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Optimization of effective parameters on Siemens reactor to achieve potential maximum deposition radius: An energy consumption analysis and numerical simulation

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ABSTRACT

We perform numerical simulations to study effects of alternating current (AC) frequency on thermal stress evolution during the Joule heating process in a 48-rod Siemens reactor. The characteristics of temperature, current density, and stress distributions within the rods located in different rings are analyzed first. A Joule heating model using AC is then proposed for flexible power adjustment. The voltage-current curves are obtained from analysis of rod radius, location, and skin depth, as well as the properties of the polysilicon. The results indicate that, during the Joule heating process, large stresses typically occur in the central regions of the silicon rods. The highest stress occurs at the center of the silicon rods located in the outer ring when a standard power frequency of 50 Hz is utilized. The results further indicate that von Mises stress significantly decreases as AC frequency increases. Additionally, we propose a novel Joule heating method that is useful for producing larger high-purity polycrystalline silicon rods by considering both low frequency and high frequency power. Based on an analysis of energy consumption during the Joule heating process, we recommend optimized power supplies for the 48-rod Siemens reactor.

1. Introduction

Recently, a high demand for high-purity polycrystalline silicon has been created by its widespread application in the form of silicon wafers, particularly in solar cell production [1–4]. Siemens (Sm) method is the preferred method for bulk growth of large-scaled and high-quality polysilicon rods [5–7] because it is a relatively mature technology compared to other methods, such as the metallurgical process [8,9] and silane process [10,11]. However, defects caused by thermal stresses, such as cracks and breakdowns, remain and negatively affect polycrystalline quality and productivity [12].

Numerical investigations of the chemical vapor deposition (CVD) process have been performed by many researchers [13–17] over the past few decades. These studies mainly concentrated on the silicon growth process in relation to the effect of gas flow and heat transfer in a Siemens reactor. Ramos et al. [18] investigated the effects of wall emissivity and gas distribution on temperature distribution and product quality, and presented a thermal model for the Siemens process. Liu et al. [19] proposed a Monte Carlo ray tracing method to design and optimize the Siemens reactor to achieve the goal of energy conservation. Ni et al. [20] calculated the distributions of gas velocity, the temperature, and the species concentrations in a Siemens reactor, and then performed a sensitivity analysis for the key factors controlling the growth rate of silicon. Li et al. [21] modulated the flow pattern and temperature field in a reactor, aiming to minimize homogeneous nucleation in the Siemens reactor. Huang et al. [22] developed a three-dimensional CFD theoretical model to describe the various transport phenomena in the Siemens reactor, and then analyzed the production cost and growth rate of the traditional CVD process.

These previous studies on gas flow and heat transfer provide valuable insights into the characteristics of the Siemens reactor. Major contributors to the high energy consumption of the CVD process are the combined effects of heat dissipation due to radiation, convection, and reaction. The power generated by the Joule heat supply must instantly compensate for these heat dissipations. Therefore, the electric heating process is also critical for the production of polycrystalline silicon rod. When power is supplied at a frequency of 50 Hz, 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 because the center is thermally insulated by the outer region or "skin" of the rod. This

