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PHYSICO-CHEMICAL MODELING OF PHASE SEPARATION IN FE-21.4 CR STEEL WITH 1.14 MO TAKING INTO ACCOUNT CROSS FACTORS

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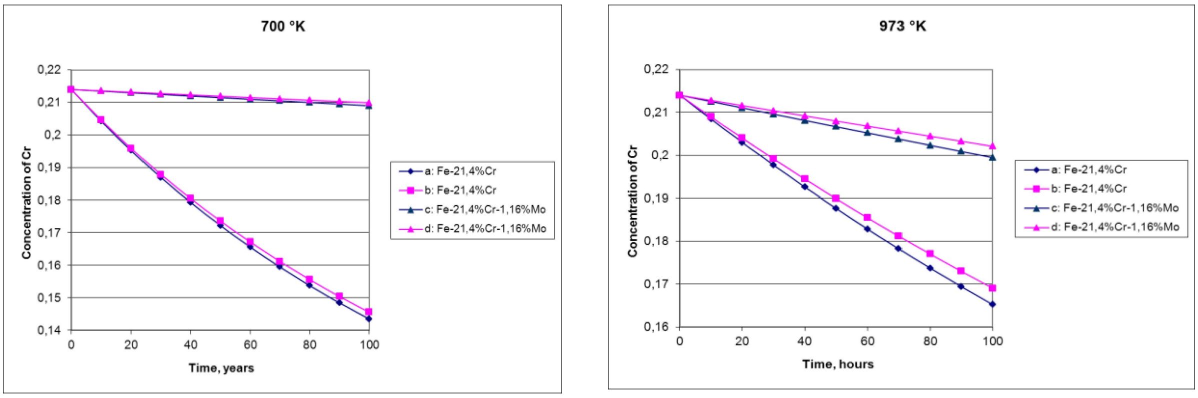
Introduction. The use of ferritic-martensitic steel*s* as structural material for steam generator rotors has been advocated due to their relatively low rate of swelling at elevated temperatures*,* for example, Fe-Cr and Fe-Cr-Al alloys [1, 2]. Because of the high Cr-content, the alloys are not suitable for use at temperatures around 500 °C as the microstructure decomposes into a Fe-rich (α) phase and a Cr-rich (α') phase due to the miscibility gap in the Fe-Cr system [3, 4]. Phase separation in such alloys can also be prevented by doping with elements that impede the segregation of chromium. To quantify the effect of elements on phase separation, multi-scale modeling is required.

Research results. In this work, the object of research is Fe - (16.1-21.4) % Cr alloys with 1.16% Mo in comparison with Fe - (16.1-21.4)% Cr alloys. The chromium content in the alloys exceeds 15%, ensuring their high corrosion and heat resistance [5]. The diffusion coefficients for these alloys at different temperatures are known in the literature [6]. The calculated parameters of the Arrhenius equation for the diffusion of iron and chromium in the studied alloys are given in Table 1. It is already clear from these data that the diffusion of chromium has a high activation energy in alloys with molybdenum, i.e. diffusion of chromium occurs more slowly in the complex alloy. Direct calculations, of course, fully confirm this position.

Table 1 – The parameters of the Arrhenius equation for the diffusion of iron and chromium in the studied alloys

Alloy composition	Parameters of the chromium diffusion		Parameters of the iron diffusion	
	A_0, m²/s	U_0, J	A_0, m²/s	U_0, J
Fe – 16,1 % Cr	$2{,}1 \cdot 10^{-5}$	204232	$10{,}6 \cdot 10^{-5}$	234517
Fe – 21,4 % Cr	$1{,}2 \cdot 10^{-5}$	201008	$14{,}0 \cdot 10^{-5}$	238309
Fe – 16,1 % Cr – 1,16 % Mo	$20{,}9 \cdot 10^{-5}$	232825	$5{,}7 \cdot 10^{-5}$	226905
Fe – 21,4 % Cr – 1,16 % Mo	$22{,}1 \cdot 10^{-5}$	235484	$12{,}6 \cdot 10^{-5}$	237344

