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DEVELOPMENT OF THE Fe–Al ALLOY PHASE EQUILIBRIUM SYSTEM AND THE Fe–Al–C TRIPLE SYSTEM IN THE THERMO-CALC PROGRAM

Shohruh RAKHMATALIEV[1,*[0000-0003-3781-1336]], Marton BENKE[1[0000-0002-1354-8660]]

[1]Institute of Physical Metallurgy, Metalforming and Nanotechnology, University of Miskolc, Miskolc, Hungary

Abstract

In this study, the phase diagrams of the Fe–Al binary and Fe–Al–C ternary systems were analyzed using the Thermo-Calc program. Based on Gibbs free energy, enthalpy, and other thermodynamic parameters, the stability of intermetallic phases under various temperature and compositional conditions was investigated. The results indicate that an increase in aluminum concentration raises Gibbs free energy, thereby reducing the likelihood of phase formation. In contrast, increasing temperature decreases Gibbs free energy, making reactions thermodynamically more favorable. The optimal conditions were observed in the temperature range of 1368–1428 K with 41–49 wt% aluminum, where AL_2Fe and AL_5Fe_4 intermetallic phases are stabilized, enhancing the wettability of aluminum coatings on steel surfaces. In the Fe–Al–C system, an increase in carbon content was found to raise Gibbs free energy, leading to weaker adhesion of the aluminum coating. These findings provide important insights for optimizing aluminized steel coatings by identifying the most favorable thermodynamic conditions.

Keywords: *Fe–Al system, Fe–Al–C system, Gibbs free energy, aluminizing, intermetallic phases, Thermo-Calc*

Introduction

The Fe–Al alloy system still holds a prominent position among binary systems for high-temperature materials and surface engineering, thanks to its unique combination of properties such as oxidation resistance, low density, and high melting points, which make it suitable for various industrial applications like turbine components, heat exchangers, and corrosion-resistant coatings. Historically, among ordered intermetallic phases, Fe_3Al and FeAl have been acknowledged for the ability to improve surface stability while maintaining sufficient mechanical strength at high temperatures [1–3]. The low solubility of hydrogen and sulfur in these intermetallics further enforces their usage in harsh environments [3]. Steel surface protection via aluminum-based coatings is a widely researched and practiced approach to enhancing oxidation and corrosion resistance. The formation of intermetallic layers at the interface can promote adhesion and thermal stability of the coating when aluminum diffuses into the iron lattice [2]. Thermodynamically, the formation of these intermetallic compounds is determined by Gibbs free energy minimization, a fundamental principle in phase stability prediction and guidance for coating optimization [4]. The usage of advanced modelling techniques, in particular, the CALPHAD (Calculation of Phase Diagrams) method, has made it possible to accurately anticipate phase equilibria and Gibbs energy alterations over wide ranges of temperature and composition by blending experimental data with computational databases [5–6]. This

