SSN COLLEGE OF ENGINEERING
KALAVAKKAM-603110

Interdisciplinary Project

Predictive Modeling of Gas Flow Dynamics in Crystal Growth Processes

Project Report

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Project Summary:

Objective:

The main reason for the crystal growth is producing silicon crystals for photovoltaic cells or solar cells. Crystalline silicon is the most commonly used material for solar cells due to its abundance, efficiency, and reliability.

Process:

Multi Crystal Silicon is grown using Directional Solidification method. The Silicon feedstock is melted at 1500 C (1414 C exact) in a container and frozen in a regular interval. The freezing process shouldnt be sudden and should be unidirectional. Hence Directional Solidification method is used.

Multi Crystal is used as the cost for growing it is less compared to growing a single crystal.(1:5 ratio). Low quality feedstock is enough for the DS method which commercially has 6N purity. The crucible is of 3N purity (SiO2).

To optimize the growth process we must have information on factors affecting the crystal growth such as the impurities formed. Certain impurities are intentionally added to the silicon melt as dopants to modify its electrical conductivity and semiconductor properties.

The materials used inside the container should have a melting point above 1500 C and should be cheap. Hence Graphite is used.

We get oxygen from quartz or silica crucible, carbon from Graphite.

Diffusion and dissolution takes place. When oxygen is diffused it reacts with silica crucible at high temperature and forms SiO (gas) and SiO2 (solid). The gas diffuses up and reacts with the graphite and forms carbon monoxide (CO). This CO separates into C and O when it comes in contact with the melt in high temperature and forms SiC along with SiO and SiO2 again. This cycle repeats again.

$SiO2 + O_2 \rightarrow SiO + SiO_2$ (Inside Melt at high temperature)

$SiO+C \rightarrow CO$ (Reaction with graphite)

$CO \rightarrow C+O$ (Inside Melt at high temperature)

$Si+C \rightarrow SiC$

$SiO2 + O_2 \rightarrow SiO + SiO_2$

The rate of Silica FeedStock commercially is 40 dollars per Kg. We use 800 Kgs in this process. We don't use the power supply in the furnace, instead diesel is used (7000L approx).

1cm/hour growth is happening.

How to reduce the impurities? Flowing Argon gas.
This argon gas being an ideal gas pushes all the other gasses outside as it flows. Hence reducing the SiO upward flow and CO downward flow. The research is therefore on how it affects the purity and growth of the silicon crystal at various parameters (reaction at different lpm of argon gas).

In case of real time operation, it takes more than 30 Lakhs to run this process. The software to monitor the furnace and simulate also costs money(Rs 2000 / day) to operate. Hence number of trial and errors performed with the software increases the cost consumption.

Hence to reduce this cost consumption and simulate the optimal conditions for each parameter we are creating an ML model to simulate this process and find how different parameters affect the Crystal Growth process. The pre existing real time software is also time consuming. But an ML model can predict the same outcome in less time making it both cost and time efficient.

Our work is focused on the gases flowing upward, downward, outward and gases being taken out.