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COMPUTER MODELING OF THE PHYSICAL AND CHEMICAL PROPERTIES OF RAILCAR STRUCTURES TO PREDICT THE REMAINING SERVICE LIFE

The article reveals the peculiarities of the importance of research work on determining the friability of steel components and parts in transport operating under static or cyclic loads in the field of elastic deformation. The issue of ensuring the safety and reliability of rolling stock is of particular importance in the context of intensive railway transport operation. Carriage structures are constantly subjected to significant mechanical and climatic loads and gradually lose their original properties. Therefore, timely forecasting of their service life is critical to preventing emergencies, optimizing repair and maintenance costs, and increasing the efficiency of transport operations. The problem of assessing the residual life of rolling stock components and parts is not new. At the same time, it is still relevant today. Cyclic loading causes the destruction of metals at a stress that is not only less than the tensile strength, but also less than the yield strength and elasticity.Metal destruction under cyclic loading is localized. The ability of a metal to resist repeated alternating loads is characterized by the cyclic toughness of the metal. It describes the ability of metals to absorb energy in an irreversible form. The deformation curves during loading and unloading do not coincide with each other, but form a hysteresis loop. It has been theoretically shown that the material's friability (porosity, defectiveness) can indeed be a key parameter for assessing the residual life of structures, especially after prolonged operational loading or exposure to aggressive environments. From a practical point of view, there is a fundamental possibility of developing devices based on certain regularities of physical properties of metals in relation to friability, which are most suitable for real components and parts and conditions during operation. Based on the above, it is possible to create an effective methodology for monitoring and diagnosing the residual life of steel parts and assemblies, which will significantly improve the efficiency of the railway industry and avoid accidents and large-scale disasters.
Keywords:*transport, railway transport, wagons, automation, computer modeling, steel friability, service life.*

Topicality.

In conditions of intensive operation of railway transport, the issue of ensuring the safety and reliability of rolling stock acquires particular importance. Carriage structures, constantly exposed to significant mechanical and climatic loads, gradually lose their original properties. Therefore, timely forecasting of their service life is critically important for preventing emergency situations, optimizing repair and maintenance costs, as well as increasing the efficiency of transport.

It is in this context that conducting research and practical work on computer modeling of the physicochemical properties of railcar structures becomes extremely relevant. The use of modern computer modeling methods allows for high-precision reproduction of complex physical and chemical processes occurring in railcar structural materials under the influence of various operational factors.

The problem of estimating the residual resource of components and parts of rolling stock structures is not new. However, it does not lose its relevance even at the present time. Since the pace of technical re-equipment of industrial equipment lags behind the pace of its aging, the relevance of developing reliable methods for estimating the residual resource increases.

Analyzing the currently available methods for estimating the residual resource, two main approaches can be distinguished:

1. Probabilistic methods based on failure statistics.
2. Technical methods based on destructive and non-destructive testing methods.

It is obvious that the zones of increased stress concentration are the most probable areas of destruction. It is in them that pre-defect changes in the structure begin to occur. According to the authors of the work, ignoring structural changes is one of the significant shortcomings of existing methods for estimating the residual resource [1]. Existing methods based on the analysis of the kinetic diagram of fatigue fracture [2] are losing their relevance due to the fact that the dynamics of fatigue crack development most often has an "explosive" character.

The relevance of research in this area is emphasized by the constant growth of requirements for the safety of railway transportation and the need to reduce operating costs. The introduction of advanced computer modeling methods into the practice of designing and operating railcar structures will contribute to increasing their competitiveness and ensuring the sustainable development of railway transport in Ukraine.

Analysis of information sources on the topic under study.

The article [3] presents an analysis of modern developments in the field of determining the residual resource of transport structures and equipment operated under conditions of long-term practice, uncertainty and risk when making final conclusions. It is emphasized that the strategy for the development of technical diagnostics requires the exclusion of dependence on the human factor and subjective observation of changes in the physical, mechanical and operational properties of controlled objects. The use of non-destructive testing and flaw detection methods for assessing the residual resource is analyzed, and the limitations of these methods at the early stages of defect development are revealed.

