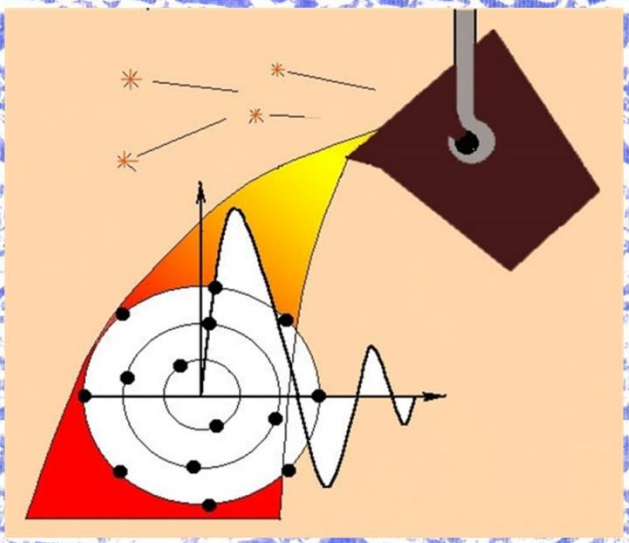
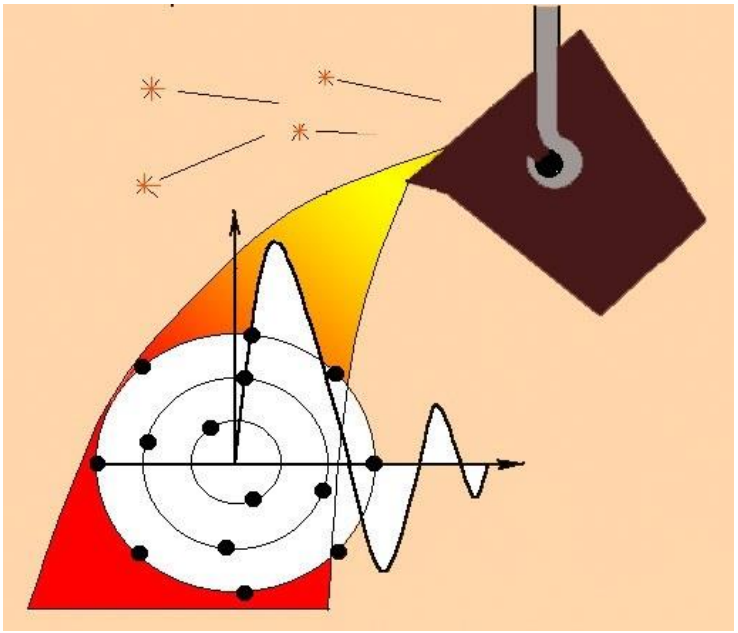
BOOK OF ABSTRACTS
OF THE INTERNATIONAL CONFERENCE
MELTS



September 12-18, 2021
Ekaterinburg, Russia



Book of Abstracts of the International Conference MELTS

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This Book of Abstracts contains brief information on modern research works devoted to modeling, calculating and experimental studying the structure and properties of disordered systems in a condensed state, as well as setting the relationship of liquid, crystalline, nanocrystalline and amorphous states.

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LINSEIS THERMAL ANALYSIS

Preface

The purpose of the MELTS Conference is to bring together scientists from the fields of chemistry, physics, materials science, and metallurgy who deal with the actual problems of disordered condensed state that includes molten materials and other related systems.

This conference follows the traditions of the All-Union (later All-Russian) Conference on the Structure and Properties of Liquid Metals and Molten Slag, which had been held regularly under the leadership of Academician Nikolai Vatolin since 1974 and was one of the largest national scientific forums on fundamental theoretical and experimental research of metal and slag systems.

The program of the event consists of the following sessions:

1. Modeling and calculation of structure and properties of disordered systems in condensed state
2. Experimental study of structure and properties of disordered systems in condensed state
3. Relationship of melts, crystalline, nanocrystalline and amorphous states.

There are no parallel sessions. Instead, they are arranged in time sequentially one after another.

All the oral communications fall into two categories: Plenary Lectures and Oral Contributions.

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THERMODYNAMIC MODELING OF Fe-Si-O SYSTEM

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Nowadays iron-silicon alloys are widely used as materials with special electrical properties. One of the main properties of this group of alloys is their high corrosion resistance. It should be noted that the melts of the Fe-Si system have been extensively studied both experimentally and using various model representations [1]. However, it is very important to study the behavior of these materials in extreme conditions and aggressive environments. One of the most effective ways to solve this problem is to use thermodynamic modeling, which reduces the amount of expensive experimental investigations.

The behavior of Fe-Si compounds (FeSi, $FeSi_2$, Fe_3Si, and Fe_5Si_3) in the oxygen atmosphere in the temperature range of 300-4000 K and pressures of 10^5-10^8 Pa is studied using the thermodynamic modeling methods and the TERRA software package [2-3].

It is shown that the compounds FeSi and Fe_3Si are sufficiently resistant to oxidation up to a temperature of 3400 K, at which their decomposition occurs. When interacting with oxygen, $FeSi_2$ is destroyed, and FeSi, Si, and SiO_2 are formed. The Fe_5Si_3 compound is stable only in the temperature range 700-1800 K, at other temperatures the condensed phase consists mainly of Fe_3Si and FeSi. The interaction of FeSi with oxygen at different initial oxygen content was studied. It is shown that at the ratio FeSi:O_2=60: 40 (wt.%) complete oxidation occurs, and the condensed phase consists exclusively of oxides and double oxides: SiO_2, Fe_2O_3, Fe_3O_4, Fe_2SiO_4.

The temperature dependences of the enthalpy, entropy, and internal energies of the Fe-Si-O system at different pressures are investigated. It is shown that these dependences are not monotonic. The graphs of the dependences I(T), S(T), and U(T) show sharp fractures at temperatures corresponding to significant changes in the chemical composition of the condensed and gas phases.

When analyzing the results obtained, it should be taken into account that the calculation method used is intended for modeling extremely equilibrium states of complex systems and does not allow finding the "trajectory" of the transition to the equilibrium state.

The work was carried out according to the state assignment for IMET UB RAS

1. Ilinykh N. I., Kulikova T. V., Moiseev G. K. Composition and equilibrium characteristics of metal melts of binary systems based on iron, nickel and aluminum. - Yekaterinburg: Ural Branch of the Russian Academy of Sciences, 2006. - 236 p.
2. Sinyarev G. B., Vatolin N. A., Trusov B. G., Moiseev G. K. Application of computers for thermodynamic calculations of metallurgical processes. - Moscow: Nauka, 1983. – 263 p.
3. Trusov B. G. Program system for modeling phase and chemical equilibria at high temperatures // Vestnik MSTU im.n. E. Bauman.Ser. Priborostroenie, 2012. – P. 240-249.