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Thermodynamic simulation of oxidation process of the Mo_{ss}-Mo_3Si hypoeutectic alloy, doped with scandium or neodymium

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Abstract

In order to study the effect of yttrium additives on the oxidation of molybdenum silicide alloys, thermodynamic modeling of the interaction in Mo-Mo_3Si-Sc_5Si_3 и Mo-Mo_3Si-NdSi systems with dry and moist air was performed in the temperature range 25-2000 °C. The calculations were performed using the HSC Chemistry 6.12 software, into the database of which the calculated missing thermochemical characteristics silicates, molybdates of scandium and neodymium were entered. Based on the obtained dependences of the composition of phases on temperature and charge of the oxidant (air or vapor-air mixture), the sequence of phase formation was determined and the compositions of oxidation products were estimated. It is shown that, under equilibrium conditions, the oxidation process with dry and moist air proceeds almost equally, since the interaction of the components of the alloy with oxygen is thermodynamically preferable than with water vapor. According to the obtained thermodynamic models, the oxidation process of the Mo-5Si-3(Sc, Nd) (wt.%) alloys involves a sequence of the following chemical transformations: at the beginning Mo and Sc (Nd) silicides oxidize forming Sc_2O_3 (Nd_2O_3), SiO_2 and elemental Mo, then molybdenum is oxidized to MoO_2 and Sc_2O_3 or Nd_2O_3 interacts with SiO_2 with the formation of appropriate silicates $Sc_2Si_2O_7$ или $Nd_2Si_2O_7$. As a result of the complete oxidation of the alloy, MoO_3 and $Sc_2(MoO_4)_3$ or $Nd_2Mo_4O_{15}$ are added to the condensed product, and molybdenum oxide $(MoO_3)_n$ vapor appears in the gas phase. In addition, the formation of $Nd_2Mo_2O_7$ and Nd_2 $(MoO_4)_3$ is possible. During the oxidation of the Mo-5Si-3Nd alloy at T > 1700 °C, $Nd(OH)_3$ can be formed in the condensed reaction products. According to the results of complete thermodynamic analysis, the formation of silicates and molybdates of scandium and neodymium can promote to the formation of a protective film on the surface of the alloys, which limits the diffusion of oxygen in them, and as a result, the oxidation resistance of alloys should increase.

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