The Rate of SiO Formation by the Reaction of Methane with Silica

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The MSc task

One of the main tasks in the Kiselrox Project is to develop the kinetic model(s) describing the reduction of the silicon oxide. Since the project has been approved under the program GASSMIX, the application of natural gas in oxide reduction should be set in the priority. In order to establish the kinetic models, experimental information is indispensable.

In the course of SiO_2 reduction, SiO play an unique and vital role. Over 90% of the energy is consumed for the conversion of SiO_2 to SiO. The rates of SiO formation by reduction of silica in hydrogen and CO/CO_2 mixture have been studied extensively in the past decades. Schwerdtfeger[1] examined the behaviour of silica at 1500^{o}C in a stream of H_2 and CO/CO_2 mixtures. For H_2 containing gases he observed that the reaction rate increased with increasing mass transfer coefficient, indicating that mass transfer in gas phase is rate controlling. Ozturk and Fruehan[2, 3] conducted experiments similar to those of Schwerdtfeger at temperature of 1650°C. The rate of silica reduction in H_2 was found to be controlled by gas phase mass transport in accordance with Schwerdtfeger. However, the rate of SiO formation by reaction of SiO_2 with CH_4 (natural gas) has never been reported in the literature. The reactions between silica and methane are therefore poorly understood, and no valid model for the kinetics of the reactions has been established.

In the present task for master student, the rate of SiO formation will be measured experimentally according to following reactions:

$$SiO_{2(s)} + CH_{4(g)} = SiO_{(g)} + CO_{(g)} + 2H_{2(g)} \quad (1)$$

Reaction $3SiO_{2(s)} + CH_{4(g)} = 3SiO_{(g)} + CO_{(g)} + 2H_2O_{(g)}$ is unlikely happened since the Gibbs energy of this reaction are positive at normal pressure and elevate temperatures. In order to avoid CH_4 decomposition, the contents of reduction gas mixture must be carefully designed. From the stoichiometry of the reaction (1), the SiO flux can be approximately expressed to:

$$J_{SiO} = J_{CO} = 0.5J_{H2} \quad (2)$$

where CO and H_2 fluxes can be determined by taking the MS online measured P_{CO} and P_{H2} into account. Appling the similar experimental technique as that of Ozturk and Fruehan[2, 3], one is able to define the rate of SiO formation under CH_4 and SiO_2.

Based on the experimental work, a kinetic model for the SiO formation can thus be set up.

Qualifications and requirements

For the qualifications and requirements, the master student in major of materials science can be assigned to the present task. Before laboratory investigation, basic knowledge of kinetics and high temperature experiments are pre-required.

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Reference

1. Schwerdtfeger, K., Transactions of the Metallurgical Society of AIME, 1966. **236**: p. 1152-1156.
2. Ozturk, B. and R.J. Fruehan, *The rate of formation of SiO by the reaction of CO or H2 with silica and silicate slags.* Metallurgical Transactions B, 1985. **16**(4): p. 801-806.
3. Ozturk, B. and R.J. Fruehan, *Kinetics of the reaction of SiO(g) with carbon saturated iron.* Metallurgical Transactions B, 1985. **16**(1): p. 121-127.