GAS-PHASE KINETIC MODELLING IN THE $AlCl_3$-CO_2-H_2-HCl SYSTEM IN VIEW OF THE CHEMICAL VAPOR DEPOSITION OF Al_2O_3

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ABSTRACT

For a specific set of conditions applied in experimental hot-wall reactor investigations to deposit α-Al_2O_3 from precursor gas mixtures containing $AlCl_3$, kinetic modelling of the gas-phase reactions was carried out on the basis of rate parameters collected or estimated by Catoire and Swihart.

Calculations are presented for upward flow rates of 20 and 0.41 slh through a vertical tube reactor (27 mm i.d.) with a 450 mm isothermal zone (1050 °C) and with varying concentrations of $AlCl_3$, CO_2, H_2 and HCl in the feed gas. The results show that $AlCl_3$ decomposes by reacting with CO_2 and H_2 to form AlOCl as the major intermediate species. The water gas shift reaction

$$CO_2 + H_2 = CO + H_2O$$

is found to take place very slowly at short residence times, but much faster with lower gas flow-rates. The H_2O generation apparently increases with the AlOCl content in the gas phase.

The results may be helpful in understanding the complex reaction mechanisms involved in alumina CVD