ISCRE25 FLORENCE 2018
BRIDGING SCIENCE & TECHNOLOGY
The 25th International Symposium on Chemical Reaction Engineering
20-23 May 2018
Florence, Italy
www.aidic.it/iscre25

A Hot-Wall Tubular Reactor for Silane Pyrolysis: Modeling and Simulation

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Highlights

- The equipment comprises a hot-wall tube reactor and a refitted ingot furnace.
- The tube reactor realizes 100% silane conversion yielding more than 90% silicon fines.
- The feedstock of pure silane is allowed without any carrier gas.
- The flow field is specially modulated for silicon fines stagnation and melt.

1. Introduction

Silane is an excellent starting material for manufacturing electronic-grade (EG) and solar-grade (SoG) polysilicon. We have been working for 10 years on the R&D of ultrapure silane production, and successfully constructed a 600 tons per year pilot plant in China. [1-4] Recently, we proposed a novel idea on silane-based crystalline silicon. The previous studies mainly focused on thin film silicon in low pressure and plasma enhanced CVD reactor at low temperature (around 200 °C) and on granular silicon using fluidized bed reactor (FBR) [5-7]. The thin film generally results in amorphous silicon with a low PV efficiency less than 10%, though some modest improvements have been reported by depositing the crystalline (nano or micro) silicon thin film. [8] The FBR process has faced several challenges with porosity, impurities, and fines formation. [9] Particularly the hassles in heating and fluidization are difficult to handle in scale up.

In traditional industrial practice, silicon containing gas is firstly transformed to rod-like or granular silicon, which are melted in the next to grow crystalline silicon ingot. This process is long, suffering product contamination, and energy-intensive. In this work, we built a direct ingot casting reactor (DICR) for manufacturing crystalline silicon ingot from silane in one step as shown in Figure 1. Since silicon powder formation can not be avoided, the goal is 100% conversion to fines. The equipment comprises a hot-wall tube reactor and a refitted ingot furnace. The operation is intermittent. Silane is converted to fines completely in the tube reactor, the fines then enter the ingot furnace and stagnates and melts in the crucible. Then the molten silicon grows crystalline silicon ingot under controlled cooling condition. This technique leaves out many intermediate steps thus is expected to be very energy efficient.

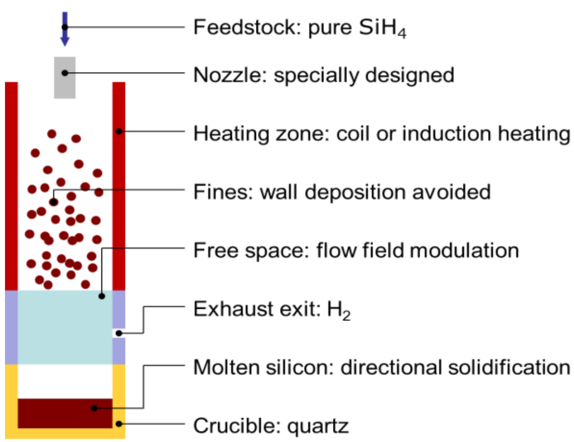

Figure 1. Conceptual design of direct ingot casting reactor (DICR).

2. Methods

At an early stage we simulated silane pyrolysis in the tube reactor using CFD technique. In the next, experimental study will be performed to evaluate the technical feasibility. Now the equipment design is already underway.

3. Results and discussion

In contrast to bell jar reactors, the DICR route pursues silicon fines formation as much as possible while the least silicon deposition inside the tube wall. We have investigated the effects of tube reactor geometry and operating condition on silane pyrolysis (results not included due to the limit of space). Preliminary simulation indicates that the deposition ratio can be maintained below 10% under a typical operating condition: $T_{\text{hot-wall}}$ = 1000 °C, P = 1.2 atm, silicon fines productivity = 35 kg/h. As shown in Figure 2, due to exothermic silane pyrolysis plus continuous heat from the hot-wall, gas temperature peaks near the outlet where the gas flow is accelerated. The tube reactor is 1 m in length, while the concentration field indicates silane runs out at about two thirds position.

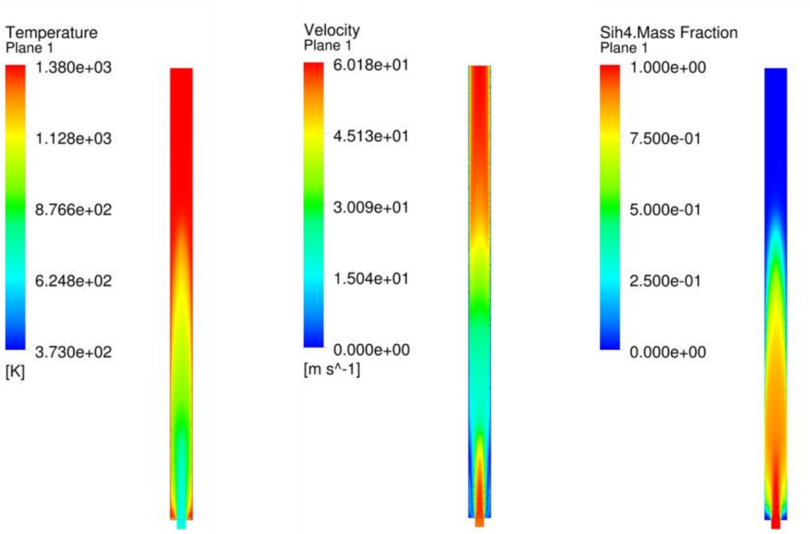

Figure 2. Snapshots of temperature, velocity, and silane concentration fields.

4. Conclusions

CFD simulations confirmed that more than 90% silane converted to gaseous silicon fines. Since the design and construction of experimental setup is still underway, and the key is realizing sufficient stagnation and melt of silicon fines in the crucible, we expect to present more experimental findings on the conference.

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Keywords
Silane; Polysilicon; Crystalline silicon; Ingot furnace.