

UOT: 620.193

DOI: <https://doi.org/10.30546/09085.2026.01.557>

PHYSICAL MODELING OF PROCESSES AFFECTING THE DIFFUSION MECHANISM DURING CORROSION

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ARTICLE INFO	ABSTRACT
Article history: Received:2025-10-08 Received in revised form:2025-10-21 Accepted:2025-11-24 Available online:2026-06-30 Keywords: Diffusion; Adsorption; Adhesion; Corrosion; Mathematical modeling. JEL Classification: L61, O32, C63	The article analyzes the mechanism of the diffusion process, which is one of the fundamental kinetic stages occurring during the corrosion of metals and alloys. In this research, the temperature dependence of the diffusion coefficient, point defects in the crystal structure, phase transitions, and the thermodynamics of grain boundaries were investigated; furthermore, the relationship between the diffusion coefficient and both crystal structure and thermodynamic factors was analyzed using mathematical models. Specifically, the influence of excitation processes occurring at the atomic and nuclear levels, magnetic properties, and adsorption-adhesion phenomena on diffusion kinetics was analyzed from a physico-mathematical perspective (through mathematical modeling). These results indicate that a comprehensive, multiscale analysis of the diffusion mechanism (at the atomic, crystalline and nuclear levels) enables a more accurate prediction of corrosion processes. Furthermore, the proposed physico-mathematical approach provides an effective theoretical framework for evaluating the integral impact of various external factors on diffusion kinetics.

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1. INTRODUCTION

One of the most pressing issues in modern materials science is to gain a profound understanding of the dynamics of corrosion processes and to manage them effectively. One of the primary kinetic stages determining the corrosion rate is the diffusion process, which facilitates mass transport. The parabolic nature of mass transport, crystal lattice defects, and interphase transitions are factors that account for the complexity of this process [3,5]. Recent studies indicate that the phenomenon of corrosion is closely linked not only to macroscopic changes but also to changes occurring at the microscopic and subatomic levels. The state of nucleons (neutrons and protons) in the nucleus, energy distribution, and temperature variations across discrete levels can act as stimulating factors for the diffusion mechanism within a corrosive environment [1,2].

The diffusion process can occur through different mechanisms in various directions, which directly affects the dynamics of corrosion. The article provides a mathematical description of the mechanism of diffusion variation in different directions and examines results obtained from the

computer modeling of phenomena occurring at the atomic and nuclear levels during the initial stage of the process. It has been determined that under constant potential conditions, intranuclear processes do not significantly influence diffusion due to the weakness of the interaction between neutrons and protons. However, during moments of excitation and throughout nuclear reactions, magnetism and rising temperatures intensify the diffusion mechanism. Excitation states arising against the background of a constant nucleon potential lead to the distribution of energy across discrete levels within the nucleus and variations in temperature, which directly influence diffusion kinetics.

2. PHYSICAL AND MATHEMATICAL ANALYSIS

The analysis of factors stimulating corrosion and physical modeling for their prevention are of particular importance. Accordingly, one of the factors affecting the mechanism of the corrosion process is the mechanism of diffusion. However, a more complex and intriguing issue concerns the factors that influence the diffusion mechanism itself. In this regard, it is essential to investigate the parabolic nature of the mechanism, the influence of crystal structure on the diffusion coefficient, temperature dependence, interdiffusion, and thermodynamic factors.

The variation in diffusion mechanisms across different directions impacts the overall corrosion mechanism [1,7]. The mathematical description of the variation in diffusion mechanisms across different directions is expressed by the following equations:

$$\frac{\partial C(r,\tau)}{\partial \tau} = \frac{1}{r^n} * \frac{\partial}{\partial r} * \left(r^n D \frac{\partial C(r,\tau)}{\partial r} \right) \quad (1)$$

$$\frac{\partial C(r,\tau)}{\partial \tau} = D * \frac{\partial^2 C(x,\tau)}{\partial x^2} \quad (2)$$

$$\frac{\partial C(x,y,z,\tau)}{\partial \tau} = D \nabla (\nabla C(x,y,z,\tau)) = D \Delta C(x,y,z,\tau) \quad (3)$$

