THERMODYNAMIC MODELING OF NICKEL-BASED SELF-FLUXING MATERIALS

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Using the TERRA and ThermoCalc software, thermodynamic modeling of self-fluxing powder materials based on nickel was carried out in the temperature range of 300-6000 K in an atmosphere of various plasma-forming gases: argon, nitrogen, air and mixtures "92 vol. % air + 8 vol. % propane" at a total pressure of $P = 10^5$ Pa. The initial composition of the simulated systems corresponded to the composition of nickel-based powder self-fluxing materials (wt. %): Ni – 79.3, C – 0.5, Cr – 15, Si – 3.2, B – 2 (PG-SR2), Ni – 74.3, C – 1, Cr – 17, Si – 4.1, B – 3.6 (PG-SR4). When preparing the initial data for modeling, the average technological parameters of the plasma spraying unit were taken into account: plasma gas consumption - 1 l/s, powder consumption – 1 g/s, 5 g/s and 10 g/s. The modeling took into account the possibility of the existence of elements, ions, compounds (oxides, carbides, silicides, and others) in condensed and gaseous states.

The temperature dependences of the components of the condensed and gaseous phases are calculated. It is revealed that the distribution of the components of the condensed and gaseous phases changes significantly with variations in the initial content of the powder material in the working fluid and the composition of the plasma-forming gas.

The temperature dependences of integral thermodynamic characteristics - enthalpy (I) and entropy (S) – for the PG-CP2 (PG-CP4) + gas (gas – Ar, N_2, air, air + propane) systems are constructed. It is shown that an increase in the consumption of powder material leads to an increase in enthalpy and a decrease in entropy for both systems. These trends become more pronounced at high temperatures (T > 3000 K), when active evaporation of the main components of the system occurs and a sharp increase in the partial pressures of the components of the gas phase is observed. A comparison of the temperature dependences of the condensed and gas phases and the thermodynamic characteristics shows that there is a correlation between them: kinks in the graphs are observed at the same temperatures. This can be explained by the phase transformations that occur in the condensed and gaseous phases, in particular, melting and evaporation.

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