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Thermodynamical Calculation of Residual Air Pressure in the Working Chamber of a Circulation Setup

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Abstract

The paper shows that the presence of aluminium oxide is conditioned by the residual air content in the chamber, which deteriorates the coating quality. In this connection, the residual pressure and content of aluminium oxide were calculated in the chamber of the circulation setup.

Keywords: Heat-resistant and heat-proof coatings; Circular method; Residual pressure; Diffusion saturation of metals and alloys; Aluminium oxide; Oxygen getter

Introduction

The main requirement to the coatings on gas turbine engine blades is the ability to resist high-temperature gas corrosion over the predetermined lifetime of the turbine [1-3]. During the operation, the coatings suffer violent exposure to the gas flow. This results in non-reversible physicochemical processes, which further lead to consequent failure of the coatings. The duration of these processes depends on the structure, composition and thickness of the coating and operating temperature.

The elaboration of new coatings and corresponding technological processes for their application is impossible without robust theoretical and calculation methods [4]. The compounds deposited on the surfaces and their formation rate depend on the composition of the saturating medium and protected alloy, the temperature and duration of the process. The determination of precise quantitative relations between the technological parameters and generated structure of the coating is useful for prognosticating operational properties of the products, selecting required technological regimes and creating control systems of thermochemical treatment (TCT) [5].

Mathematical experiment planning is used to receive additional information on the studied phenomenon and property or to save time and material resources due to the complexity and unclear mechanism of the process [6]. The experiment planning is aimed at determining the necessary number of tests that would completely unveil the impact of various variable factors (the composition of the saturating medium, temperature, pressure, etc.) on the parameter under study. The object of the study is described by the model represented as 1st-, 2nd- and 3rd-order polynomial; these models do not consider the TCT mechanism. The statistic models give no information about the process kinetics and are used, as a rule, to solve specific problems.

Any model is just the reflection of a real process; the range of made assumptions obviously necessitate experimental studies of TCT processes with the application of new calculation methods.

At the early stage of the calculations using the laws of equilibrium thermodynamics, the modeling was ultimately simple. The majority of works determining the parameters of coating deposition implement the thermodynamical calculations of the probability of chemical reactions by determining the sign of Gibbs energy. Let us exemplify this by the following reaction:

$$a\,A + b\,B \rightleftarrows c\,C + d\,D \quad (1)$$

$$_{\nabla}G^0_{reaction} = c\,_{\nabla}G^0_C + d\,_{\nabla}G^0_D - a\,_{\nabla}G^0_A - b\,_{\nabla}G^0_B \quad (2)$$

The calculations are applicable only in the case when the composition of the reaction products within the studied range of parameters is defined only by this chemical equation.

The method of equilibrium constants is a no go when calculating reactions in multi-component systems of random composition, multi-stage processes and in the presence of a condensed phase, because the diffusion saturation relates to complex multi-component heterogeneous systems.

The work presents an effective algorithm for numerical solution of equations describing the equilibrium in multi-component systems, which allows using a PC (TERRA software) to calculate the equilibrium compositions of the formed substances, including their thermodynamical data [7]. The collected thermodynamical data enable researchers to determine with higher accuracy necessary conditions of diffusion processes, yield of the target products and amount of secondary products and other characteristics. The calculation method is based on the determination of phase and chemical equilibrium using the principle of maximum entropy.

The work presents the thermodynamical calculation of the working media with a due consideration of residual air and its impact on the coating structure.

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Theory and Methods

It was elucidated that the occurrence of aluminium oxide is due to the presence of water and air (H_2O and O_2), which in calculations were introduced in different amount.

The presence of Al_2O_3 aluminium oxide in the coating was tested by micro-X-ray spectroscopy. The analysis of the impurities identified aluminium in the form of aluminium oxide. The content of other particles was not studied. Other unwanted particles in the coatings can be solid particles of chromium nitride and aluminium nitride. Nitrogen gets into the chamber with air and due to the dissociation of ammonium chloride NH_4Cl.