In the scientific paper [4], an optimized maintenance planning for emergency and rescue railway cars using a genetic algorithm was developed. The study was conducted on the example of a railway company in Iran. The aim of the study is to minimize maintenance costs and increase the reliability of railway transport. The genetic algorithm is used to optimize maintenance schedules taking into account various constraints and factors. The results of the study demonstrate the effectiveness of the proposed approach for improving maintenance management.

The article [5] discusses the development of an intelligent decision support system for locomotives. The system structure and the assessment of the quality of its operation are described. The system is designed to improve the efficiency and safety of locomotive operation. The paper presents data processing algorithms and decision-making methods.

The article [6] presents a method for theoretical assessment of the safety of new freight cars against derailment. The study focuses on the analysis of the dynamic characteristics of cars and their interaction with the track. Factors affecting the risk of derailment, such as speed, track geometry and car parameters, are considered. The proposed method allows assessing the safety of cars at the design stage. The results of the study can be used to improve the design of cars and increase the safety of rail transport.

The scientific and applied work [7] investigates theoretical and practical aspects of determining the parameters of onboard capacitive energy storage devices for underground rolling stock. The requirements for energy storage devices in underground mining conditions are considered. Different types of storage devices and their characteristics are analyzed. Methods for calculating the optimal parameters of storage devices to ensure the effective operation of underground transport are proposed.

The article [8] considers the issues of determining the rational parameters of the system of capacitive energy storage for underground railway rolling stock. The influence of the storage parameters on the energy efficiency and operational characteristics of trains is studied. Methods for optimizing the choice of storage capacity and power are proposed. The technical and economic aspects of implementing such systems are considered.

The authors of the publication [9] analyze the operational reliability of railway vehicles in the context of derailment safety. Different methods for determining safety assessment criteria are considered. A comparative analysis of these methods is carried out to assess their effectiveness. The study is aimed at improving methods for assessing the risk of derailment and increasing railway safety.

European Standard [10] describing test and simulation methods for the acceptance of the running gear characteristics of railway vehicles. The standard covers running and static tests. It sets out requirements for test procedures and assessment criteria. The application of this standard is essential for ensuring the safety and compatibility of railway vehicles.

Standard [11] UIC (International Union of Railways) which defines the procedures for testing and approving railway vehicles in terms of their dynamic behaviour. The standard covers aspects of safety, track impact and running performance. It establishes methodologies for assessing the dynamic performance of vehicles. The application of this standard is essential for ensuring the safe operation of railway transport. The document is key for railway designers, manufacturers and operators.

In [12], an experimental approach to assessing the safety of freight cars against derailment is presented. The authors describe conducting experiments to study the dynamic behavior of cars. The results of the experiments are used to analyze the factors affecting the risk of derailment. The study contributes to a deeper understanding of the mechanisms of derailment and the development of measures to prevent them.

The scientific study [13] examines the modernization of railway cars with the aim of increasing customer satisfaction and ensuring safety. The authors analyze the impact of modernization on various aspects of the operation of cars. Technological solutions and innovations aimed at improving comfort, reliability and safety are investigated. The article emphasizes the importance of modernization for increasing the competitiveness of railway transport.

At the same time, it is precisely with structural changes that changes in the physical and chemical properties of steel are associated. In this work, we focused on the fatigue loads to which steel parts made of steel grade 09G2S are subjected under normal conditions (room temperature and normal atmospheric pressure).

Research methods

Analysis of literary sources allows to systematize existing knowledge about the physical and chemical properties of materials of car structures and factors affecting their durability. Construction of computer models involves the use of finite element methods to simulate loads, temperature effects and corrosion processes acting on car structures. Verification and validation of models is carried out by comparing the results of modeling with experimental data obtained in laboratory or field conditions. Conducting a series of model experiments with varying load parameters, climatic conditions and material properties allows to assess their impact on the service life of structures.

Object and subject of research.

The object of research is railcar structures and the processes of changing their physicochemical properties under the influence of operational factors.

The subject of the study is the patterns of changes in the physicochemical properties of materials of car structures (mechanical, corrosion, fatigue, etc.) and their relationship with the service life, which are studied using computer modeling methods.

