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Electric heating of the silicon rods in Siemens reactor

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ABSTRACT

In the Siemens reactor, all the energy is supplied by the heat generation on silicon rods which are heated up by the passage of current, the center of the rods will become hotter than the surface which is maintained ideally at 1373 K. Understanding the thermal and electrical behaviors of silicon rods in electric heating process is crucial for an optimal operation of the Siemens reactor. In the present paper, the electric heating model of silicon rod for the 24-rod Siemens reactor has been developed. In order to verify the present model valid, calculated results by application of the model were compared with industrial data. The results show that comparing to the industrial data obtained using a 24-rod Siemens reactor, the relative error of theoretical calculations are 7.32% and 9.41% for the rods located in the inner ring and outer ring, respectively. Based on the developed model, the influence of the location of silicon rods within Siemens reactor and reactor wall emissivity during electric heating process has been investigated. Interesting results show that the temperature gradient of silicon rods located in the outer ring is larger than the inner ones when the rods are heated up by direct current (DC). The temperature gradient within the rod becomes smaller and the required voltage and current decreases when the emissivity of the reactor wall surface decreases. Two interesting ways to reduce energy consumption can be deduced: increasing radius of the rod at the end of the process and decreasing the wall emissivity by wall surface treatment or/and selecting more appropriate materials.

1. Introduction

With the development of solar energy technology, the market for polysilicon is currently subject to profound changes due to the expansion of the photovoltaic (PV) industry [1,2]. Many processes for producing polysilicon have been tested and reported [3–5], among which the Siemens process presently dominates the production of the polysilicon. Almost 80% of the polysilicon produced worldwide are obtained by the popular technology [6,7]. The bell-jar reactor is employed to produce polysilicon, in which several high-purity silicon slim rods with a radius of 0.5 cm initially are heated by an electric current flowing through them. The seed rods grow to about 6–7 cm at the end by polysilicon deposition through the thermal decomposition of trichlorosilane (TCS) in a hydrogen environment.

Although the Siemens process has obvious advantages, including high quality, safe and mature technology, the high cost and energy consumption are the main challenges presently [2,3]. The power consumed in the Siemens reactor is the sum of the following contributions: power loss through convection, power loss through radiation and the power consumed by the chemical reaction. Many researches have been carried out and published in the open literatures. Huang et al. [8,9] have carried out a series of theoretical studies to investigate the radiative heat transfer between the rods and the inner shield in a novel polysilicon CVD reactor. The simulation results show that improving the polysilicon growth rate, enlarging the reactor capacity and decreasing the inner shield emissivity can reduce the energy loss of the CVD reactor. del Coso et al. [10–12] have conducted a series of theoretical and experimental studies on the non-homogenous temperature profile within the silicon rods in a 36-rod Siemens reactor and evaluated the effects of the frequency of the current supply, which shows that the maximum rod diameter limitation can be overcome by using high-frequency current sources. Based on the del Coso developed model for radiative heat loss, Ramos et al. [13–14] presented a new model for convective heat loss, and the model is validated by comparison with experimental results obtained using a laboratory-scale CVD reactor. Pazzaglia et al. [15] proposed a thermal shield for use in a Siemens reactor to block the thermal radiation emitted from heated silicon rods. Gum et al. [16] opened a patent in which the power loss is reduced by a thin layer of gold

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inside a reactor chamber. In our previous works, the comparison for radiative heat loss and convective heat loss in an industrial Siemens reactor of 24 rods already studied [17]. Vallerio et al. [18] formulated and solved a robust optimal control problem of a CVD reactor based on the evaluation of Lyapunov equations and studied the trade-off among productivity and energy cost via a multi-objective (MO) scalarization method for polysilicon production.

It is noted that the research works mentioned above mainly focused on power losses in Siemens reactor. The total power is supplied by Joule heat through silicon rods, thus the main challenges in electric heating process are to estimate the power losses in the Siemens reactor and to obtain current–voltage curves. However, the thermal and electrical behaviors of silicon rod in Siemens reactor have rarely been studied at present. Li et al. [19] investigated the thermal and electrical behaviors within the silicon rods during production, and proposed a method for minimizing the power required to maintain the deposition temperature. Hou et al. [20,21] investigated the temperature profile of silicon rod heated by DC, and analyzed the thermal stress within the rod. Kozin et al. [22] developed a detailed mathematical model to calculate the radial temperature profile in silicon rods by heating currents of different forms. As the control of rods temperature in Siemens reactor is a dynamic process, an advanced process control technique for the Siemens reactor has been discussed by Viganò et al. [23]. They presented a real-time model based predictive control applied to a laboratory-scale Siemens reactor. Those works mentioned above mainly focused on the temperature profile within silicon rod in the electric heating process regardless of the influence of rods' location and reactor wall emissivity. On the contrary, the objective of the present investigation was focused on the effect of silicon rod's location and reactor wall emissivity on current–voltage curve and temperature profile within the rods. It is hoped the optimum current–voltage curve is obtained for the rods located in different rings in the 24-rod Siemens reactor with different wall emissivity. In our model, all the energy required to maintain these rods at the operating temperature comes from the DC passing through them.