The thermodynamical calculations were traditionally made to determine the possibility of reactions and transition of the coating components in a reasonable temperature range. The thermodynamical calculations of gas medium composition did not consider the impact of residual air on chemical reactions in the circulation setup reactor [8]. Thus, we could not determine the roles of oxygen and water vapor in the formation of the coating structure.

The real chemical factor is a complex multi-component heterogeneous system where takes place the chemical interaction of halide source and residues of moist air with all chemical elements in the working volume, saturated melts, sources of coating elements, materials of attachments and reactor's internal surface. The interaction in such complex system can lead to the formation of both gaseous and condensed compounds that, after introducing into the coating, adversely change its phase composition and structure. Primarily, these are brittle inclusions of oxides, nitrides, silicides, etc. Since a bunch of parallel reactions occur in the reactor (tens and more), the analysis of the equilibrium state by conventional methods (method of equilibrium constants) becomes unavailable due to cumbersomeness of the calculations.

This necessitates theoretical, calculation and experimental studies (phase analysis and chemical composition of the impurities) that will allow identifying the causes of unaccounted impurities.

The work presents the calculation of the mass content of residual oxygen O_2 that prevents the formation of Al_2O_3 in the circulation setup with the muffle working volume of 0.23 m^3 and working pressure of 10^5 Pa. The sources of moist were represented by the moist that remains after incomplete evacuation of air from the muffle. The pressure of the setup is ~3 Pa.

Initial data: $NH_4Cl+Al+Cr+N_2+O_2+H_2O$. Calculations using TERRA software have allowed determining the equilibrium state for such systems with a due regard to the real bulk load of reacting components. For the calculations, the following assumptions were made: initial atmospheric contents are at 10^5 Pa, residual pressure after evacuation by a fore pump is 3 Pa, consequent evacuation down to 0.3 Pa and additional evacuation down to 0.03 Pa. The results of the thermodynamical calculations are presented in Table 1.

The density of the working gas at the saturation temperature of 1000°C in regard to the circulation setup was determined as:

$$\rho_{1000^0 \tilde{N}} = \frac{\rho_0}{(1+\alpha_\rho \cdot t)} \cdot 0^{5},$$

where $\rho_{1000°C}$ is the medium density at the saturation temperature of 1000°C,

ρ_0 is the density of the gas mixture in the working chamber at 1 atm. (0.001293 g/cm^3),

α_ρ is the coefficient of the gas medium expansion (0.00367 1/t°C).

Results and Discussion

The content of oxygen in regard to the circulation setup was not more than 0.07 g. Also, the influence of yttrium as the getter for oxygen in the working chamber was studied.

The calculations allowed determining the maximum acceptable residual pressure (~3 Pa) of moist air (moisture) in the setup working chamber and admissible minimum amount of aluminum oxide (10^{-4}-10^{-5} mol/kg). The results are given in Table 1 and in Figure 1. Evidently, the decrease of the residual atmosphere reduces the content of impurities in the setup muffle in solid state for Al_2O_3; the further reduction of the residual atmosphere content lower that ~3 Pa has no effect on aluminium oxide content. Presumably, the impurities can be presented by other substances revealed by the calculations.

Additional results of the calculation given in Table 2 testify that even at low oxygen and moisture content (0.001 mole after system evacuation), aluminium oxidizes with the formation of Al_2O_3 with appreciable fixation of O_2 and H_2O. Hence, the formation of Al_2O_3 particles is conditioned by the presence of moisture and oxygen in the working chamber. In addition, aluminium oxide is used in the powder method as inert filler and can get into the coating structure along with the particles of the powder mixture. In this connection, deeper cleaning of the working gas medium from oxidizers requires implementation of active oxygen getters.

