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Deposition reactors for solar grade silicon: A comparative thermal analysis of a Siemens reactor and a fluidized bed reactor

A. Ramos [a,*], W.O. Filtvedt [b], D. Lindholm [b], P.A. Ramachandran [c], A. Rodríguez [d], C. del Cañizo [a]

[a] Instituto de Energía Solar – Universidad Politécnica de Madrid, ETSI Telecomunicación, 28040 Madrid, Spain
[b] Institute for Energy Technology -IFE-, Kjeller, Norway
[c] Washington University, MO, USA
[d] Departamento de Ingeniería Química, Universidad Complutense de Madrid, 28040 Madrid, Spain

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ABSTRACT

Polysilicon production costs contribute approximately to 25–33% of the overall cost of the solar panels and a similar fraction of the total energy invested in their fabrication. Understanding the energy losses and the behaviour of process temperature is an essential requirement as one moves forward to design and build large scale polysilicon manufacturing plants. In this paper we present thermal models for two processes for poly production, viz., the Siemens process using trichlorosilane (TCS) as precursor and the fluid bed process using silane (monosilane, MS). We validate the models with some experimental measurements on prototype laboratory reactors relating the temperature profiles to product quality. A model sensitivity analysis is also performed, and the effects of some key parameters such as reactor wall emissivity and gas distributor temperature, on temperature distribution and product quality are examined. The information presented in this paper is useful for further understanding of the strengths and weaknesses of both deposition technologies, and will help in optimal temperature profiling of these systems aiming at lowering production costs without compromising the solar cell quality.

1. Introduction and scope

In the last years production of solar cells has by far surpassed microelectronics as the main consumer of polysilicon in the world market [1]. Although the exponential growth in world production capacity made the silicon prices drop dramatically, they are foreseen to become stable in the next years [2,3] and significant growth in polysilicon consumption is expected in the medium-long term [4,5]. As the production of silicon feedstock is responsible of about 25–33% of the energy cost of an installed silicon based solar cell module [6,7], the importance for polysilicon producers to reduce production costs is revealed [8].

The most common means of obtaining polycrystalline solar grade silicon (SoGSi) is via decomposition of a silicon containing reactant gas through heating. The currently favoured method is the chemical route from trichlorosilane (TCS), named the Siemens process, which leads to high quality polysilicon at the expense of high energy consumption. Thus, low-cost technologies of obtaining polycrystalline silicon are coming on the scene: i.e. monosilane (MS) based fluidized bed reactors (FBR). In short, at present two main trends in polysilicon production exist: increase efforts to reduce the ratio kilowatts-hour per kilogram (kWh/kg) of polysilicon produced through the traditional process and support the new low-cost technologies development to make the lower energy consumption a sufficient advantage compared to other process disadvantages [9].

1.1. Scope

CVD processes are complex; thermodynamics, radiation, fluid-dynamics, kinetics and chemistry are involved [10–13]. Understanding of the fundamental reactions and how they influence product quality at the same time as to comprehend the phenomena responsible of the energy consumption, is key in order to aid further development in polysilicon CVD.

Although a debate in the polysilicon community about the benefits and drawbacks of these different deposition technologies exists [1,2], there is a lack of reliable data, based on rigorous models, and contrasted experimentally in similar conditions [14–16]. Also, some of the shortcomings of the FBR in terms of material quality are related to the nature of the process. In this paper theoretical models of heat losses of a Siemens reactor and a FBR

* Corresponding author. Tel.: +34 91 453 35 49; fax: +34 91 544 63 41.
E-mail address: alba.ramos@ies-def.upm.es (A. Ramos).

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prototype are developed and the thermal distributions within a fluidized bed and a Siemens reactor are explored; both experimental data and associated modelling are presented. The thermal conditions within the reactors are directly linked to the decomposition and deposition sequence which in turn influences the quality of the produced silicon. Any reduction in silicon price cannot come at the expense of a reduction in solar cell performance. It is therefore essential to know how the thermal distribution is within different reactor concepts and how these distributions may be altered in order to promote favourable growth and suppress competing unwanted mechanisms.

As has been established earlier by others, the solar cell efficiency will ultimately depend on the concentration of impurities in the material, not to disregard other defects and the passivation of the surfaces [17]. Of these contributions the impurity concentration level is linked to the feedstock route while the other contributions are linked to the crystallisation and cell processing. The question is therefore not if impurities may influence the possible obtainable efficiency of the solar cells, but if these levels are relevant as current limitation for the efficiency. A further question may be that for high efficiency cell concepts if sufficient material quality is obtainable through low cost routes.

