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Numerical modeling study on the epitaxial growth of silicon from dichlorosilane

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ABSTRACT

Computer simulations play an important role in determining the optimal design parameters for chemical vapor deposition (CVD) reactors, such as flow rates, positions of the inlet and outlet orifices, and rotational rates, etc. Reliability of the results of these simulations depends on the set of chemical reaction used to represent the process of deposition in the reactor. Aim of the present work is to validate the simple empirical reaction to model the epitaxial growth of silicon for a Dichlorosilane-H_2 (DCS)-H_2 system. Governing equations for continuity, momentum, energy, and reacting species are solved numerically using the finite volume method. The agreement between experimental and predicted growth rates for various DCS flow rates is shown to be satisfactory. The increase in growth rate with the increase in pressure is in accordance with the available data. Based on the validated chemical reaction model, a study was carried out to analyze the uniformity of the silicon layer thickness for two different flow rates in a planetary reactor. It was concluded that, based on the operating conditions, the uniformity of the silicon layer over the wafer is independent of the satellite rotational rate in the reactor.

1. Introduction

Dichlorosilane (SiH_2Cl_2, DCS) has high deposition rates at moderate temperatures and it decomposes without H_2 addition [1]. This makes it a favorable precursor for silicon deposition. Another advantage of DCS is that it allows selective epitaxial growth (SEG) without the addition of HCl. Regolini et al. [2] observed that crystal growth remained selective with no nucleation without HCl addition for temperatures ranging from 650 °C to 1000 °C. Lee et al. [3,4] have also studied the selective epitaxial growth by rapid thermal processing and concluded that for DCS fraction lower than 2%, SEG can be attained without the addition of HCl. Many experimental studies have been performed in the past to estimate the reaction rate constants and dominant chemical species involved in the silicon growth from a DCS-H_2 mixture [5–8]. Morosanu et al. [1] determined the silicon growth rates for DCS-H_2 systems by dividing the operating temperatures into low, intermediate, and high temperature ranges. They showed that at all temperatures, with low and normal H_2 partial pressure, Si growth rate was proportional to the DCS concentration in the gas phase. Later, Coon et al. [7] provided a comprehensive silicon growth model by including gas and surface phase chemical reactions. Their model concurred with the experimental results by Regolini et al. [2,5]. Coon et al. have also shown that at temperatures above 1173 K, the silicon growth rate was proportional to the incident flux of DCS.

Recent advancements in the field of computational fluid dynamics have provided a tool to study the reactive flows at different operating conditions. Hierlemann et al. [8] proposed some modifications in the reaction mechanism proposed by Coon et al. [7] to account for the effect of carrier gas and decomposition of the DCS in the gas phase at a higher temperature. Coupling of their model with the detailed thermal fluid environment showed good agreement with the experimental values over a wide range of temperatures and pressures. In contrast to Hierlemann et al. [8], Knutson et al.[9] proposed two pathways for the gaseous decomposition of DCS: $SiH_2Cl_2 \rightarrow SiCl_2 + H_2$ and $SiH_2Cl_2 \rightarrow SiHCl + HCl$. However, their model over-predicted the silicon growth rate for higher DCS inflow concentrations.

A major problem in modeling the epitaxial growth rate of the silicon from the reacting species is determining the exact chemical reactions involved in the process. Therefore, an attempt has been made to use a simple reaction model in cases where it is not important to determine the concentration of other by-products. Kastelic et al. [10] used simple reactions to model the growth and etching of the silicon in the DCS-HCl-H_2 system at an operating pressure

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Nomenclature

C_P	specific heat capacity
$D_{k,m}$	mass diffusion coefficient
E	internal energy
GR	average weight of silicon per unit area of a wafer
g_i	vector of gravitational acceleration
H	specific enthalpy
h^*	normalized height
J_k	diffusion flux
k	thermal conductivity
P	pressure
Pe	Peclet number
R_k	net rate of production of species
Re	Reynolds number
r^*	normalized radius coordinate based on the wafer diameter
S_k	rate of creation by addition from the dispersed phase plus any user-defined sources
T	temperature
u_i	velocity component in the ith direction
v	specific volume of the system

Greeks

μ	viscosity
ρ	density

of 150 torr. Their results were in good agreement with those from the experiments. In previous studies, the activation energy for the growth rate of silicon from the DCS-H_2 system ranges between 40 and 50 kcal/mol [2].

