Molecular Dynamics Studies on the SiO_2-C Reaction System using the ReaxFF Reactive Force Field

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Silicon as raw material for solar cells is industrially produced in electric arc furnaces by carbothermal reduction of silicon dioxide SiO_2 (silica) according to the simplified reaction equation: $SiO_2 + 2C \dashrightarrow Si + 2CO$. 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. In order to optimize the highly energy consuming process of silicon production, it is essential to understand the reaction mechanism. A new promising approach for molecular dynamics (MD) studies of chemical reactions is the use of the reactive force field ReaxFF [1, 2] that introduces a bond distance/bond order concept into the molecular model. Thus, we will present our studies on the capability of ReaxFF to describe the SiO_2-C reaction system. This includes simulations to examine the ability of ReaxFF to reproduce the morphologies of bulk silica and carbon over a wide temperature range. We have also studied the structure of the simulated silica surface upon heating in terms of defects such as over-coordinated silicon atoms or small ring sizes, considering different silica modifications and heating rates. We will then present ReaxFF simulation results for chemical reactions between silica and carbon, and how they are influenced by structural defects of the surfaces as chemically reactive sites.

[1] A.C.T. van Duin, S. Dasgupta, F. Lorant and W.A. Goddard III, J. Phys. Chem. A 105, 9396-9409, 2001.
[2] A.C.T. van Duin, A. Strachan, S. Stewman, Q. Zhang, X. Xu and W.A. Goddard III, J. Phys. Chem. A 107, 3803-3811, 2003.