Experimental and Molecular Simulation Studies of Silicon Production in a Microwave Furnace

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Introduction
Silicon as a raw material for solar cells is industrially produced in an electric arc furnaces by carbothermic reduction of SiO2 according to the simplified reaction equation

$$SiO_2 + 2C \rightarrow Si + 2CO$$  

However, the underlying reaction mechanism is still subject of discussions, as it involves a complex system of reactions between solid, liquid and gaseous compounds and by-products such as SiC and SIO. Due to the complex reaction system of silicon production, it is believed that the heating of a mixture of silica and carbon in the ratio 1:2 in a laboratory furnace will either result in the production of SiO or SiO2, but in Si metal or SiC. Contrary to these observations, we present an approach for silicon production in a laboratory microwave furnace leading to silicon metal [3]. A new promising approach to get insight into the complex reaction mechanisms are MD simulation studies using the reactive force field ReaxFF [4, 5]. We here also present studies on its capability to describe the SiO2-C reaction system.

Experimental Setup
We developed a special designed microwave furnace with a microwave power up to 6 kW and a high-temperature resistant cavity. Experiments can be carried out under vacuum and inert-gas atmosphere, while cavity’s pressure, incoming and absorbed microwave power, flow of inert-gas, and temperature (by IR thermometer and thermocouples) can be measured. Since the absorbed microwave power depends on the electric field strength, much effort was put into the cavity’s design. Therefore, we used simulation techniques [6] to model the electric field, and simulations results were found to be in good agreement with experiments.

Experimental Results
With carbon being a very good microwave absorvent we started measuring its heating rates at different microwave powers. Results indicate heating rates of the core of more than 500 K/min with a microwave power of 900 W as shown in figure 1. As the thermocouple wires affect the microwave field, measurements were taken after turning off the microwave power. Due to this, cooling of the sample has to be taken into account. Thus, the temperature drop of the surface was observed by the IR during the time we needed to obtain the value from the thermocouple. We then assumed that the cooling in the core of the sample and at the surface is the same.

Simulations of Pure Materials in the System SiO2-C
We examined the ability of the reactive force field ReaxFF by van Duin et al. [5] to reproduce properties of pure compounds in the reaction system SiO2-C, i.e. SiO2, SiC, silicon and carbon, and the gaseous compounds CO, CO2, O2 and SiO [7]. For all solid compounds the simulated structural parameters are in good agreement with literature values. As SiO is stated to be one of the most important intermediates in silicon production, we also tested the ability of the ReaxFF model to reproduce the formation of gaseous SiO [8]. As shown by figure 3, gasous SiO molecules were formed in the simulation at temperature between 1,000 and 1,500 K, which ist in good agreement with experiment.

Chemical Reactions
To identify reactive sites on SiO2 surfaces, we added carbon atoms in a simulation box above a defective SiO2 surface and followed their reaction paths. Figure 5 shows different reaction steps during the reaction of a carbon atom with the SiO2 surface, where carbon forms gaseous CO in contact with the SiO2 surface.

Conclusions
Although the new process still requires fundamental investigation, we have shown the ability of producing silicon metal in a microwave furnace, which is a promising approach to increase both the energy efficiency of silicon production and the silicon quality. MD-simulation results suggest, that the ReaxFF is well suited for simulation studies on the SiO2-C reaction system to get insight into the mechanisms reaction of silicon production. Acknowledgment
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References