*Corresponding author: shohruh.rahmataliev@uni-miskolc.hu

thermodynamic modelling plays an important role in understanding phase evolution during coating processes and in determining the optimum conditions for alloy additions. Recent studies still give the CALPHAD-based thermodynamic method significant credit in complex alloy systems, such as the Al–Co–Cr–Fe–Ni high-entropy alloys [1,7]. Since the binary Fe–Al system, the Fe–Al–C ternary system has a lot of clutter, with carbon, the main element in steel metallurgy, part of the picture, as its interaction with the other elements leads to phase changes and microstructural development. Depending on the amount of carbon and the temperature at which processing is done, it can form carbides or graphite, with different effects on mechanical and tribological properties. The carbide event in the alloy can strengthen the alloy, but excessive graphite may weaken its mechanical performance [7]. Analyzing these interplays requires precise thermodynamic evaluation, especially for steels of practical industrial importance. For this, we have used Steel 45, a medium-carbon structural steel commonly used in mechanical and structural applications, and Thermo-Calc software to study the Fe–Al–C system. The analysis focuses on mapping phase equilibrium regions, changes in Gibbs free energy, and the roles of aluminum and carbon in the system's stability. A lot of attention is paid to areas where aluminum has a high affinity for iron surfaces, thereby promoting the growth of intermetallic layers that are resistant to corrosion. The ternary phase diagram shows that the liquid, FCC, BCC, and graphite phases coexist in different proportions, indicating the complexity of the thermodynamic interactions involved. The most recent experimental examinations of the aluminizing treatment of steel surfaces have pointed out that the dense Fe–Al intermetallic layers (e.g., Fe_2Al_5, $FeAl_3$) are formed and have also looked into their growth kinetics as well as the different processing conditions under which, among others, thermodynamics and kinetics have the impact on the performance of the coating to be an [2,15]. Also, studies based on first principles have revealed the mechanical and interfacial properties of the Fe–Al intermetallic compounds, again stressing the role of atomic-level understanding in the design of advanced materials [1]. Nonetheless, it is still necessary to perform systematic thermodynamic modelling that links phase stability, intermetallic development, and coating optimization in medium-carbon steels, especially in light of the recent advances in computational and experimental techniques from 2023 to 2025. The present study, via the association of the computational predictions with the thermodynamic fundamentals, not only facilitates the understanding of intermetallic formation and phase evolution in Fe–Al–C systems but also provides a pathway to the development of advanced coatings that would be able to enhance service life, structural reliability, and resistance to harsh environments.

Materials and Methods

Structural encoding and data representation

Thermodynamic modeling of the Fe–Al binary and Fe–Al–C ternary systems was carried out using Thermo-Calc software (version 2024a), a powerful, advanced computational platform commonly used to determine phase equilibria, thermodynamic properties, and phase transformation behaviour in metals [8,9]. In this case, the calculations were performed according to the Open-CALPHAD approach, which is an advancement over the classical CALPHAD method, in which Gibbs free energy descriptions of different phases are obtained by fitting polynomial expressions to experimental and critically assessed data [10–12]. In this manner, the total Gibbs free energy of the system is minimized at each temperature and composition to determine stable phase assemblages in equilibrium conditions. This method has been confirmed many times in multicomponent systems, including steels, intermetallics, and advanced high-temperature alloys [8,9,13]. Thermo-Calc consists of two main components: (i) an engine that does the calculations and provides the results of equilibrium and phase diagrams, and (ii) internal thermodynamic databases that are consistently regarded as the best. In this research, the TCFE15 and SSOL6 databases were selected for use because they contain detailed, critically evaluated descriptions of Fe-, Al-, and C-containing phases, including ordered intermetallic,

carbides, and solid solutions [10,12]. The credibility of these databases has been proved in the recent thermodynamic evaluations of Fe–Al and Fe–Al–C systems [11,14].

Fe–Al Binary System Calculations

The calculations of equilibrium phases for the Fe-Al binary system were carried out with the help of the Binary Calculation module of Thermo-Calc. The calculation of the phase diagram was done at a constant pressure of 1 bar and a temperature from 300 °C to 1500 °C, which included the key solid–solid and solid–liquid transformations relevant to aluminizing and high-temperature processing. To represent both the disordered and ordered intermetallic phases like α-Fe (BCC), Fe_3Al (DO_3), FeAl (B2), and Fe_2Al_5, the TCBIN v1.1 parameter set and TCFE15 database were used properly [8,9]. Through Gibbs energy minimization, the equilibrium phase fields were determined, and the phase boundaries were found by following the ranges of stability of these phases as a function of temperature and composition. The results were confirmed with the help of recent experimental data and other sources [15–17].

Fe–Al–C Ternary System Development

In order to analyze the impact of carbon on the stability of phases as well as the formation of carbides, the Fe–Al–C ternary system was simulated by the Ternary Calculation module of Thermo-Calc. The calculations took place at a pressure of 1 bar over a temperature span from 600 °C to 1400 °C, covering the critical phase transitions in the case of medium-carbon steels during aluminizing and heat treatment [18]. The TCFE15 database was picked due to its exhaustive accounting of carbide and carbonaceous phases, which comprise Fe_3C (cementite), Fe–Al carbides, and graphite (C) [12,18]. The generation of equilibrium diagrams was done through isothermal sectioning, as well as liquidus projections, to show the Fe, Al, and C phase relations at varied temperatures. Special focus was given to the stability of the intermetallics FeAl (B2) and Fe_3Al (DO_3) with the entry of carbon. The Gibbs free energy differences (ΔG) were calculated in order to determine the thermodynamic preference of the transformations between the intermetallic and carbide phases, for instance:

