Prediction of thermal and electrical behavior of silicon rod for a 48-rod Siemens reactor by direct current power

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\begin{abstract}
In the present work, a Joule heating model by direct current (DC) has been developed for the rods arranged in a 48-rod Siemens reactor (SMS-48). The combined effect of heat dissipation (radiation, convection and reaction energy) and heat conduction produced by Joule effect has been examined by application of the developed model, taking into account variations of the rod radius and wall emissivity. The influence of the rod location, rod radius and wall emissivity on temperature profile and voltage-current curves during the electric heating process have been studied. Furthermore, the thermal and electrical behavior of silicon rod arranged in the SMS-48 and SMS-24 has been compared with each other. The dimensionless parameter (\(p\)) has also been introduced to investigate the effect of the number of rods and their arrangement on energy consumption. The interesting results show that the temperature profile of the rod arranged in the inner ring within SMS-48 is flatter than that in the SMS-24. The curve of current increases and becomes lower for the inner ring and keeps a linear relation for the outer ring in a manufacturing process. The required current and voltage increase when the wall emissivity increases. Enlarging the reactor capacity and meanwhile decreasing the dimensionless parameter (\(p\)) is an effective method to decrease energy consumption.
\end{abstract}

1. Introduction

Solar energy is one of the most sustainable and clean energy sources available, the effective utilization of it has become vitally important [1–3]. As one of the most dominant materials for photovoltaic (PV) industry, the ultra-purified silicon, known as polysilicon, has been devoted to making solar energy more competitive with various sustainable energy sources in recent years, and more than 80% of commercial solar cells are made of polysilicon [4–6]. Thus, the low direct manufacturing cost of feedstock is vital to the further promotion of the PV industry.

Many processes exist for the production of polysilicon, such as the Siemens process [7], metallurgical process [8], silane process [9], among which the Siemens process is the main technology for the production of polycrystalline silicon in rod form for photovoltaic (PV) industry [10]. The polysilicon serves as starting material in the fabrication of monocrystalline silicon by means of crucible pulling (Czochralski or CZ method) or by means of zone pulling (float zone or FZ method) [11]. It is noted that the Siemens process has been to deposit silicon on starter filaments by thermal decomposition of the trichlorosilane (SiHCl\textsubscript{3}), so as to produce silicon rods. Such a process occurs in a cooled, bell-jar reactor, so-called Siemens reactor (SMS), in which a large number of electrodes are arranged on a circular plate, and several silicon starter filaments with a radius of 0.5 cm are arranged in an inverted U-shaped form [12]. In such silicon deposition systems, a power supply is used to pass current through the rods for such heating of the rods. At a temperature of several hundred degrees or more, the reactant gas decomposes and deposits on the heated filaments to form larger-diameter silicon rods.

Additionally, approximately 20\% of the manufacturing cost of crystalline silicon PV modules and systems corresponds to the polysilicon feedstock [13,14]. Therefore, a decrease in costs of polysilicon production in the Siemens process is essential in enabling large scale PV power generation and making this popular technology more competitive among various processes in the near future [15]. Furthermore, current price levels also press polysilicon manufacturer to reduce their production costs even more if they are seeking a sustainable development. The heat dissipation in the SMS can be classified into three parts, including convective heat dissipation, radiative heat dissipation and the heat dissipation by the chemical reaction [16].

Many valuable contributions to the literature in terms of heat transfer inside the CVD reactor. del Coso et al. [17] analyzed the...
radiative heat loss in an SMS-36 and proposed some proposals for diminishing the energy loss, including enlarging the reactor capacity, improving the properties of the reactor wall and introducing thermal shields. Ramos et al. [18–21] addressed the heat consumption modeling in a CVD laboratory prototype for polysilicon production, their work focused on the heat loss in the CVD process and developed a novel theoretical model for convection heat loss. Ni et al. [22] simulated the epitaxial growth of silicon in an SMS-24, and constructed a mathematical model to describe the multi-species thermal fluid transport, based on the model, the distributions of gas velocity, temperature and species concentrations in the reactor were predicted numerically. Huang et al. [23,24] proposed a three-dimensional computational fluid dynamics theoretical model to describe various transport phenomena in a novel CVD reactor, their simulation results demonstrated that the flow pattern of the gas mixture in the novel reactor approximates a plug flow model and that the temperature field can be controlled by changing the operating parameters. Liu et al. [25] built a model basing on Monte Carlo ray tracing method to analyze the radiative energy loss in the polysilicon CVD reactor. Their results show that the average saving energy rate is 39% when the rod number changes from 36 to 72, and it can reach 58% after using a thermal shield in 72 rods reactor.