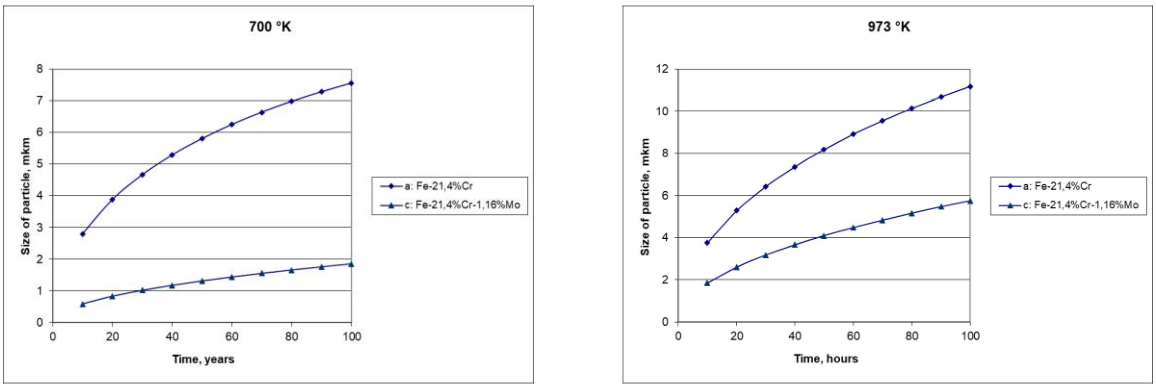
In this work the current concentrations of chromium and iron in a solid solution were found by numerical integration of Fick's equations at two temperatures - working 700 ° K and increased - 973 ° K [7, 8]. Calculations were carried out without and taking into account cross factors [8]. The calculation results are shown in Fig. 1 and 2 respectively.



a) b)

Figure 1 – Change in chromium concentration in solid solution of steels Fe – 21,4 % Cr and Fe – 21,4 % Cr – 1,16 % Mo at a temperature 700 °K (a) and 973 °K (b), lines a, c - without cross factors, lines b, d - with cross factors

Conclusions. The calculation results shows, that the thermal stability of the Fe - 21.4% Cr alloy with 1.16% Mo is much higher than without molybdenum. At an operating temperature of 700 ° K, the concentration of chromium in the solid solution of the Fe - 21.4% Cr alloy decreases from 21.4% to 16.1% in about 70 years of operation, with the formation of σ-phase inclusions about 7 microns in size (Fig. 2). In the Fe - 21.4% Cr - 1.16% Mo alloy, the chromium concentration changes insignificantly during the same operating time.



a) b)

Figure 2 – Changing the size of inclusions in steels Fe – 21,4 % Cr and Fe – 21,4 % Cr – 1,16 % Mo at a temperature 700 °K (a) и 973 °K (b)

At an elevated operating temperature of 973 ° K, phase separation is observed in both alloys. The concentration of chromium in the solid solution of the Fe - 21.4% Cr alloy decreases from 21.4% to 16.1% in about 120 hours of operation, while inclusions of the σ-phase with a size of about 12 microns are formed.

In alloy Fe – 21,4 % Cr – 1,16 % Mo at a temperature of 973 ° K, the chromium concentration during the same operation time decreases three times slower with the formation of inclusions of the σ-phase about 6 microns in size.

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Abstract. Physicochemical modeling of diffusion phase transformation and determination of the long-term microstructural stability of the Fe-21.4 Cr alloy with 1.16 Mo taking into account cross factors has been carried out. A conventional Fe-21.4 Cr alloy is used as a reference material. The article proposes an integral approach to modeling phase separation in chromium alloys, combining the determination of diffusion coefficients and fluxes of elements, taking into account their dependences on the concentration and an assessment of the mutual diffusion of elements. The calculated values of diffusion fluxes are used to calculate the current concentrations of carbon and chromium in the alloy and the size of chromium formations. They show that the thermal stability of the Fe - 21.4% Cr alloy with 1.16% Mo is much higher than without molybdenum. In alloy Fe – 21,4 % Cr – 1,16 % Mo at a temperature of 973 ° K, the chromium concentration during the same operation time decreases three times slower with the formation of inclusions of the σ-phase about 6 microns in size.

Key words: Physicochemical modeling, phase transformation, fluxes, chromium alloys, nonequilibrium thermodynamics, diffusion coefficients.