Metal cladding of friction surfaces in liquid media

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Abstract. On the basis of the quantum-chemical method, the possibility of using a liquid lubricant containing a fine powder of the Al-Mg-Li system is considered. It provides a high-quality process of metal cladding of steel friction surfaces and, as a result, an increase in the resource of a single application of a liquid lubricant and the resource characteristics of the tribological system "wheel rail".

1. Introduction
Strong mechanical stresses that arise during the operation of the locomotive lead to the damage to the rolling surface of the wheel-set of railway rails. The destruction of the tire, the occurrence of cracks on the rail head can lead to an emergency situation on the railway tracks. Intensive wear of rails and wheel flanges of the rolling stock is the main threat to the safe train movement.

According to the rules of technical operation of the railways of the Russian Federation, it is forbidden to include carriages on long-distance passenger trains with tire wear of more than 7 mm, local traffic of more than 8 mm, and for freight carriages of more than 9 mm. It is forbidden to use locomotives for trains with tire wear over 7 mm, and for tender tires over 9 mm [1].

Timely turning of wheel-set tires restores the working profile of locomotive wheel-sets and allows prolonging their service life [2].

The resource costs of wheels and rails can be cut almost threefold by turning wheel rims on the rolling surface. Figure 1 and 2 show the types of railroad wheel turning, where \( h_0 \) is the wheel turning depth along the rolling surface equal to no more than 10 mm, and \( h_0'' \) is the wheel turning depth along the ridge equal to at least 30 mm.

Reducing the wear of wheels and rails by 3-4 times and energy consumption for traction up to 10% is achieved by applying lubrication technologies for the wheel flanges and the side surface of the outer rail. Existing lubrication technologies are performed with the help of railroad cars, railroad locomotives, suburban trains, stationary track lubricators, traction rolling stock equipped with onboard ridge lubricators. Increasing the efficiency of lubrication is also achieved through the improvement and unification of lubricants (taking into account the regions of application) [3].
The main problem with this lubrication technology is that the liquid lubricant has a short lubrication service life, i.e. it does not remain on lubricated surfaces for a long time because it flows down into the ballast prism, polluting it and everything around.

Metal-plating of steel friction surfaces in liquid media makes it possible to create modern lubricants for stationary track lubricators that increase the resource characteristics of the wheel-rail tribosystem. It means that it increases the resource of a single application of a lubricant on the friction surface [3]. Powders of soft metals and their alloys are used as cladding elements. There are processes of creating a dynamic effect on the friction system in the form of external, natural vibrations or frictional natural oscillations of contacting micro- and macro-roughness in the friction zone. In addition, there can be processes of suppression of "natural vibrations" of contacting micro- and macro-roughness. The total contact stiffness also changes when the direction of the relative sliding of the friction surfaces shifts [4].

We assume that a fine powder of the Al-Mg-Li system in a liquid medium of a lubricant will be in a suspended state, i.e. it will neither precipitate nor float due to its unique density (2.47 g·cm$^{-3}$) [5].

When selecting a fine-dispersed powder based on aluminum-lithium alloys in such a way that the specific gravity of the lubricant and the aluminum-lithium powder are close in value, which will ensure high-quality metal-coating of friction surfaces in a liquid lubricant and, accordingly, will increase the efficiency of the lubrication technology with stationary track lubricators working with liquid lubricants.

On the basis of quantum-chemical methods, calculations of the strength of chemical bonds of various polyatomic objects (molecules and solids) were performed with an accuracy comparable to the accuracy of instrumental measurements of the firmness of such objects. In the case of solids, this statement refers mainly to defect-free structures that do not have local defects.

In this work, quantum-chemical methods were applied to study materials that are promising for application on the rolling surface of railway wheels. To study this issue, we carried out numerical experiments using methods based on the DFT approximation. Nowadays the accuracy of such methods is quite high, which makes it possible to consider the results obtained with their help as a fairly reliable guideline when designing various materials. In this work, we used the ADF-BAND program complex [6], which was previously used in our group to investigate the strength of steel grain boundaries [7].

2. Purpose and objectives of the study
Based on the quantum-chemical method, consider the possibility of using a liquid lubricant containing a fine powder of the Al-Mg-Li system to ensure a high-quality process of metal plating of steel friction surfaces and, as a result, increase the resource of a single application of liquid lubricant and the resource characteristics of the wheel-rail tribological system.
3. Materials and research methods

To calculate the strength of the objects studied in this work, we used the following ratio:

$$E_{\text{strength}} = \frac{\{E(I) - E(II) - E(III)\}}{S}$$

where $E(I)$, $E(II)$, $E(III)$ are the energies of the initial object and its two desoldered parts, $S$ is the area of desoldering (figure 3). Thus, $E_{\text{strength}}$ is the energy required to separate a body into two parts, referred to the division surface.

It is important to note that the model used in our calculations (figure 3) is quite simple. In the direction of the vertical axis, 5-6 layers of atoms are considered, and the horizontal layers represent an infinite two-dimensional periodic structure. Figure 3 displays nine cells of this structure.

To confirm the accuracy of the results obtained using this model, it is necessary to compare them with already known experimental data. We chose the following parameters for this purpose: the first one was the melting point, which integrally characterizes the strength of interatomic bonds in the metal; and the second one was the ultimate mechanical strength of metals, which also depends on the strength of interatomic bonds. The melting temperature should be considered a more reliable experimental value in this case, since it depends on the defectiveness of metals to a much lesser extent than the ultimate strength.