$$3FeAl + C \rightarrow Fe_3C + Al, \quad (1)$$

$$Fe_3Al + C \rightarrow Fe_3C + Al. \quad (2)$$

The calculations indicate that above approximately 900 °C, Fe–Al intermetallics remain more stable than Fe_3C, implying limited carbon solubility under equilibrium conditions [18,19]. The ternary diagrams also show that carbon preferentially stabilizes BCC solid solutions and carbides within restricted compositional ranges rather than forming new ternary compounds. These findings align with recent CALPHAD studies of Fe–Al–C systems [19,20].

Summary of Computational Parameters

The computational parameters used in this study are presented in Table 1.

Table 1. Parameters summary

Parameter	Description
Software	Thermo-Calc 2024a
Calculation types	Binary and Ternary (Phase Diagram)
Databases	TCFE15, SSOL6, TCBIN v1.1
Pressure	1 bar
Temperature range	300–1500 °C (binary), 600–1400 °C (ternary)
Considered phases	Fe_3Al (DO_3), FeAl (B2), Fe_2Al_5, Fe_3C, Graphite
Method	Gibbs free energy minimization (Open-Calphad)

Results and Discussion

Figure 1 illustrates the calculated Fe–Al binary phase diagram developed using the Thermo-Calc software. The diagram demonstrates the equilibrium phase relationships across a wide range of aluminum concentrations (0–100 mass%) and temperatures (200–2000 K). Several distinct phase regions and transformation lines can be observed, indicating the complex interaction between Fe and Al in different compositional and thermal conditions.

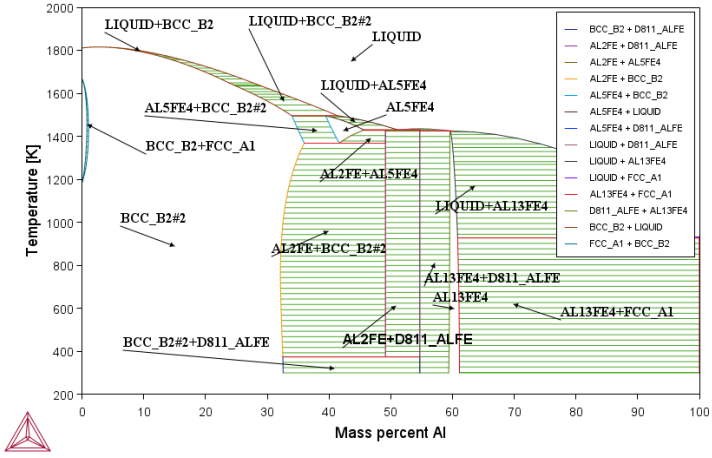

Fig. 1. Calculated Fe–Al phase diagram using Thermo-Calc software

The major phase for low Al contents (mass% under ~25) according to table 2 is BCC_B2, which below the melting point gradually gives way to BCC_B2 + FCC_A1 by separating the two phases. This transformation is an indication of B2-type intermetallics forming in Fe-rich blends. The range of 30-50 mass% Al has many intermetallics like Al_5Fe_4, Al_2Fe, and $D8_{11}$_AlFe noted. The Al_2Fe + $D8_{11}$_AlFe zone represents a solid-state equilibrium that gives rise to ordered Fe–Al intermetallics, which are characterized by high hardness and oxidation resistance. The persistent nature of the Al_5Fe_4 and $Al_{13}Fe_4$ phases in the intermediate Al compositions has been corroborated by experimental data from earlier studies. In the case of high Al contents (mass% > ~70), the phase region of $Al_{13}Fe_4$ + FCC_A1 comes into view that signifies the mixing up of the Fe–Al intermetallic and aluminum-rich solid solution phases. If further heated, the regions turn into liquid + $Al_{13}Fe_4$ or liquid + FCC_A1 ones, thus revealing the liquidus boundaries that delineate the melting behavior of Fe–Al alloys and at the same time showing the finite behavior of the phase diagram that is consistent with the known binary Fe–Al systems and proving the used Thermo-Calc thermodynamic database's correctness. The generic topology of the phase diagram matches the known binary Fe–Al systems, confirming the trustworthiness of the Thermo-Calc thermodynamic database employed. The calculated findings lay a dependable base for the research continuation in the Fe–Al–C ternary system, which will provide a more profound comprehension of the role of carbon in phase equilibria, intermetallic stability, and microstructure evolution.