Statement of the problem

Wear and destruction of car structures under the influence of complex physicochemical processes is a serious problem in the railway industry, which leads to significant economic costs and increases the risk of accidents.

Traditional methods of assessing the service life, based on empirical observations and field tests, are long, expensive and do not always allow obtaining comprehensive information about the behavior of materials in various operating conditions. In this regard, the development and implementation of computer modeling methods that allow studying the physicochemical properties of car structures at the micro- and macro-levels is becoming relevant.

Computer modeling opens up opportunities for detailed analysis of corrosion processes, metal fatigue, wear of friction surfaces and other factors affecting the durability of wagons. It allows predicting changes in the mechanical properties of materials under the influence of external factors, such as temperature fluctuations, humidity, aggressive environments and mechanical loads. However, to obtain reliable modeling results, it is necessary to take into account the complexity of physicochemical processes occurring in real operating conditions.

Purpose and objectives of the study.

The aim of the study is to present the results of computer modeling of the physicochemical properties of railcar structures, allowing for a detailed study of their behavior under the influence of various factors. This helps to identify potential weaknesses and failure mechanisms of materials. Based on the data obtained, it is possible to accurately predict the service life of railcars and optimize their maintenance.

To achieve the set goal, the following tasks were solved:

- simulation modeling of cyclic loads on welded joints of the car to predict the appearance and development of fatigue cracks;
- a predictive model of the residual resource of a railcar based on the integration of computer modeling data of physical and chemical properties and operational parameters;
- the corrosion process of the metal of the car under the influence of various atmospheric conditions was investigated in order to determine the factors that most affect the rate of destruction;

Presentation of the main material.

Most steel assemblies and parts in industry and transport operate under static or cyclic loads in the elastic deformation range. The main regularities of the fatigue failure process of metals under cyclic loads include the following.

Cyclic loading causes the failure of metals at stresses that are not only less than the ultimate strength, but also less than the yield and elastic limits. The lower the stress, the more stress changes (cycles) are required to cause the specimen to fail. The relationship between stress and the number of cycles that cause the specimen to fail is depicted as a fatigue curve (Wohler curve) [14].

The destruction of metal under the influence of cyclic loading is local in nature.

The ability of a metal to resist repeated alternating loads is characterized by the cyclic viscosity of the metal. It characterizes the ability of metals to absorb energy in an irreversible form. The deformation curves during loading and unloading do not coincide with each other, but form a hysteresis loop. The area of the hysteresis loop characterizes the work that the metal is able to absorb in an irreversible form in one cycle.

According to the kinetic strength theory [15], the destruction of a material is considered as a thermofluctuation process, in which thermal fluctuations help overcome the energy barrier necessary to break atomic bonds.U_0

Energy barrier U_0 is the activation energy that must be overcome to break a bond in the absence of external stress.

The effect of stress σ– external stress reduces the effective energy barrier, facilitating fracture.

The connection between and $U_0 \sigma$– usually described by a linear or nonlinear dependence, for example:

$$U(\sigma) = U_0 - \gamma\sigma \tag{1}$$

where is the structure-sensitive coefficient that takes into account the effect of stress on the activation energy.γ

The rate of destruction isThe probability of overcoming the barrier is described by the Arrhenius law:

$$\tau = \tau_0 \exp\left(\frac{U_0 - \gamma\sigma}{kT}\right) \tag{2}$$

where:

τ– time to destruction,

τ_0– pre-exponential factor (characteristic time of atomic vibrations),

k- became Boltzmann,

T– absolute temperature.

According to [15], cyclic loading can be divided into three main stages, characterized by different mechanisms of deformation and fracture: the stage of cyclic microfluidity, the stage of cyclic fluidity and the stage of cyclic strengthening (weakening). The tendency of metals to cyclic strengthening or weakening is determined by the ratio of the tensile strength σ_B to the conditional yield strength $\sigma_{0.2.}$

If the ratio $\sigma_B / \sigma_{0,2} \leq 1.2$, then weakening occurs, for $\sigma B / \sigma_{0,2} \geq 1.4$, strengthening occurs, for $1.2 \leq \sigma_B / \sigma_{0,2} \leq 1.4$ both strengthening and weakening can occur. In the first two stages, although changes in the structural state occur, the mechanical properties practically do not change. At the stage of cyclic strengthening or non-strengthening, an intensive change in mechanical properties occurs.