Figure 3. The disintegration of the original complex into two parts under the action of a power load.

4. Results and discussion

In each column of table 1 below you can find relative values (with respect to the maximum value of this parameter for each metal) along with experimental and calculated data.

Table 1. Calculation results and comparison with already known experimental data.

| Chemical elements | Calculation - specific cohesive energy, eV/A2 | Experimental data on the ultimate strength, MPa | Experimental melting point, K |
|-------------------|---------------------------------------------|-----------------------------------------------|-------------------------------|
| Fe                | 0.48                                        | 250                                           | 1808                          |
| Cu                | 0.25                                        | 220                                           | 1356                          |
| Al                | 0.19                                        | 80                                            | 934                           |
| Zn                | 0.15                                        | -                                             | 692                           |

To make it crystal clear, these results are demonstrated in graphical form (figure 4). The qualitative agreement between theoretical and experimental data is obvious. It was found out that the obtained group of metals Fe, Cu, Al, Zn fully agrees with the already known experimental data, when arranged
according to a decrease in their strength. This fact allows supposing that the results presented below, that have been obtained using the same model, are also close to reliable values.

5. Calculations of cohesion and adhesion in a multilayer system

As a specific example, let us consider a system consisting of several layers of atoms of various elements and their compounds. To make things clear, let us choose a system consisting of iron atoms (the base element), as well as aluminum and aluminum oxide. Our task in this case is to carry out a comparative analysis of the strength of the layers of each of the elements of the system and the intermediate layers between them. To assess the strength of the inner layers of the metal, the cohesion energy was calculated; the strength of the intermediate layers was estimated by determining the adhesion energy.

When calculating the energy of adhesion, it was assumed that the atoms of the first layers of a chemical element applied to the base metal have the same symmetry as the atoms of the base metal (space-centered cube (SCS) in the case of iron and aluminum). In addition, the diffusion of atoms of the deposited element into the surface of the main element was taken into account. For this purpose, the atoms of the applied element were introduced into the upper layer of atoms of the main element.

![Figure 4. Comparison of the data on cohesion energy obtained using the model with experimental data on the ultimate strength and melting point of various elements.](image)

Below, tables 2 and 3, as well as figure 5 and 6 display the results of calculations of the energy of aluminum adhesion on iron and aluminum oxide on aluminum. The rest of the results are summarized in table 4.

| Lattice symmetry | Number of layers | Layer energy, eV | Energy of system (3Fe,2Al), eV | Sell dissociation energy, eV | Specific cohesive energy, eV/A² |
|------------------|-----------------|-----------------|-------------------------------|----------------------------|-------------------------------|
| Fe SCS           | 3               | -55.21          | -73.77                        | 4.19                       | 0.36                          |
| Al SCS           | 2               | -14.37          | -                             | -                          | -                             |
Table 3. Adhesion of aluminum oxide to aluminum.

| Lattice symmetry | Number of layers | Layer energy, eV | Energy of system (3Fe,2Al), eV | Sell dissociation energy, eV | Specific cohesive energy, eV/A² |
|------------------|------------------|------------------|-------------------------------|-----------------------------|-------------------------------|
| Fe SCS           | 3                | -3.05            | -63.20                        | 1.80                        | 0.11                          |
| Al SCS           | 2                | -38.35           | -                             | -                           | -                             |

Figure 5. Decomposition of the 3Fe + 2Al complex.

Figure 6. Decomposition of the 3Al+AlO₂ complex.

Table 4. Summary of the obtained Results.

| Elements       | Bond type  | Bond energy, eV/A² |
|----------------|------------|--------------------|
| Fe-Fe          | Cohesion   | 0.48               |
| Fe-Al          | Adhesion   | 0.39               |
| Al-Al          | Cohesion   | 0.19               |
| Al-AlO₂        | Adhesion   | 0.11               |

Table 4 shows the corresponding values of energies and types of bonds for the corresponding elements of the investigated layers. As a result of the analysis of the data obtained, a consistently decreasing strength of chemical bonds in the system of layers (Fe, Fe), (Fe, Al), (Al, Al), (Al, AlO₂) is clearly visible. Thus, during friction, the outer layer of AlO₂ with the lowest adhesion energy will serve as the ‘primary lubricant’. When it is wiped off, the next layers of the system will be sequentially wiped off, protecting the base element (iron) from destruction.

6. Conclusion

When using stationary lubricators on the road network of Russian Railways, it is important to use modern liquid lubricants that increase the resource of the wheel-rail tribosystem. Such lubricants include oils containing cladding elements, such as finely dispersed powders of metals and their alloys.

It has been determined that the results of calculating the strength of the studied elements Fe, Cu, Al and Zn obtained by the quantum-chemical method are fully comparable with the already known experimental data, such as cohesion energy, experimental ultimate strength and melting point.

A comparison of the calculated values of the adhesion energies of the intermediate layers and the cohesion energies of the inner layers of a multilayer system revealed a decrease in the value of the strength of chemical bonds in the considered systems of layers (Fe, Fe), (Fe, Al), (Al, Al), (Al, AlO₂).
A lubricant containing a metal-plating additive in the form of a fine powder of the Al-Mg-Li system increases the efficiency of the lubrication technology when using stationary track lubricators. The effectiveness of lubrication consists in keeping the lubricant on the rolling surfaces of wheels and rails.

References
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