The determination of Gibbs free energy of the Fe–Al system at 300 K provides a value of -37495.22 J, which makes it clear that the Fe and Al components interaction has already started. The negative enthalpy value of the system at this temperature and composition indicates the Fe–Al reaction to be exothermic, meaning the interaction is spontaneous and the formation of stable phase at low temperature is facilitated. For instance, in the Al_2Fe + BCC_B2 phase region, at 700 K it was observed that with the increase of aluminum concentration the Gibbs free energy of the system also rises, which is a sign of reduced reactivity. However, the rising temperature causes the Gibbs energy to drop, which means that the reaction tendency and phase stability are being improved. Consequently, it is inferred that temperature is a key factor in making the intermetallic phase formation more thermodynamically favorable. As the

main goal of this study is to apply an aluminum coating to iron surfaces in order to reduce or prevent corrosion, the systems with BCC phase were not considered for detailed discussions.

Table 2. Key features and mechanisms of generative deep learning models for molymer design

	Quantities	**Measuring unit**		
Mass percent Al	32.56508	[Mass percent]		
Temperature	300.00721	[K]		
System				
Moles	1.00000			
Mass	41.41794	[g]		
Temperature	300.00721	[K]		
Total Gibbs Energy	-37495.22285	[J]		
Enthalpy	-30994.40488	[J]		
Volume	0.00000	[m³]		
Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
Al	0.49988	0.32565	0.00001	-28257.68957
Fe	0.50012	0.67435	5.84431E-6	-30057.78206
Stable Phases				
	Moles	*Mass*	*Volume Fraction*	
BCC_B2#2	1.00000	41.41794	0.00000	
Composition				
Component	*Mole Fraction*	*Mass Fraction*		
Fe	0.50012	0.67435		
Al	0.49988	0.32565		

This is because the BCC (body-centered cubic) phase of iron has been proven to be more prone to corrosion than the ordered intermetallic structures. At 1400 K, in the Al_2Fe + Al_5Fe_4 phase region, the increase of aluminum concentration lead to an increase of the Gibbs free energy (therefore, reactivity is lessened), while the rise in temperature caused a decline in Gibbs energy (thus, increasing reactivity). Identification of a similar trend was done in the single-phase area of Al_5Fe_4 at 1430 K where increase in aluminum concentration raised the Gibbs energy and rise in temperature lowered it, thus the whole thing again supported that the upsurge in temperature by means of diffusion facilitated the intermetallic growth and consequently improved the thermodynamic stability. Gibbs energy was positive in the case of the $Al_{13}Fe_4$ + FCC_A1 phase analysis at 800 K with a direct dependence on aluminum concentration and an indirect, caused by the temperature, one—this again proving that high temperature drives the process of phase formation. The same behavior was noted in the Liquid + $Al_{13}Fe_4$ phase at 1200 K, where Gibbs energy rose with aluminum concentration but fell as temperature increased pointing out that thermal activation leads to both phase equilibrium and chemical bonding being strengthened in the system. In the single-phase field of $Al_{13}Fe_4$ at 1000 K, an identical trend was confirmed: higher aluminum content raised Gibbs energy while temperature elevation lowered it. As a whole, the results are indicative that while aluminum promotes the intermetallic phase formation, the excessive aluminum content not only increases the Gibbs energy but also reduces the reaction spontaneity of the system. From a statistical thermodynamic standpoint, it is commonly accepted that when the Gibbs energy of a reacting system is around –100,000 J the chemical interaction among the components is the most efficient. The Fe–Al system in this research reached its highest stability at 1368–1428 K with 41-41% and 41-49 mass% of aluminum, where the Gibbs energy of the system was between –93090 J and –96063 J. In such a situation, the aluminum-coated iron substrate has turned the interface into a liquid-bonding area with much better contact. A more detailed investigation of the phase diagram does reveal that the Gibbs energy of all phases increases with the growing concentration of aluminum; however, on the other hand, the effect of the rising temperature is the opposite – the Gibbs energy decreases. Consequently, it can be said that aluminum enrichment is a factor that hampers the formation of phases while temperature is a factor that accelerates the process. Thus, to create corrosion-resistant intermetallic phases in the Fe–Al system, it is very important to find the point at which the Gibbs energy is the most negative. The peak thermodynamic condition was characterized at 1428 K and 45.51 mass% Al, where the Gibbs energy was –96946 J. This