$$\frac{\partial C(x,y,z,\tau)}{\partial \tau} = D \left(\frac{\partial^2 C(x,y,z,\tau)}{\partial x^2} + \frac{\partial^2 C(x,y,z,\tau)}{\partial y^2} + \frac{\partial^2 C(x,y,z,\tau)}{\partial z^2} \right) \quad (4)$$

$$\frac{\partial C(x,\tau)}{\partial \tau} + \frac{\partial j(x,\tau)}{\partial x} = 0 \quad (5)$$

$$\frac{\partial C(x,y,z,\tau)}{\partial \tau} + \text{div } j(x,y,z,\tau) = 0 \quad (6)$$

$$V = \frac{dq}{d\tau} = DS \frac{\partial C(x,\tau)}{\partial x} \quad (7)$$

$$j = -D \text{grad} C(x,y,z,\tau) = -D \nabla C(x,y,z,\tau) \quad (8)$$

$$\text{Grad} = \nabla = \bar{i} \frac{\partial}{\partial x} + \bar{j} \frac{\partial}{\partial y} + \bar{k} \frac{\partial}{\partial z} \quad (9)$$

$$j = \frac{dq}{Sd\tau} \quad (10)$$

$$j_x = -D \frac{\partial C(x,\tau)}{\partial x} \quad (11)$$

$$\frac{dC(x)}{dx} \approx \frac{C_2 - C_1}{\Delta x} = \frac{\Delta C}{\Delta x} = \frac{C\left(x + \frac{\Delta x}{2}\right) - C\left(x - \frac{\Delta x}{2}\right)}{\Delta x} \quad (12)$$

$$dq = -DS \frac{\partial C(x,\tau)}{\partial x} d\tau \quad (13)$$

It is evident from the mathematical descriptions that diffusion varies in different directions depending on various parameters. These variations are associated with point defects, inter-defect interactions, phase transitions, and the thermodynamics of grain boundaries [4,6]. Furthermore, adsorption and adhesion phenomena, as well as environmental factors, significantly influence the process.

The diffusion mechanism is influenced by intra-atomic energy and magnetic moments, electron-nuclear interactions, and the state of nucleons (neutrons and protons) [2,8]. Let us examine the mathematical description of the processes occurring within the nucleus. As a result of computer modeling, the energy distribution function of the processes occurring in the nucleus has been described by equation (14):

$$\rho F(E_x) = \frac{\sqrt{\pi}}{12a^{1/4}E_x^{5/4}} e^{2\sqrt{aE_x}} \quad (14)$$

From this, it is clear that under a constant potential, neutrons and protons generally do not interact with each other [2, 5]. Where E^x - represents the excitation energy, and a - is the coefficient characterizing the magnetic properties between neutrons and protons. Naturally, in this case, the processes occurring in the nucleus will not significantly affect diffusion:

$$\lambda = \exp \left[a_0 + \sum_{i=1}^5 a_i T_9^{\frac{2i-5}{3}} + a_6 \ln T_9 \right] \quad (15)$$

As can be seen, in this case, it fully characterizes the duration of nuclear reactions during moments of excitation within the nucleus. This moment, as observed, indicates the point at which magnetism and temperature increase. At this stage, the diffusion mechanism and the diffusion from the corrosion-inducing source will intensify:

$$N(A, Z) = \sum_i \int_0^T \lambda_i(t) \cdot \prod_j y_j(t) dt u \quad (16)$$

This is the mathematical description of the time at which neutrons leave the nucleus during this moment of excitation:

$$\lambda(T) = \sqrt{\frac{8}{\pi M}} \frac{N_A}{(kT)^{3/2} G(T)} \int_0^\infty \sum_p \frac{(2I^p+1)}{(2I^0+1)} \sigma^p(E) E \exp\left(-\frac{E+E_x^p}{kT}\right) dE \quad (17)$$

$$G(T) = \sum_p \frac{(2I^p+1)}{(2I^0+1)} \exp\left(-\frac{E_x^p}{kT}\right) \quad (18)$$

