Mars Exploration (3)
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RESEARCHES ON REACTION DYNAMICS OF MG/CO2 POWER SYSTEM FOR MARS EXPLORATION

Abstract

The Mg/CO2 power system is a very promising propulsion mode in future Mars exploration due to the abundant carbon dioxide resources in the atmosphere of Mars. At present, much of research on Mg combustion in CO2 has focused on the ignition and combustion characteristics at the macro level; however, few databases exist for the research on their micro-reaction characteristics. In this study, the heterogeneous and homogeneous reaction characteristics of the Mg/CO2 system as well as the coexisting Mg/CO system were investigated by thermal analysis kinetics and quantum chemical calculation methods, respectively. The corresponding kinetic parameters were subsequently obtained according to detailed theoretical calculations. The results showed that the heterogeneous reactions between Mg and CO2 as well as CO are both controlled by the first-order reaction model (F1), that is, linear kinetics controlled. The apparent activation energies are 132.4 kJ•mol-1 and 100.2 kJ•mol-1, respectively; and the pre-exponential factors are 1.376104 s-1 and 2.386102 s-1, respectively. There are two intermediate transition states in the homogeneous reaction between Mg and CO2, and the reaction energy barriers are 114.4 kJ•mol-1 and 226.0 kJ•mol-1, respectively. However, the suitable transition state structure was not found in the homogeneous reaction between Mg and CO. The total energy barrier of this reaction is 850.9 kJ•mol-1, which is significantly higher than that of Mg/CO2 reaction system. In addition, the rate constant of Mg/CO2 homogeneous reaction is much higher than that of Mg/CO homogeneous reaction, the former is 10 to 17 orders of magnitude higher than the latter, in the temperature range between the boiling point of Mg and 2000 K. These results indicate that the gas phase reaction of Mg in CO2 environment is mainly the reaction between magnesium vapor and CO2, while the reaction between Mg and CO mainly occurs on the surface of molten magnesium droplets. The conclusions are valuable for the combustion models of Mg/CO2 system, which is expected to contribute to the structural design and optimization of Mg/CO2 rocket engines or Mg/CO2 burners for Mars exploration.