particular point lies in the domain of the $Al_2Fe + Al_5Fe_4$ phases. Table 3 presents the calculated parameters for the equilibrium condition.

Table 3. The calculated parameters for this equilibrium condition are presented below

Quantity	Value	Unit
Mass percent Al	45.51969	[%]
Temperature	1428.12783	[K]
Total Gibbs Energy	–96946.20298	[J]
Enthalpy	15617.98665	[J]
Mole Fraction (Al / Fe)	0.63361 / 0.36639	–
Stable Phases	$Al_2Fe + Al_5Fe_4$	–

This thermodynamic state represents the most stable condition, characterized by minimal Gibbs energy and enhanced interfacial adhesion between aluminum and iron. Consequently, the $Al_2Fe + Al_5Fe_4$ phase, at around 1428 K and 45–49% Al, is considered the optimal thermodynamic condition for producing durable, corrosion-resistant aluminized coatings on iron substrates.

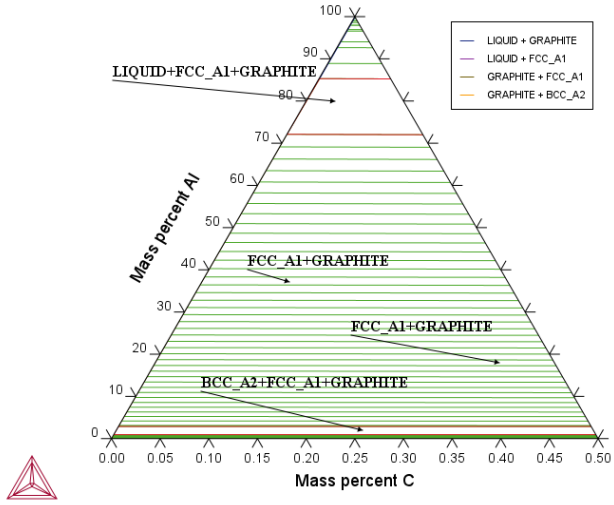

Fig. 2. Ternary phase diagram of the Fe–Al–C) system showing equilibrium regions among Liquid, FCC_A1, BCC_A2, and Graphite phases

To further analyze the coating behavior of aluminum on carbon-containing steel (Steel 45), the Fe–Al–C ternary phase system was investigated. Figure 2 shows the Fe–Al–C ternary phase diagram generated using Thermo-Calc software, illustrating the phase equilibria between iron, aluminum, and graphite (carbon) at high temperature. This diagram helps understand how carbon affects the phase stability and thermodynamics of aluminized steel systems.

The diagram consists of several multi-phase regions, including:

- Liquid + FCC_A1 + Graphite
- FCC_A1 + Graphite
- BCC_A2 + FCC_A1 + Graphite
- Graphite + BCC_A2

The presence of carbon (in the form of graphite) is very crucial in dictating the diffusion and phase formation at the interface of steel and aluminum in this system. Increasing the mass percent of carbon (from the left-hand side of the diagram to the bottom-right corner) stabilizes phases containing graphite,

