SILANE PYROLYSIS IN A NOVEL BELL-JAR REACTOR: A CFD STUDY

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Abstract
A 3D computational fluid dynamics (CFD) model was developed for modeling the chemical vapor deposition (CVD) of silane in bell-jar reactors with and without cooling jackets. Detailed insights into the temperature distribution, gas flow behavior and rod growth rate were obtained. Effect of various operating conditions on silane conversion and homogeneous pyrolysis selectivity was predicted. The information obtained by the CFD model can be utilized for further optimizing design of silane based bell-jar reactors.

Introduction
Low-cost solutions to increase the accessibility of high-purity polysilicon are vital to the developments of Photovoltaic (PV) and modern electronics industries. At present, electronic grade silicon which requires a typical purity of 99.999999999% mainly relies on the so-called Siemens process, involving trichlorosilane (TCS) CVD in bell-jar reactor, while silane based fluidized bed reactor (FBR) route is still struggling in meeting the solar grade purity requirement of typically 99.99999% (Filtvedt, W., 2012). Actually, silane based bell-jar reactor route appears to give ideal possible purity while maintaining acceptable low operating cost, however relevant comprehensive numerical model is still missing. The present work developed a 3D CFD model in which silane pyrolysis kinetics available in literature was implemented, for predicting the CVD process in silane based bell-jar reactor and the effect of reactor configuration on it.

CFD Model Development
The gas flow modeling was based on the steady state RANS equations. The RNG $k-\varepsilon$ turbulent model and the discrete ordinate model were used to solve turbulent viscosity and radiative transfer equation respectively. The heterogeneous kinetic models proposed by Hashimoto et al. (1990), Iya et al. (1982) and Furusawa et al. (1988) were separately evaluated with experimental data and the first one was finally adopted, while the homogeneous kinetics proposed by Furusawa et al. (1988) was employed. A rate formula was derived based on local concentration and averaged thermal velocity for modeling gaseous silicon deposition on rod.

$$D = \frac{1}{4} C_{\text{Si(g)}} v_{th} \text{ [mol/(m^2·s)]}$$ (1)

where $C_{\text{Si(g)}}$ represents the gaseous silicon concentration and $v_{th}$ is its thermal velocity.

Results and Discussion
Comparative simulation cases were conducted in bell-jar reactors with and without cooling jackets (Figure 1), the calculated rod growth rates, silane conversion and homogeneous pyrolysis selectivity were listed in Table 1.

<table>
<thead>
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<th>Table 1. Material balance calculation</th>
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<tr>
<td>$G$, $\mu$m/s</td>
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<td>Reactor A</td>
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<td>Reactor B</td>
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As shown in Figure 2, steady temperature fields around rods are achieved in Reactor A, so it is convenient to extend the configuration to large scale reactors, while the temperature distribution in Reactor B is rather chaotic and substantially higher, which explains the considerable increase of homogeneous pyrolysis selectivity as shown in Table 1.

As shown in Figure 3, steady flow fields along the rods was apparent in Reactor A, resulting a uniform residence time distribution. The gas collision and recirculation are evident in Reactor B, resulting in shorter residence time, which is expected to cause the lower silane conversion as shown in Table 1.

As shown in Figure 4, the axial growth rate in Reactor A is declining due to gradual decline in silane concentration. The vicinities of U-bends present lower growth rate due to the reactant dilution as discharged from the channels. The chaotic profile in Reactor B is apparent and the overall rate is substantially lower due to lower silane conversion.

A series of simulation cases were conducted in Reactor A to predict silane conversion and homogeneous pyrolysis selectivity for various combinations of inlet flow rates, operating pressures, inlet silane mole fractions and cooling wall temperatures, as shown in Figure 5.

Conclusion

In this work, a 3D CFD model was developed and successfully applied to silane based bell-jar reactor modeling, in which detailed insights into the CVD process were obtained for various operating conditions.

References