Scientific research in the work on the influence of carbon on the physical and mechanical properties of 09G2S steel in the production of freight car frames. According to DSTU 8541:2015, the main chemical composition of steel (in %) and the optimized composition of steel are given in Table 1.

Table 1 Chemical composition of steel 09G2S, wt %.[16]

Chemical composition of steel 09G2S	Mass fraction of elements % mass.							
	C	Si	Mn	Cr	Ni	Cu	P	S
DSTU 8541:2015	≤0.12	0.17-0.37	1.4-1.8	≤0.3	≤0.3	≤0.3	-	-
Optimal chemical composition	≤0.091	≤0.23	≤1.71	≤0.027	≤0.027	≤0.201	≤0.009	≤0.007

Under normal conditions, carbon is in a solid solution with iron and in the form of a chemical compound - cementite (Fe3C). An increase in the percentage of C in steel leads to an increase in the carbide phase, therefore, to an increase in hardness and strength and, as a result, a decrease in the plasticity and toughness of steel. From a physical point of view, an increase in the proportion of carbon leads to an increase in electrical resistance and coercive force, and a decrease in magnetic permeability. According to [14],The atoms of the alloying elements distort the crystal lattice of ferrite, increasing its strength. The dependence is described by the Fleck-Hahn equation:

$$\Delta\sigma_s = \sum_{i=1}^{n} Ki \cdot Ci^n \quad (3)$$

Ki– strengthening coefficient (MPa/at.%),

Ci– element concentration (at.%),

n≈ 1 (for most elements).

The values of the ferrite strengthening coefficients are given intables 2

Table 2The values of the strengthening coefficients of ferrite by various elements dissolved in it

Element	Coefficient Ki, MPa/at.%	Impact on ferrite
C	4890	Strong hardening, but low solubility (<0.02%).
Si	87	Significant strengthening, increases the yield point.
Mn	73	Moderate strengthening, improves hardenability.
Ni	27	Reduces the brittle transition temperature.
Cr	16	Increases corrosion resistance, weak strengthening.
Cu	45	Greatly slows down tempering, increases heat resistance.

As can be seen from Table 2, the greatest strengthening effect is associated with carbon.The quantitative degree of ferrite strengthening depends on the type and concentration of alloying elements, and their combination allows you to achieve the desired level of steel strength.

From the point of view of physics, elements dissolved in ferrite, in the initial state, lead to the formation of a non-equilibrium thermodynamic system, which gradually tends to pass into an equilibrium state. The main mechanism of such a transition is the diffusion of alloyed elements. The diffusion rate in this case will be determined by expression (1) and will significantly depend on the external voltage, which reduces the potential barrier, and temperature. Two mechanisms of carbon release are possible:

1. Diffusion of carbon atoms to dislocations and grain boundaries.

2 Formation and growth of carbides.

Diffusion of carbon atoms to dislocations leads to strengthening of ferrite, it becomes "softer", steel becomes plastic. The growth of carbides, on the contrary, leads to the fact that the proportion of the "hard" phase in steel increases, the total hardness increases, embrittlement occurs. This state is the most dangerous and critical. The probability of brittle fracture becomes the greatest. An additional factor affecting the diffusion process is the grain size. If the grain size is smaller, then the diffusion process is faster. Carbon needs to travel a shorter path to reach the grain boundary. Accordingly, the concentration of carbon also has a certain influence. The more carbon, the faster the diffusion process

The degree of degradation (embrittling) of the strength properties of a material can be assessed by changing its hardness. It was noted that under the influence of operational factors, the structure and mechanical properties of the material change (embrittling). The change in the structure and mechanical properties of the material (embrittling) occurs not only under alternating loads, but also under the influence of static loads.

Looseness as an objective criterion of residual resource. The creation of objective control over the technical condition of steel assemblies and parts involves the development of a method of prompt and reliable diagnostics. One of the options for such control may be a method based on a change in the physicalco-chemical properties of metals, in particular, on the nature of changes in the structural looseness of steel, which is an indicator of its thermodynamic stability.