which acts as a barrier to the diffusion of aluminum into iron. On the other hand, in the region with higher aluminum content (upper part), the phase equilibrium shifts toward liquid + FCC_A1 + graphite, indicating a stronger affinity between aluminum and iron, with carbon pushed to the interface. The spot of equilibrium for Steel 45 (about 0.45 mass% C) is adjacent to the FCC_A1 + Graphite and BCC_A2 + FCC_A1 + Graphite borders. It means that the microstructure of the steel during aluminizing is mainly composed of α-Fe (BCC_A2), γ-Fe (FCC_A1), and graphite phases, forming a mixture. The presence of these phases indeed promotes the drawing of aluminum into the substrate at a moderate rate, while maintaining good coating adhesion. This happens at high temperatures (more than 1200 K), where the ternary system moves towards Liquid + FCC_A1 + Graphite, and it is here that aluminum starts to take up the molten phase, facilitating wetting and spreading on the steel surface. During cooling, the system's aluminum reacts with iron, forming intermetallic compounds such as FeAl and Fe_2Al_5, while graphite remains an inert phase at the grain boundaries. This behavior is advantageous because it leads to the formation of aluminum-coated protective layers with better resistance to oxidation and corrosion. From a thermodynamic perspective, the introduction of carbon leads to a slight increase in the system's Gibbs energy compared to the binary Fe–Al system, primarily because of the limited solubility of carbon in aluminum and the formation of graphite. Nevertheless, carbon also contributes to microstructure refinement and improved interfacial bonding, which, in turn, leads to stronger adhesion of the coating. The evaluation of the ternary phase diagram Fe–Al–C indicates that for Steel 45 the equilibrium of phases is the most favorable within the BCC_A2 + FCC_A1 + Graphite region. This composition is a guarantee of stable aluminide formation, balanced diffusion behavior, and improved coating performance. The intermetallics of Fe–Al and the phases containing graphite work together to provide the aluminum-coated steel surface with both corrosion resistance and mechanical strength.

Conclusion

The thermodynamic evaluation of the Fe-Al and Fe-Al-C alloy systems using Thermo-Calc (Open CALPHAD methodology) highlighted three aspects: phase stability, intermetallic formation, and the effect of carbon on phase equilibria. The binary system Fe-Al showed: the binary phase diagram designated the stability areas of the main intermetallic compounds, i.e., Al_5Fe_4, Al_2Fe, and $Al_{13}Fe_4$, over a vast aluminum concentration range (0-100 wt%). Increasing the aluminum concentration shifts the phase boundary between the ordered and disordered structures, promoting the formation of DO3 (Fe_3Al) and B2 (FeAl) phases, which in turn contribute to increased hardness, oxidation resistance, and thermal stability. The melting of the alloy starts at about 900 °C and lasts until 1450 °C, depending on the aluminum content, which is very important for the coating to be optimized through controlled thickening. The ternary system Fe-Al-C witnessed with the addition of carbon a significant modification of the binary Fe-Al phase equilibria with the result being the creation of regions containing graphite and carbide. The computations based on the Gibbs energy reveal that the Fe-Al intermetallics remain the thermodynamically favored over Fe_3C even at temperatures above 900 °C, suggesting that the intermetallic matrix has very low carbon solubility under equilibrium conditions. The occurrence of graphite phases in addition to FCC_A1 and BCC_A2 solid solutions suggests the possibility of composite-like coatings with higher wear resistance and better thermal conductivity. Practical Implications: The study reveals that applying aluminum coatings to medium-carbon steels (such as Steel 45) not only prevents corrosion but also extends the material's lifespan at high temperatures and maintains its strength. Theoretical calculations enable varying the parameters of the aluminizing process, such as temperature and aluminum content, to achieve the desired intermetallic layer thickness and phase composition. Limitations and Future Work: The present research assumes thermodynamic equilibrium, whereas actual industrial processes may involve kinetic barriers, such as slow diffusion rates and non-equilibrium phase formation. A future direction would be to conduct experimental validation of intermetallic growth kinetics, along with investigating the influence of other alloying elements, namely Cr, Ni, or Si, on phase stability and coating performance. To summarize, the work in this project provides a numerical and forecasting foundation for creating Fe–Al-based steel coatings,

thereby advancing protective layers with excellent corrosion resistance, structural stability, and high-temperature performance.

Designing and discovering new polymeric materials has become easier because of the use of generative models in polymer research. Exploring the vast chemical space of polymers has been enabled by these models, including diffusion models, Generative Adversarial Networks (GANs), and Variational Autoencoders (VAEs).

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