtained

\[
R_{cr} = \frac{6Gb_0^2 \left[ \frac{E_1}{E_1 + E_2} \right]}{\pi(1 - \mu)(f_{s,1} + f_{s,2} - f_b)}, \tag{11}
\]

where \( E_2 > E_1 \).

In this case, the upper bound \( \frac{R_u}{R_{cr}} \) for \( E_2 >> E_1 \) will be
Dependencies (10) and (12) show that a decrease in the contact temperature \( T \) contributes to the prevention of adhesion, especially for metals with a relatively low melting point \( T_m \). The increase in the Burgers vector of a fictitious dislocation \( b_f \) has a positive effect, which in practice can be achieved by the use of surface films that separate surfaces. It is also advisable to use metals with a low energy of crystal lattice defects proportional to the multiplier \( Gb^2 \) in friction pairs.

These conclusions correspond to the practice of developing and operating friction pairs, which indicates the prospects of the approach described in this article for developing ways to improve them.

### Conclusions

The onset of the moment of seizure is associated with the formation of thermodynamically stable adhesion points, the dimensions of which exceed some critical values determined by the physical-mechanical properties of the metals of the friction pair.

The formation of thermodynamically stable adhesion points can be considered as a phase transition, as a result of which the “surface” phase disappears and the “bulk” phase appears.

Theoretically substantiated measures to prevent the adhesion of metals, such as: reducing the contact temperature, the use of surface films, the use of friction pairs of metals with low energy defects of the crystal lattice.

### References

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