Journal of Crystal Growth 394 (2014) 145–152

Contents lists available at ScienceDirect

Journal of Crystal Growth

journal homepage: www.elsevier.com/locate/jcrysgro

Numerical and experimental evaluations on new direct growth process of polycrystalline silicon wafer from liquid silicon

BoYun Jang [a,*], SeungWon Shin [b,**], JinSeok Lee [a], JoonSoo Kim [a]

[a] Energy Materials and Convergence Research Department, Korea Institute of Energy Research, Daejeon 304-343, Republic of Korea
[b] Department of Mechanical and System Design Engineering, Hongik University, Seoul, 121-791, Republic of Korea

ARTICLE INFO

Article history:
Received 24 October 2013
Received in revised form
10 January 2014
Accepted 3 February 2014
Communicated by D.W. Shaw
Available online 25 February 2014

Keywords:
A1. Polycrystalline
A1. Solidification
A2. Growth from melt
B2. Semiconducting silicon
B3. Solar cells

ABSTRACT

A new polycrystalline silicon (Si) wafering process directly from Si melt is introduced. As Si is known to have high latent heat, maintaining the steady state solidification condition in target area could be a main issue to achieve proposing wafering process. In addition, as the proposed process is based on horizontal growth, another critical issue is to keep grains growth parallel to the wafer growth direction, which results in large grain sizes. At first, simple numerical modeling was used to evaluate the possibility of realizing this new conceptual process, and to determine the main process parameters. From the simulation results, growth velocity and heat transfer rate at the solidification zone was identified as main process parameters for the steadily grown Si wafer within target area. Based on the simulation results, a growth system was set up experimentally, and the feasibility of the process was examined. A Si wafer with dimensions of $156 \times 156 \times 0.3$ mm^3 was successively obtained and grains growth parallel to wafer growth direction as calculated in the simulation were observed.

1. Introduction

Even though majority of Si wafers for photovoltaics is produced by multi-wire sawing [1–6], the direct growth of a polycrystalline Si wafer (also called a ribbon) from liquid Si has also been investigated over 30 years [7–20]. There is theoretically no kerf-loss from direct growth method. It does not require an ingot because a wafer can be produced directly from the liquid Si thus can be very cost effective. Basically, vertical and horizontal growth directions of a Si wafer from liquid Si can be possible. This growth direction becomes the most important parameter for the quality and the production cost of the Si wafer. If the grains grow parallel to the wafer growth direction, they would have sufficient time to grow, which results in larger grains. Larger grain size, i.e. fewer grain boundaries, is very important, because the grain boundary is a representative defect that worsens the quality of a wafer.

Dendrite web growth, string ribbon growth, and edge-defined film-fed growth (EFG) can be categorized as vertical growth methods. In the case of EFG, typical grain size is larger than several millimeters. In spite of large grains, the production cost is relatively high, because the typical growth velocity of this method is as low as 1–2 cm/min [9,20]. Lower growth velocity results in a longer process time, which mainly determines the cost. Alternatively, the growth velocity is as high as 600 cm/min in the horizontal growth method [10,11,20]. Ribbon growth on substrate (RGS) and silicon sheet from powder are well known horizontal growth methods. In this process, heat is transferred by contact between the liquid Si and a substrate, which makes the liquid Si solidify very quickly. In addition, grains grow perpendicularly to the wafer growth direction, because grains grow from the substrate. Therefore, the grain size is strongly dependent on the substrate. However, previous research revealed that there is a limitation in the grain growth in horizontal growth process [13–15]. For example, the maximum grain size of wafer by RGS method was 200 μm [20].

If grains grew parallel to the wafer growth in the horizontal growth process, it would be possible to obtain both good quality and low production cost. A new growth model should be based on the horizontal process, because the growth velocity determines the tact time and the production cost. At the same time, the grains must grow parallel to the wafer growth during the process. A new horizontal growth model with parallel grain growth to the wafer growth direction can be established by modifying the continuous mold casting process. Continuous mold casting is a representative industrial manufacturing process for steel or copper slabs that features high production speed [21–23]. In addition, little material is lost during the casting. However, this process is known to be

* Corresponding author. Tel.: +82 42 860 3476; fax: +82 42 860 3133.
** Co-corresponding author.
E-mail address: byjang@kier.re.kr (B. Jang).

http://dx.doi.org/10.1016/j.jcrysgro.2014.02.006
0022-0248

effective for thick and ductile metals, whereas a Si wafer is usually thinner than 500 μm, and Si is very brittle because of its covalent bonding properties. Furthermore, Si has a high latent heat of 427.8 cal/g which makes it difficult to solidify a Si melt [24].