It is evident from these mathematical descriptions that if static equilibrium is established within the nucleus, no changes occur in the concentration of particles, and the energy distribution among neutrons remains constant. It is clear that nuclear reactions vary under the influence of temperature. However, simultaneously, the temperature within the nucleus rises during moments of excitation, and the energy distribution also changes depending on the discrete levels of these excitation moments. It has been clarified that the emergence of excitation moments during a constant nucleon potential is related to magnetic properties. The variation of energy and temperature across discrete levels within the nucleus during these different excitation moments directly impacts the diffusion mechanism during corrosion. However, the optimal solution to the stated problem involves investigating the influence of changes occurring in particles - especially within crystal lattices - on the diffusion mechanism for each excitation state. During these moments of excitation, the diffusion coefficient, as well as the thermodynamics, kinetics, and other specific mechanisms of diffusion, undergo a complete transformation.

The rise in temperature and changes in magnetism during excitation moments arising from nuclear reactions increase the diffusivity of the corrosion source. The research demonstrates that the excitation states occurring during a constant nucleon potential are directly linked to magnetic properties. In these cases, structural changes within the crystal lattices entirely alter the diffusion coefficient, as well as the thermodynamics and kinetics of the process.

One of the primary processes affecting the diffusion mechanism during corrosion is the mechanism of adsorption. Naturally, for an optimal solution to the problem, let us examine the physical description of the process:

$$dF^\alpha = -S^\alpha dT - p dV^\alpha + \sum \mu_i dN_i^\alpha \quad (19)$$

$$dF^\beta = -S^\beta dT - p dV^\beta + \sum \mu_i dN_i^\beta \quad (20)$$

$$\gamma = \left(\frac{\partial F}{\partial A}\right)_{T,V,N_I} \quad (21)$$

$$dF = -S dT - p dV + \sum \mu_i dN_i + \left(\frac{\partial F}{\partial A}\right)_{T,V,N_I} dA \quad (22)$$

It is clear from this description that in a heterogeneous system during adsorption, the very low number of molecules preserves the property of additivity; thus, if the adsorption mechanism proceeds via a certain pathway in one part, it tends to follow that same pathway in other parts. However, this mechanism varies due to several factors. The primary reasons for this include factors such as the nature of adsorption dynamics, the thermal effect, adsorption forces, variations in potential energy during adsorption, processes occurring in adsorption layers under the influence of temperature, and differential changes depending on temperature.

Certainly, during subsequent analysis, the individual examination of each parameter paves the way for an optimal solution to the problem.

One of the main processes and mechanisms that affect corrosion is the adhesion process and the formation of an adhesion layer. As such, the adhesion mechanism inherently influences the process. Let us examine the general mechanism of adhesion:

$$W_{adhesion} = \sigma_{s.t.c.} (1 + \cos \phi) \quad (23)$$

Simultaneously, the formation of the adhesion layer exerts a significant influence on the corrosion process. From this mechanism, it is evident that the adhesion process depends on the surface tension coefficient of the liquid ($\sigma_{s.t.c.}$) and the contact angle of the solid surface ($\cos \phi$). However, an optimal solution for investigating the influence of the adhesion process on the diffusion mechanism can only be found by examining the factors that affect these specific parameters. Analyses indicate that the adhesion strength depends on the energy per unit surface area (E) and the number of active bonds (N):

$$W_a = EN \quad (24)$$

These parameters, in turn, are closely linked to the state of the crystal lattice and processes occurring at the atomic-nuclear level; they vary depending on the nature of the bond, the condition of the crystalline lattice, and surface processes, consequently altering the adhesion mechanism.

Variations within the general mechanism - namely diffusion, adsorption, and adhesion - subsequently affect the corrosion process.

3. CONCLUSION

1. Although intranuclear processes do not significantly affect diffusion under constant potential conditions, increased temperature and magnetism during moments of excitation substantially accelerate the diffusion mechanism.
2. The distribution of molecules and the preservation of the additivity property during adsorption alter the character of the diffusion layers.

3. Adhesion strength influences corrosion resistance depending on the energy per unit surface area and the number of bonds.
4. Complex modeling of diffusion, adsorption, and adhesion mechanisms facilitates the discovery of optimal technological solutions for the corrosion protection of metal structures.

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