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Iron sulfide stoichiometry as a monitor of sulfur fugacity in gas-mixing experiments

Astrid Holzheid[1,*] and Katharina Lodders[2]

[1]Institut für Geowissenschaften, Universität Kiel, 24098 Kiel, Germany
[2]Planetary Chemistry Laboratory, Department of Earth and Planetary Sciences and McDonnell Center for the Space Sciences, Washington University, Campus Box 1169, One Brookings Drive, Street Louis, Missouri 63130-4899, U.S.A.

Abstract

We explore a method to utilize the stoichiometry of iron sulfide to determine the sulfur fugacity in experiments containing CO-CO_2-SO_2 gas mixtures. The Fe-S phase diagram shows that the stoichiometry of iron sulfide melts is closely related to the sulfur fugacity f_{S_2} at a given temperature and ambient pressure. We derive equations that relate the sulfur fugacity to the mole fraction of sulfur X_S in the iron sulfide from available literature data, and a solution model using the Redlich-Kister approximation for the excess Gibbs energy of mixing. We test the method by exposing iron sulfide to CO-CO_2-SO_2 gas mixtures and subsequently analyzing the "Fe-S monitor" for its stoichiometry. Most sulfur fugacities calculated from the equilibrium gas composition agree within 5–10% (1200 °C) and 1–4% (1400 °C) with those derived from the sulfur mole fraction in the monitor and literature data calibration, which is consistent with the spread observed in literature data. There were no suitable literature data for a full calibration at 1300 °C, so we combined the available literature and our data to find the sulfur fugacity as a function of mole fraction sulfur. Overall the Fe-S monitor technique is a convenient method to determine the sulfur fugacity in high-temperature experiments containing CO-CO_2-SO_2 gas mixtures as long as oxygen fugacities remain below that of the iron-wüstite or iron-magnetite buffer.

Keywords: Iron sulfide, stoichiometry, sulfur fugacity, f_{S_2} monitor