One of them is yttrium. According to the calculations, the introduction of yttrium in the amount of 0.01 mole completely fixes O_2 and H_2O in the form of yttrium oxide Y_2O_3. We suggest, when performing the evacuation (down to 3–6 Pa) of residual air, removing it by NiY alloy that fixes the residual oxygen and moisture into yttrium oxides (YO, Y_2O, Y_2O_3) (Table 2). The initial composition of the reagents (in moles) and reaction products (mol/kg) at the temperature of 1000°C are presented in Figures 2 and 3.

Pressure [Pa]	Substance content (Al_2O_3) [mol/kg]		
	Temperature, 1200 K	Temperature, 1300 K	Temperature, 1400 K
0.03	$4.56 \cdot 10^{-6}$	$4.56 \cdot 10^{-6}$	$4.56 \cdot 10^{-6}$
0.3	$4.56 \cdot 10^{-6}$	$4.56 \cdot 10^{-6}$	$4.56 \cdot 10^{-6}$
3	0.000224	0.000224	0.000119
30	0.004533	0.004364	0.001667
300	0.045165	0.045165	0.044885

Table 1: Calculation of acceptable residual air pressure in the setup working chamber preventing the formation of oxides (Al_2O_3) in the coating.

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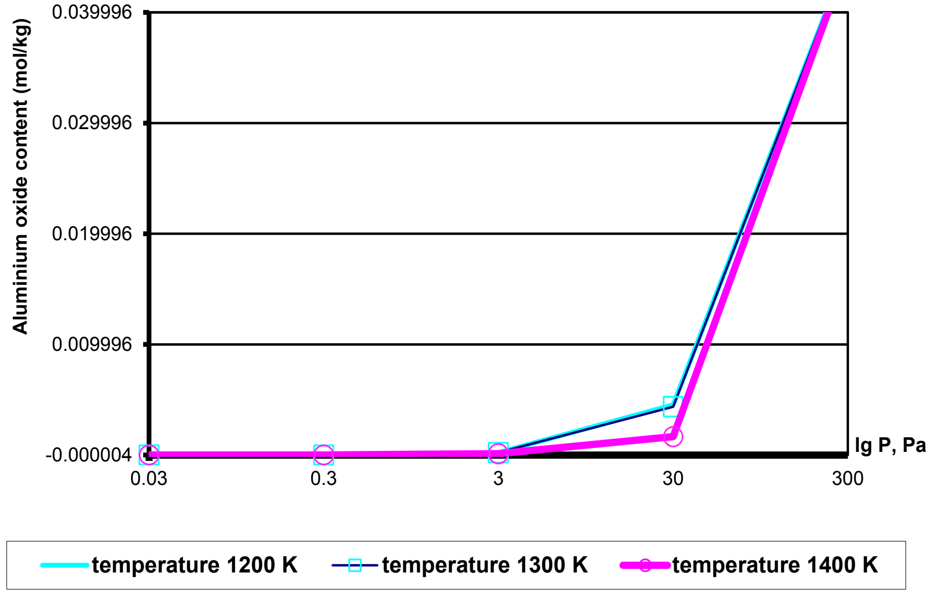


Figure 1: Maximum permissible residual pressure (~3 Pa) of moist air and minimal admissible content of aluminium oxide in the working chamber of industrial circulation setup.

Initial data							Reaction products			
T °C	Ni	Y	O_2	h=2	$NiCl_2$	Al	Al_2O_3	Y_2O_3	O_2	H_2O
1000	5	0	0.001	0.001	1	1	0.02	0	0	0
1000	0.025	0.005	0.001	0.001	1	1	0.0055	0.013	0	0
1000	0.01	0.002	0.001	0.001	1	1	0.014	0.005	0	0
1000	0.05	0.01	0.001	0.001	1	1	0	0.019	0	0
1000	0.1	0.02	0.001	0.001	1	1	0	0.018	0	0
1000	0.25	0.05	0.001	0.001	1	1	0	0.017	0	0
1000	0.5	0.1	0.001	0.001	1	1	0	0.015	0	0
1000	1	0.2	0.001	0.001	1	1	0	0.012	0	0
1000	2.5	0.5	0.001	0.001	1	1	0	0.008	0	10^{-15}
1000	5	1	0.001	0.001	1	1	0	0.005	0	10^{-10}

Table 2: Impact of yttrium on the composition and content of oxides (mol/kg).