Looseness indirectly characterizes the energy of interatomic interaction. The stronger the chemical interatomic bonds and the higher their energy, the more pronounced the effect of "tightening" the atoms into a compact crystal lattice (structure) is and the smaller the corresponding value of its structural looseness will be [17]. Weak chemical bonds of a compound indicate a lower energy of their connection and, therefore, a higher structural looseness. It is obvious that looseness is a value inverse to the energy density of a substance.

In the scientific literature and, in particular, in the work [17], a fairly large number of correlation dependences of physical parameters on structural looseness are presented. The structural looseness ω of a crystalline substance has the form of the formula:

$$\omega = \frac{M}{n \times p} \tag{4}$$

where: M - molecular mass (g/mol); ρ - steel density (g/cm3); n is the number of atoms in the compound formula[17].

As an example, we will give the calculation of the structural looseness of cementite (Fe3C) of steel 09G2S according to the optimal chemical composition.[16]

$$\omega_1 = \frac{54,632 \times 3 + 12,011}{4 \times 7,85} = 5,61 \frac{cm3}{gr \times atom} \tag{5}$$

For ferrite, which has, for example, one carbon atom in its bcc lattice, the looseness can be calculated as follows:

$$\omega_2 = \frac{54,632 + 12,011}{2 \times 7,85} = 4.24 \frac{cm3}{gr \times atom.} \tag{6}$$

If there are two carbon atoms in the bcc lattice of ferrite, then:

$$\omega_3 = \frac{54,632 + 2 \times 12,011}{3 \times 7,85} = 3,33 \frac{cm3}{gr \times atom.} \tag{7}$$

The integrated looseness of steel in the general case can be found by the formula:

$$\omega \quad = x_1 \omega_{1+} x_2 \omega_2 + \cdots .. \tag{8}$$

where x1 is the fraction of iron carbide in steel, x_2 is the fraction of ferrite with one carbon atom dissolved in the lattice, ω_1 and ω_2 are the looseness of the corresponding phase. In principle, the sum (8) can be supplemented with other inclusions.

During carbon diffusion, the carbide fraction x_1 may increase, and the alloyed ferrite fraction x_2 may decrease. Depending on which term in expression (8) increases faster, the overall structural looseness will also change. During embrittlement of steel, looseness decreases.

The choice of the looseness parameter was due, first of all, to the fact that work [9] presents a fairly large number of correlation dependences of physical parameters on structural looseness: 1) melting temperature, 2) relative hardness, 3) absolute Vickers hardness, 4) surface energy, 5) Young's modulus, 6) shear modulus, 7) modulus of comprehensive volumetric compression, 8) coefficients of thermal linear and 9) volumetric expansion, 10) volumetric compressibility, 11) sound propagation velocity, 12) refractive index, 13) crack resistance, 14) effective fracture energy, 15) boundary interatomic electron density, 16) electron work function, 17) thermal conductivity, 18) maximum atomic vibration frequencies, 19) heat capacity. It is possible that the above list of physical parameters can be expanded by deriving the corresponding dependencies.

It is possible that the given list of physical parameters can be expanded with the derivation of the corresponding dependence. As an example, Figure 1 shows a graph of the dependence of Young's modulus on structural looseness, constructed according to the correlation dependence (9):

$$\ln E = -1.854 \times ln\omega \quad + 8.808 \tag{9}$$

From (Fig.1) it is seen that with decreasing looseness, Young's modulus increases (fragility increases)

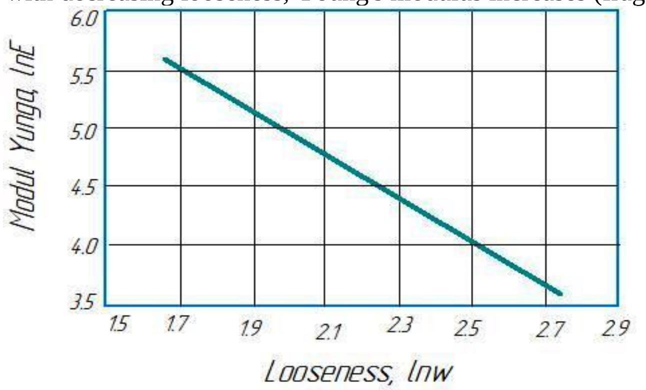

Fig.- 1 Dependence of Young's modulus of crystalline matter on structural looseness

Structural looseness ω increases the average distance between atoms, which reduces Young's modulus. In addition, with decreasing looseness, relative and absolute hardness, surface energy, shear modulus, sound speed increase, the coefficient of thermal linear expansion and heat capacity decrease, etc.