There are many issues which must be considered to apply the continuous casting process for Si wafering. The first issue is whether it is possible to apply continuous mold casting for Si wafer growth (existence of steady state solidification within target region). The second is whether the grains grow parallel to the wafer growth direction when continuous casting is modified for the horizontal growth process of a Si wafer. To check the possibility of applying continuous casting to a horizontal growth process for Si wafers, we introduce a solidification model and numerically simulate the solidification behavior beforehand. The growth process with the solidification model is also simulated to observe the direction of grain growth. Main objective of the numerical simulation was to check the possibility of obtaining steady state solidification and identifying the major controlling parameters on parallel grain growth to wafer growth direction so simple model should be sufficient enough. An experimental system was set up based on the analysis from numerical simulation, and preliminarily tests were performed on the Si wafer growth process to check the feasibility. More complex modeling and boundary conditions would be necessary for realistic simulation which would generate tight connection between numerical and experimental results. This will be our future endeavor. In following section, description of the solidification model of Si in a casting mold is presented, followed by simple 2D-numerical simulations to evaluate the grain growth and possibility of applying continuous casting to a horizontal growth process for Si wafering.

2. Numerical and experimental procedures

2.1. Basic modeling

In the process introduced here, liquid Si is solidified in a mold called a solidification zone, which plays a key role in casting the Si wafer. The solidified Si is continuously pulled out of the solidification zone. The dimensions of the solidification zone determine the thickness and width of the solidified Si wafer. During this process, two types of liquid–solid interfaces can be formed in the solidification zone. Fig. 1 shows idealized solidification models for when the solid–liquid interface moves (a) perpendicular and (b) parallel

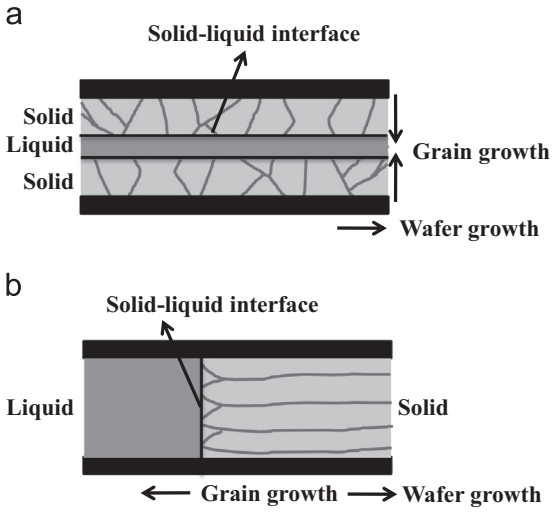

Fig. 1. Solidification models when solid–liquid interface moves (a) perpendicular and (b) parallel to wafer growth direction.

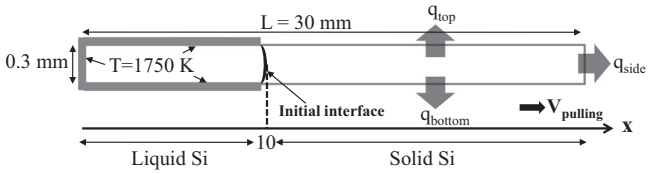

Fig. 2. 2-dimensional model of the solidification zone with dimensions of 30×0.3 mm^2.

to the wafer growth direction of the solidified Si. These models are just presented for convenience, and it is likely that a mixture of the two models exists in reality.

In the case of the interface moving perpendicular to the wafer growth direction, with the grains growing upward and downward, small horizontal grains meet at the middle of the solidification zone. These discontinuous grains are sources of recombination sites of generated electrons in a solar cell, which results in poor conversion efficiency. In contrast, grains can grow continuously when the liquid–solid interface moves parallel to the wafer growth direction, as shown in Fig. 2(b). A few long grains or even only one grain can be obtained in the solidified Si. A Si wafer with a few long grains results in improved cell efficiency. In addition, Si is known to expand in volume when it is solidified [24]. In the case of model (a), volumetric expansion occurred upward and downward, which induced high stress between the mold and solidified Si, and eventually terminated the process. In model (b), the stress induced by volumetric expansion can be released toward the liquid Si. Consequently, control of the solid–liquid Si interface in a specific direction is critical to realizing this process. However, it is impossible to observe the evolution behavior of the solid–liquid interface experimentally during the process, because the process temperature is typically higher than 1600 K. To pre-evaluate this process before actual implementation, we propose a 2-dimensional numerical simulation of the solidification process, and investigate the main process parameters to properly control the solid-liquid interface.

2.2. Numerical approach and boundary conditions

As pointed out earlier, main objective of the numerical simulation is to check the validity of continuous casting approach to Si wafering and growth direction during solidification. The final interface shape determined from temperature distribution will be critical to analyze the growth direction during solidification and the movement by the pulling velocity of the solidified Si generates internal flow of liquid Si near the entrance. To account for these rather complex conditions, full numerical analysis was necessary. With numerical solution, we can also estimate the important design variables such as required time to reach steady state as well as the final shape of the interface. This information can be used as design guide for future implementation. We have used a Level Contour Reconstruction Method (LCRM) to track the solid–liquid interface evolution. LCRM [25,26] is a hybrid form of front tracking and level set methods. It combines the advantages of explicit tracking and automatic handling of the topological changes of the interface from front tracking and level set, respectively.

The 2D governing equations for the momentum in the liquid phase and energy for both phases are as follows:

$$\nabla \mathbf{u} = 0 \tag{1}$$

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\nabla\mathbf{u}\right] = -\nabla p + \rho\mathbf{g} + \nabla\mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T) \tag{2}$$

$$\frac{\partial T}{\partial t} + \mathbf{u}\nabla T = \alpha\nabla^2 T \tag{3}$$