2. Model descriptions and simulation methods

2.1. A 24-rod Siemens reactor configuration

In industry, the TCS decomposition is conducted in a reactor chamber of 10–16 m^3 [13]. In the reactor chamber, a number of polysilicon rods are placed. These rods are heated by the Joule effect to around 1373 K in a hydrogen and TCS atmosphere. The geometric diagram of the 24-rod Siemens reactor is illustrated in Fig. 1. According to the data from Kunming Yeyan New-Material Co., Ltd, the bell-shaped reactor was 3500 mm high with an inner diameter of 1720 mm and the vertical height of each silicon rod was 2400 mm. $SiHCl_3$–H_2 mixture was introduced into the reactor from 9 inlets distributed on the bottom of the reactor and there is only one outlet in the center on the bottom of the reactor, which show that the geometry of the reactor is center-plane symmetrical.

2.2. Convective heat loss

Convective heat loss can be calculated starting from the gas's temperature distribution. This heat transferred between a surface and a moving fluid is a combination of molecular diffusion due to the concentration gradient (perpendicular to the gas flow) and bulk motion of molecules (parallel to the gas flow). The flow velocity near the surface is low (diffusion dominates), and as we move away of the surface the bulk motion increases and it becomes the dominating force. Heat transfer loss by convection, in watts per unit area, can be calculated if the convection coefficient (h), the temperature at the rod's surface (T_s) and the average temperature of the free stream (T_∞) are known:

$$q_{\text{convection}} = h \cdot (T_s - T_\infty) \tag{1}$$

The convection coefficient (h) depends on the gas mixture and the flow regime within the reactor chamber with 24 rods. Based on the data from industrial production, the estimated approximate value are $8 \sim 20\ \text{W/m}^2\ \text{K}$ for the rod located in the inner ring and $10 \sim 30\ \text{W/m}^2\ \text{K}$ for the one located in the outer ring respectively.

2.3. Radiative heat loss

A theoretical model (Surface to surface model) for radiative heat loss calculations has been adopted in the 24-rod reactor. The S2S model assumes the solid surfaces to be grey and diffuse. The 24-rod Siemens reactor has 25 surfaces: the reactor wall at $T_w = 373$ K, and 24 silicon rods at $T_s = 1373$ K, the net thermal radiation heat exchanged by the ith rod surface with the cold wall can be calculated with the following Eqs. (2) and (3) [24].

$$q_{\text{radiation}} = \xi\vartheta(T_s^4 - T_w^4) \tag{2}$$

$$\xi = \frac{F_{i\to w}}{\left(\frac{1}{\varepsilon_0} - 1\right)F_{i\to w} + \left(\frac{1}{\varepsilon} - 1\right)F_{w\to i} + 1} \tag{3}$$

where ξ is the radiation coefficient between the surface of silicon and reactor wall, which is the function of emissivity and the view factor, ϑ is Stephan–Boltzmann constant, ε_0 is silicon emissivity, ε is reactor wall emissivity, the view factor $F_{i\to w}$ is the fraction of energy leaving the ith rod surface that is incident on reactor wall surface w, $F_{w\to i}$ is the fraction of energy leaving the reactor wall surface w that is incident on the ith rod surface.

2.4. Thermal and electrical model for Siemens reactor

Consider a cylindrical silicon rod vertically placed, with an arbitrary radius R and the length L. This is a simplified, symmetric model of a rod in the Siemens reactor. Since DC passes through the silicon rod, the electric field inside the silicon rod fulfilled the following equation:

$$\nabla^2 E = 0 \tag{4}$$

where the electric field can be defined as $E(r) = dV/dz$, dV/dz is the applied voltage per unit length in axial direction.

Heat inside the silicon rod is generated by Joule effect, giving a radial-dependent temperature distribution $T(r)$. Steady state has been considered in this case and it is a good assumption based on the following reasons: although deposition takes place and changes geometry, conduction sets a temperature profile much faster; the temperature evolves much slower than the electric field. Therefore the temperature dependence on time has been neglected. Regarding the heat transfer within the semiconductor, the following equation is fulfilled under steady-state conditions [24]:

$$\nabla(k\nabla T) + q = 0 \tag{5}$$

where k is the thermal conductivity of Si, and q is the heat generation per unit of volume, defined as $q = (dV/dz)^2\sigma(T)$, $\sigma(T)$ is the electric conductivity of silicon.

Taking into account the symmetries in the problem, Eqs. (4) and (5) yield

$$\frac{d^2E}{dr^2} + \frac{1}{r}\frac{dE}{dr} = 0 \tag{6}$$