Conclusions.

1. It has been theoretically shown that the looseness (porosity, defects) of the material can indeed be a key parameter for assessing the residual life of structures, especially after prolonged operational load or exposure to aggressive environments.

2. From a practical point of view, there is a fundamental possibility of developing devices based on certain laws of physical properties of metals from looseness, which are most optimally suited for real assemblies and parts and conditions during operation. Based on the above, it is possible to create an effective method of monitoring and diagnosing the residual resource of steel parts and assemblies, which will significantly increase the efficiency of the railway industry and avoid accidents and large-scale disasters.

3. Computer modeling allows you to accurately reproduce the distribution of stresses and deformations in key nodes of the car structure under the influence of operational loads.

4. Modeling of corrosion processes, taking into account the aggressiveness of the environment, is an important tool for predicting the reduction in the bearing capacity of elements.

5. Taking into account dynamic loads that arise during movement over track irregularities increases the accuracy of predicting the fatigue strength of the metal.

6. Computer modeling makes it possible to optimize the design of a railcar at the design stage in order to increase its reliability and service life.

7. Modeling of failure processes under different types of loads (tension, compression, shear) allows to determine critical sections of the structure.

8. Comparative analysis of different design options using modeling helps to choose the most durable solution.

9. Integration of data on monitoring the technical condition of wagons into the model allows for adjusting service life forecasts and increasing their accuracy.

10. The results of computer modeling are valuable information for developing effective strategies for maintenance and repair of the railcar fleet, aimed at extending their service life.

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Стаття розкриває особливості важливості, науково-дослідних робіт, з визначення рихлитості сталевих вузлів і деталей на транспорті працює в умовах статичних або циклічних навантажень у сфері пружної деформації. В умовах інтенсивної експлуатації залізничного транспорту питання забезпечення безпеки та надійності рухомого складу набуває особливої ваги. Вагонні конструкції, постійно зазнаючи значних механічних та кліматичних навантажень, поступово втрачають свої первісні властивості. Тому, своєчасне прогнозування терміну їхньої служби є критично важливим для запобігання аварійним ситуаціям, оптимізації витрат на ремонт та обслуговування, а також підвищення ефективності транспортних перевезень.Проблема оцінки залишкового ресурсу вузлів і деталей конструкций рухомогог складу не є новою. Разом з тим, вона не втрачає актуальності і в теперішній час. Циклічне навантаження спричиняє руйнування металів за напруження, яке не тільки менше за межу міцності, а й менше за межу плинності та межу пружності.Руйнування металу під дією циклічного навантаження має локальний характер. Здатність металу чинити опір повторним знакозмінним навантаженням характеризується циклічною в'язкістю металу. Вона характеризує здатність металів поглинати енергію в необоротній формі. Криві деформації під час навантаження і розвантаження не збігаються між собою, а утворюють петлю гістерезису. Теоретично показано, що рихлість (пористість, дефектність) матеріалу дійсно може бути ключовим параметром для оцінки залишкового ресурсу конструкцій, особливо після тривалого експлуатаційного навантаження або впливу агресивних середовищ. З практичної точки зору існує принципова можливість розроблення приладів, заснованих на тих чи інших закономірностях фізичних властивостей металів від рихлості, які найоптимальніше підходять для реальних вузлів і деталей та умов під час експлуатації. На основі вищевикладеного , можливе створення ефективної методики контролю і діагностики залишкового ресурсу сталевих деталей і вузлів, яка дозволить істотно підвищити ефективність роботи залізничної галузі та уникнути аварій і великомасштабних катастроф.
Ключові слова: *транспорт, залізничний транспорт, вагони, автоматизація, комп'ютерне моделювання, рихлість сталі термін служби.*

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