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Nomenclature

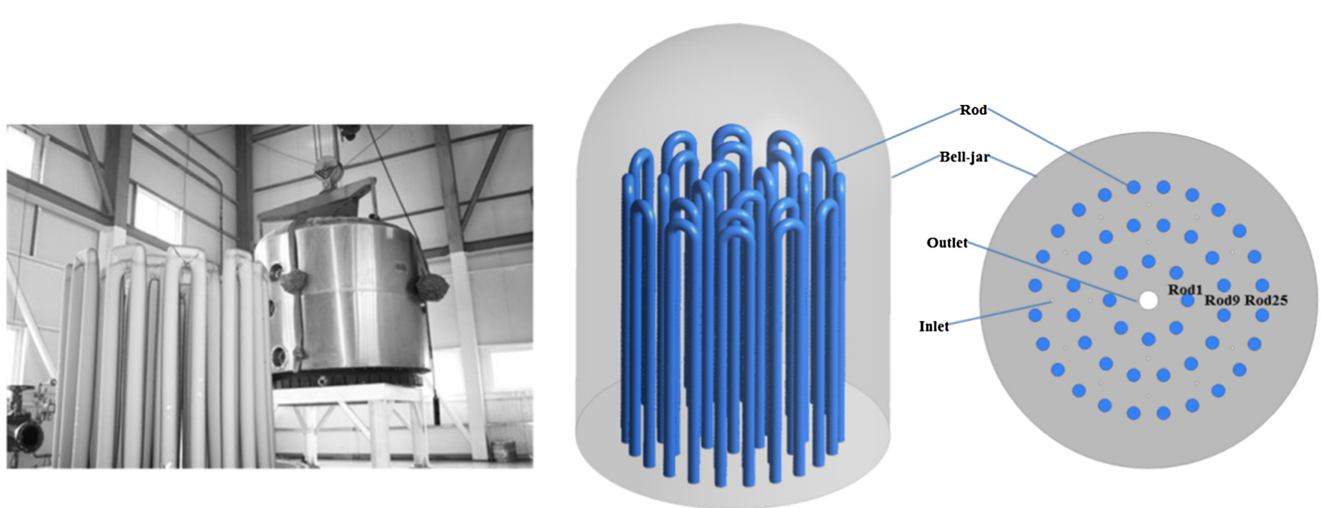
L	length of silicon rod, m	q_c	convective heat dissipation, W/m^2
R	radius of silicon rod, cm	q_{ra}	radiative heat dissipation, W/m^2
H	magnetic field intensity, A/m	q_{re}	heat dissipation via endothermic reaction, W/m^2
J	current density, A/m^2	C	elastic constant matrix
E	electric field strength, V/m	ε	strain tensor
μ	magnetic permeability, H/m	α	thermal expansion coefficient, 1/K
ω	current angular frequency, rad/s	T_{ref}	reference temperature, K
σ	electric conductivity of silicon, S/m	γ	Poisson's ratio
r	radial coordinate, cm	σ_{Mise}	Von Mises stress, MPa
κ	parameter, $\kappa^2 = \omega\mu\sigma$	S^*	average relative error
J_0	current density at the surface of a silicon rod, A/m^2	En	specific energy consumption, kWh/kg
I_{Tot}	total electrical current, A	Q	total heat dissipation from the rod surface, W/m^2
S	rod cross-sectional area, m^2	ρ	density of polysilicon, kg/m^3
δ	skin depth, cm	υ	deposition rate of polysilicon, µm/min
f	frequency of alternating current, Hz	AE	average energy consumption, kWh/kg
k	thermal conductivity of Si, W m^{-1} K^{-1}	R_f	final rod radius, cm
T_s	rod surface temperature, K		
$T(r)$	radial-dependent temperature distribution, K		
q	heat generation per unit of volume, W/m^3		

uneven temperature profile within the silicon rods creates internal stresses, causing the final rods to be brittle. The formation and propagation of stress-induced defects are highly dependent on thermal stress evolution during the electric heating process. Stress levels are determined by the nonlinear temperature gradients created by the power supply system [23,24], among which the Joule heating method, power allocation, and operation curves of the voltage-current are the most important.

Analytical studies on the Joule heating process of rods in Siemens reactors have been performed considering both direct current (DC) and alternating current (AC) power sources [25–28]. Most of these studies focused on the thermal and electrical behavior of silicon rods. However, for the Joule heating process, less theoretical work has been performed on thermal stress evolution. We aim to investigate the effects of various AC frequencies on the stress distributions within silicon rods located in different rings in a 48-rod Siemens reactor. The evolution of the temperature, current density, and stress distributions within the rod, as well as the maximum rod deposition radius, are also analyzed. Based on the results, we propose a novel Joule heating method that is useful for producing the larger high-purity polycrystalline silicon rods. Furthermore, a detailed analysis of energy consumption during the polysilicon deposition process has is performed for various final deposition rod radii. It is hoped that our findings will guide the overall design and optimization of Siemens reactors to achieve further energy consumption reduction in polysilicon industries, thereby making the Siemens process more competitive.

2. Problem description and mathematical model

A schematic of an industrial-scale Siemens reactor is portrayed in Fig. 1(a), in which the furnace periphery is shown. Of particular modeling interest in the Siemens reactor is the main furnace body, which is comprised of reactant gases, silicon rods and bell-jar (see Fig. 1(b)). As noted previously, the general process for the production of polysilicon uses a thermal reduction of a silicon containing composition. The trichlorosilane (TCS) is used as a reactant gas and hydrogen also participates in the reaction according to reaction (1).



(a) (b)

Fig. 1. (a) A 48-rod Siemens reactor operating in Kunming Yeyan New-Material Co., Ltd. (b) Three dimensional geometric model.