The research works mentioned above mainly focused on heat transfer in the CVD reactor, and from the valuable contributions, we can conclude that enlarging the reactor capacity and decreasing the wall emissivity can reduce the power consumption. In the reactor chamber, the rods are heated internally by the Joule effect, when power is supplied by a DC power, the current migrates toward the centers of the rods. The center of a rod becomes progressively hotter, relative to the surrounding outer region of the rod, since the center is thermally insulated by the outer region or “skin” of the rod. Due to this uneven temperature profile within silicon rod in turn creates internal stresses when the rods cool down the following growth, with the resulting rods being brittle and subject to breakage. Therefore it is a crucial and urgent endeavor to decrease the temperature gradient within silicon rod in order to avoid its breaking-down and to obtain the optimal current-voltages curves. However, analytical studies of the thermal-electric behavior of rods in SMS have rarely been reported at present. Li et al. [26] modeled the local variations in current and temperature within the silicon rods as they are heated up by low frequency current. Their results indicated that the energy consumption decreased with increasing silicon deposition rate and decreasing the heat losses. Nie et al. [27] similarly utilized a direct current (DC) sources to investigate the temperature profiles of silicon rods arranged in an SMS-24, and analyzed the influence of rod location and wall emissivity. del Coso et al. [28] discussed the convenience of using high-frequency current sources in a single rod CVD reactor, and analyzed the influence of current frequency and emissivity on temperature and current density profiles in a silicon rod with the radius of 7.5 cm. Kozin et al. [29] developed a new resistive heating method and analyzed different AC shapes to reduce the internal temperature gradient of the polysilicon rods within an SMS. Viganò et al. [30] discussed the process control technique and presented a real-time model for a laboratory-scale SMS since controlling the rods temperature is a dynamic process.

High AC or DC power is applied to heat silicon rods up to the reaction temperatures. The advantage of using DC (or low frequency of AC) rather than high AC power is that DC power equipment is more commercial and the voltage is much lower [31]. In case of AC heating, the temperature at the center of rod may not reach excessive values when the silicon rods grow larger because of the eddy current effect most of the current flows near the rod surface [31]. Although high frequencies are desirable at certain conditions for heating silicon rods, the self-inductance of the silicon rods, due to magnetic flux changes, may be higher than that for DC resistance [32]. Furthermore, the operating problems associated with large voltages at high frequencies represent difficult design problems. Thus, the power for the SMS is applied by the DC (or low frequency of AC) in present.

The present paper focused on the thermal and electric behavior of silicon rod heated by DC Joule heat. Some studies have been reported in the open literature and the temperature distribution within silicon rod in a laboratory-scale CVD reactor or a small size industrial SMS (24-rod SMS) have been studied in detail [26–28]. However, the SMS with more rods has been employed in industry to reduce the energy consumption and the SMS-48 becomes a priori choice. Because of the rods arranging in three rings in the SMS-48, the thermal and electric behavior of the silicon rod becomes more complicated, comparing to that in the SMS-24 with two rings.

Accordingly, the present study aims to develop a mathematical model, which is a fully coupled model between the electromagnetic and thermal equations. The transport phenomena have been studied and the parameter convective coefficient (h), and radiation coefficient (Ω) are introduced to couple the heat exchange with the ambient environment. The theoretical framework provides a deeper understanding of thermal and electrical behavior based on several key factors including: rod location, rod radius and wall emissivity. The voltage-current curves of the rod located in different rings within the SMS-48 were also obtained under different rod radii and wall emissivities. Finally, the dimensionless parameter (p) is employed to discuss the energy consumption for different configurations (SMS-24, SMS-48-A, SMS-48-B). It is hoped that the findings will guide the overall design and optimization of SMS to realize further energy consumption reduction in polysilicon industries.

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**Nomenclature**

- $L$: Length of silicon rod, m
- $R$: Radius of silicon rod, cm
- $h$: Convection coefficient, W/m²K
- $\xi$: Radiation coefficient between the surface of silicon and reactor wall
- $T_s$: Rod's surface temperature, K
- $T_{in}$: Average temperature of the free stream, K
- $q_c$: Convective heat dissipation, W/m²
- $q_r$: Radiative heat dissipation, W/m²
- $q_{ir}$: Heat dissipation by the endothermic reaction, W/m²
- $\varepsilon_o$: Emissivity of silicon
- $\varepsilon_r$: Emissivity of reactor wall
- $F_{wi}$: View factor from the ith rod surface to wall surface
- $F_{wi}$: View factor from wall surface to the ith rod surface
- $E$: Electric field strength, V/m
- $V$: Electric potential, V
- $J$: Current density, A/m²
- $a$: Electric conductivity of silicon, S/m
- $r$: Radial coordinate, cm
- $I_{Tot}$: Total electrical current, A
- $S$: Rod’s cross section area, m²
- $k$: Thermal conductivity of Si, W m⁻¹K⁻¹
- $T(r)$: Radial-dependent temperature distribution, K
- $q$: Heat generation per unit of volume, W/m³
- $\epsilon$: The average relative error
- $G$: Specific energy consumed per kilogram of polysilicon, kWh/kg
- $Q$: Total heat loss dissipation, W/m²
- $\rho_{Si}$: Density of polysilicon, kg/m³
- $\nu$: Silicon deposition rate, mm/h
- $p$: Dimensionless parameter

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- $S^*$: Theoretical model for convection heat loss. Ni et al. [22] simulated the internal temperature gradient of the polysilicon rods within an SMS. Viganò et al. [30] discussed the process control technique and presented a real-time model for a laboratory-scale SMS since controlling the rods temperature is a dynamic process.

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