THERMODYNAMIC MODELING OF Fe-Si-O SYSTEM

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MOTIVATION

The investigation of physical and chemical properties of iron, silicon and their alloys is important for production and operation of instruments and devices, which contain Fe, Si and their compositions. Besides this, it is very important to investigate the behavior of these materials on extreme conditions and aggressive media.

RESULTS

Thermodynamic modeling of the behavior of iron, silicon and compositions of Fe-Si system in oxygen in the wide range of temperatures (300 – 4000 K) at the different pressures (P = 0.1, 1, 10, 100 MPa) was carried out. As the software the program TERRA was used. The temperature dependences of the equilibrium composition of the components of the condensed phase and partial pressures of gas phase, which are formed when heating of iron, silicon and their compositions at the oxygen atmosphere were constructed. It was shown that with the increase of the temperature the chemical composition of the investigated systems undergoes substantial changes. The domains of existence of the components of the condensed and gas phases are revealed (Fig.1).

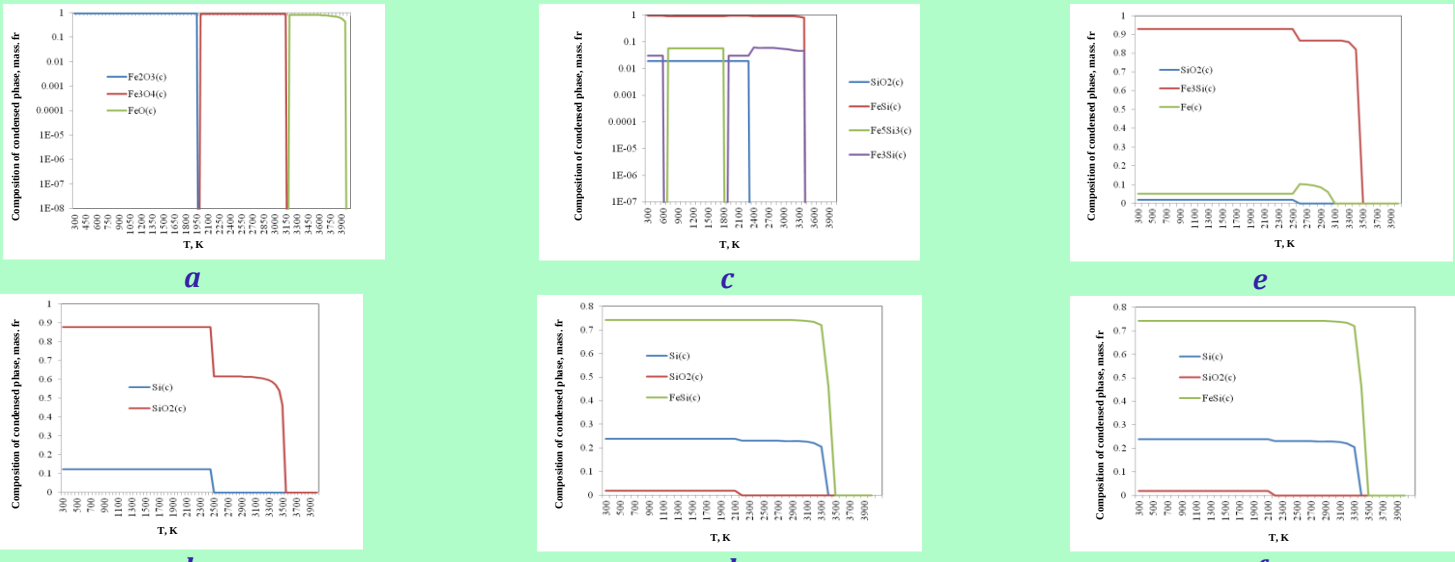

Fig.1. Temperature dependences of equilibrium composition of the condensed phase, which is formed when heating of iron (a), silicon(b), FeSi (c), $FeSi_2$(d), Fe_3Si(e) and Fe_5Si_3 (f) at the oxygen atmosphere. Common pressure: P = 1 MPa (a, b) and P = 0.1 MPa (c - f)

The temperature dependences of integral entropies, enthalpies and Gibbs energies were calculated. It was shown, that these dependencies are nonlinear. The comparison of the temperature dependences of the composition of components and thermodynamic parameters shows that there is a correlation between them: the breaks on the graphs are observed at the same temperatures. In our opinion, these breaks were caused by changes of the phase composition of the system (Fig.2).

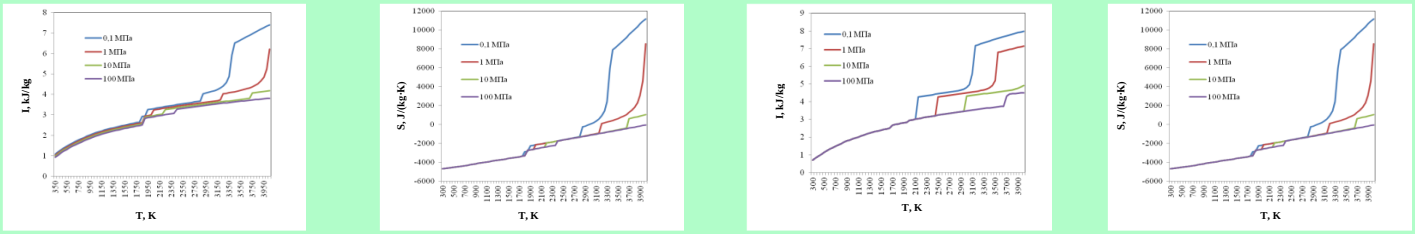

Fig.2. Temperature dependences of integral enthalpies (I) and entropies (S) for Fe-O (a, c) and Si-O (b, d) systems at different common pressures

It is shown that the steadiest composition in the studied system is FeSi. The simulation of behavior of FeSi when heating on the temperature range 300-4000 K with the different initial content of oxygen in system was carried out. It was obtained that complete oxidation occurs at the relationship of $FeSi:O_2$ = 60:40 (mass.%); the condensed phase consists exclusively of oxides and binary oxides: SiO_2, Fe_2O_3, Fe_3O_4, Fe_2SiO_4.