2. Polysilicon deposition technologies

2.1. Siemens process

The traditional route for polysilicon production consists of chemical vapour deposition (CVD) from TCS [18]. CVD of polysilicon comprises two main steps: metallurgical silicon (MG Si) transformation to TCS and purification, and TCS reduction into high purity silicon. The latter, the CVD of polysilicon itself, is the largest contributor to the energy consumption of the overall process which is in the range of 45-80 kWh/kg; the best number corresponds to large capacity plants [19–21]. From now on, we refer to the CVD of polysilicon as the Siemens process.

The Siemens process occurs inside a bell reactor containing heated silicon rods in a reactive gas atmosphere. It requires high deposition temperatures while keeping the reactor wall relatively cold. Joule's effect is responsible of the heating of the rods until the deposition temperature, that is typically, 1100–1150 °C. The initial diameter of the seed rods is less than 1 cm and the deposition process runs until rods' diameters are in the range 13–20 cm. The need for maintaining large temperature differences between the deposition surfaces and the reactor wall – to avoid homogeneous nucleation that would lead to lower quality of the resulting material – will cause a limit to theoretical reactant yield; and is the main responsible of the high energy consumption. However, several improvements have been made to the design resulting in a substantial reduction in energy consumption [22].

The Siemens process was initially developed to produce electronic grade polysilicon (EG Si), which has a purity of at least 99.9999999%, or 9N. This is the purity level needed in the microelectronics industry, though the purity requirements in the solar PV industry may be less demanding [23,24], what opens opportunities for possible modifications to reduce the energy consumption of the Siemens process.

2.2. Fluidized bed reactors

The most valued alternative to the Siemens reactor is the fluidized bed reactor (FBR) [25]. A cylindrical reactor vessel is filled with tiny silicon particles which are kept fluidized by an ascending gas flow, typically hydrogen. The column of particles in the fluidized bed is heated above 600 °C for the decomposition reaction to occur and the reactive gas, monosilane gas (MS), is inserted. The initial diameter of the silicon particles is in the range of microns, and after some dwelling time the particles have grown to a size suitable for extraction [26,27].

In the FBR, the decomposition reaction to polysilicon deposition occurs at temperatures significantly lower than in a Siemens reactor. The FBR holds the potential to become the dominating CVD reactor for production of solar grade silicon since the energy consumption per kilogram of silicon produced is estimated to be in the range of 4–16 kWh/kg [28,29]; numbers vary depending on the number of steps or energy consuming processes that have been accounted for its calculation. However, it is first necessary to address the challenges with purity and porosity, production of fine dust (fines), and to achieve good gas and temperature control, among others [30,31].

The purity of the polysilicon obtained from MS in a FBR is below that of the Siemens process, compromising its use for microelectronic devices. It can be acceptable for solar cells, provided good temperature control and low amount of fines formation achieved in the process [32,33].

3. Heat loss phenomena in SoGSi production

First, the heat loss problem associated with polysilicon CVD is addressed; all contributions to the energy consumption of both the Siemens reactor and the FBR are introduced. When applying the energy balance equation to the polysilicon CVD problem, the following contributions must be evaluated: the rate of variation of energy, the net rate of kinetic and internal energy transfer by convective transport, the net rate of heat transfer by conduction due to temperature gradient and enthalpy transport for an ideal gas, the rate of work done on the system by other molecular transport mechanism (pressure and stress) and by external forces, the heat of chemical reactions and the heat transfer by radiation [34–36]. In the following, the relevant terms contributing to the energy consumption of each particular reactor will be identified.

3.1. Siemens reactor

In the Siemens reactor heat loss is due to radiation, conduction and convection via gases and the heat consumed due to the chemical reactions taking place [37]. Of these, the major contributor is radiation heat loss [38]; contribution of the latter is typically below 1%, thus heat consumption due to chemical reactions taking place can be disregarded.

As stated above, the main challenge of the Siemens process is to reduce the ratio kWh/kg of silicon produced. On the one hand, faster deposition processes are desired to reduce this ratio. On the other hand, higher deposition rates are obtained with higher temperatures, leading to higher energy consumption. Therefore, a compromise solution is needed; it is widely accepted that the deposition temperature at which the ratio kWh/kg is minimized is between 1100 and 1150 °C [39].

3.2. FBR

Several attempts have been made to use chlorosilanes in fluidized beds for polysilicon production. However, this has so far proven challenging as there will always be a temperature distribution within a fluidized bed. This is simply because the reactant needs to be injected at a temperature below its decomposition temperature: for both TCS and MS this will typically be below 300 °C. Ideal deposition temperature will be 600–800 °C for MS, for TCS it will be 900–1100 °C [31,12]. However, whereas suboptimal deposition due to low temperature may lead to hydrogen