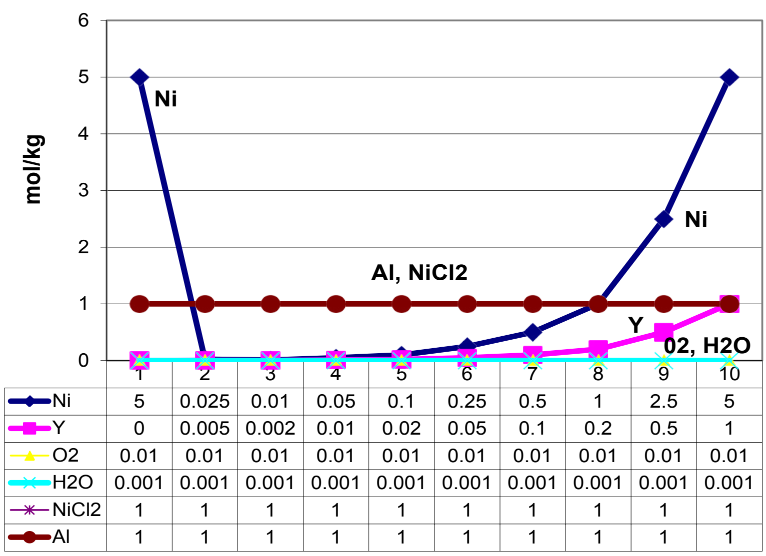
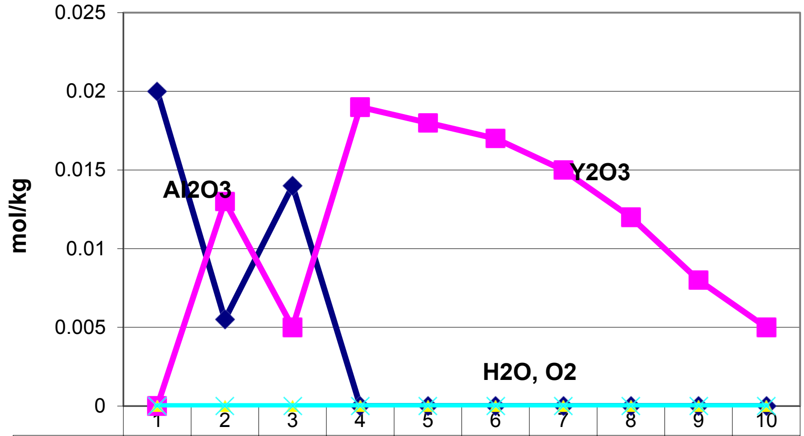


Figure 2: Initial composition of reagents in moles at the temperature of 1000 °C (content of O_2 and H_2O at residual air pressure in the chamber of ~3Pa).



	1	2	3	4	5	6	7	8	9	10
Al2O3	0.02	0.006	0.014	0	0	0	0	0	0	0
Y2O3	0	0.013	0.005	0.019	0.018	0.017	0.015	0.012	0.008	0.005
O2	0	0	0	0	0	0	0	0	0	0
H2O	0	0	0	0	0	0	0	0	1E-15	1E-10

Figure 3: Interaction products (mol/kg) at the temperature of 1273 K.

Conclusions

The work has calculated the acceptable content of oxygen and maximum permissible pressure (~3 Pa) of moist air (moisture) in the setup working chamber with a due consideration of its construction feature. Also, the admissible minimal amount of aluminium oxide was determined (10^{-4}-10^{-5} mol/kg). We suggest, when performing the evacuation (down to 3-6 Pa) of residual air, removing it by NiY alloy as the getter that fixes the residual oxygen and moisture into yttrium oxides (YO, Y_2O, Y_2O_3).

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