In the present study, the chemical kinetics of the DCS-H_2 system was modeled by two different sets of chemical reactions and their effect was compared with the experimental data. The first set of chemical reactions is based on the surface and gas phase reactions proposed by Hierlemann et al. [8], whereas the second set consists of the single reaction proposed by Kastelic et al. [10]. These reactions are given in Table 1. This study is intended to compare the two reaction models and emphasize the robustness of the single rate determining reaction to predict the growth rate of Si epitaxial growth. CVD reactors have wide applications in the industry e.g. semiconductor and related devices, film coatings, optical fibers and production of ceramic matrix composites. Keeping this usefulness in view, CVD reactors with complex geometries, the use of single reaction models will enhance the robustness of numerical analysis. Owing to the wide range of applications of CVD, e.g. Nano electronics, fiber optics, formation of composites and catalysts and powder production etc. [11–16], this development will be very helpful.

2. Case description

This study is divided into two parts. In the first part, the single reaction model is validated using the available experimental data by Hierlemann et al. [8], while in the second part, this model is applied to study the growth of silicon on a masked wafer surface in a planetary CVD reactor.

A representation diagram of Hierlemann's reactor is shown in Fig. 1(a). The gas mixture of DCS and H_2 enters from the shower head inlet at the flow rates of 50 sccm and 6 slpm, respectively.

Table 1
Chemical reaction models for silicon deposition.

Hierlemann reaction model		
Reactions	Activation energy J/kmol	Pre exponent factor
$SiH_2Cl_2 + 4Si \rightarrow 5Si(b) + 2Cl + 2H$	-1.6×10^7	0.08
$SiH_2Cl_2 \rightarrow SiCl_2 + H_2$	1.7×10^8	2.0×10^{13}
$SiCl_2 + 2Si \rightarrow 3Si(b) + 2Cl$	-4.2×10^6	0.13
$H_2 + 2Cl + 2Si(b) \rightarrow 2HCl + 2Si$	3.0×10^8	5.0×10^{20}
$2Cl + 3Si(b) \rightarrow SiCl_2 + 2Si$	3.1×10^8	3.0×10^{12}
$H + Cl + 2Si(b) \leftrightarrow 2Si + HCl$	3.0×10^8	1.0×10^{13}
$2H + 2Si(b) \rightarrow H_2 + 2Si$	2.0×10^8	9.0×10^{11}
Single reaction model		
$SiH_2Cl_2 \rightarrow Si(b) + 2HCl$	2.2×10^8	4.0×10^{26}

These gases react with the wafer positioned upside down in the reactor. For the selective epitaxial growth (SEG), 99.9 percent of the wafer is masked with SiO_2. The wafer is heated to 1123 K by radiation from tungsten lamps through the quartz window at the bottom of the reactor. The quartz window is assumed to be 850 K. For varying flow rates, the DCS flow rates are reduced from 50 sccm to 3 sccm while maintaining a constant H_2 flow rate. The operating pressure of the reactor ranges from 2 to 10 torr.

Fig. 1(b) shows the schematic diagram of the planetary CVD reactor. The left side of Fig. 1(b) shows the interior part of the full reactor, in which five silicon wafers are mounted on the satellites on the surface of the graphite susceptor. Wafers are 99.9 percent masked with SiO_2 because they are used for the selective epitaxial growth of the silicon. A mixture of DCS and H_2 at atmospheric pressure is injected into the reactor from the inlet. The temperature of the inlet gas is 300 K. The susceptor and satellite temperatures are both 1123 K. The ceiling of the reactor is continuously cooled and maintained at a temperature of 80 °C less than the satellite temperature. Two different flow rates were used to study the effect of the flow rate and DCS fraction on the silicon deposition and velocity profiles. For case 1, the flow rate is maintained at 1.2×10^{-5} kg/s and the DCS fraction is maintained at 0.0083. For the second case, the flow rate is increased to 3.91×10^{-4} kg/s while reducing the DCS fraction in the mixture to 0.0043. For each case, the satellite rotates at a speed of 1.04 rad/s in a counter clockwise direction, while the susceptor's rotational speed is maintained at 0.52 rad/s in a clockwise direction. The operating pressure of the reactor is 30 torr. Due to the symmetry of the geometry of the reactor, 1/5 of the entire geometry with periodic boundary conditions is considered in the current simulation (Fig. 1(b)). Pressure outlets are present at the bottom of the reactor, as shown in the Fig. 1(b).

3. Numerical treatment

In the present study, the unstructured finite volume code Fluent V16.1 [17] is used for the simulations. The fundamental equations governing the flow of incompressible ideal gas are solved numerically. For Hierlemann's reactor, a hexahedral mesh with 14,000 cells is used. For the CVD reactor, a polyhedral mesh with 1 million cells is used in this study, as shown in Fig. 2. Grid convergence for the first case was tested, and it was found that an increase in the number of cells beyond the 14,000 cells solution remained unchanged. Similarly, for the second case, 1 million cells are sufficient to provide converged results. The second order upwind scheme is employed for the spatial discretization of the advection terms of the governing equations.