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A novel method for gas flow and impurity control in directional solidification of multi-crystalline silicon

M.P. Bellmann [a,*], D. Lindholm [b], M. M'Hamdi [c]

[a] SINTEF Materials and Chemistry, 7465 Trondheim, Norway
[b] Institute for Energy Technology, 2027 Kjeller, Norway
[c] SINTEF Materials and Chemistry, 0315 Oslo, Norway

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ABSTRACT

In this paper the potential of a specially designed argon gas injector for controlling the gas flow and transport of impurities in directional solidification of multi-crystalline silicon is evaluated. The gas injector which consists of a valve allows one to control the flow direction independently in the vertical and horizontal directions. Based on a gas flow model derived from a semi-industrial crystallization furnace the impact of different gas injection combinations on the gas flow pattern and impurity transport is studied. Special focus is given to the SiO evacuation from the melt-free surface, the CO formation at graphite surfaces and the CO evacuation from the furnace interior. It is found that for gas flow pattern formed through horizontal rather than vertical gas injection, SiO and CO are evacuated most effectively from the furnace interior and the formation of CO is inhibited. Such a type of gas injector presents a versatile tool for controlling the flow and impurity transport in the gas phase and possibly improving the material properties of crystalline silicon.

1. Introduction

In directionally solidified multi-crystalline silicon (mc-silicon), oxygen and carbon are the impurities that are present at the highest level. Typical pathways of these impurities [1,2] are illustrated in Fig. 1. Dissolved oxygen from the silica crucible and silicon nitride coating is carried by the melt to the solid–liquid interface where it is incorporated into the solid or it evaporates as silicon monoxide from the melt-free surface. Argon gas, injected into the furnace chamber, carries the silicon monoxide (SiO) to the hot graphite fixtures where it reacts with carbon to form carbon monoxide (CO). At the melt-free surface CO dissociates into the melt and finally carbon and oxygen are incorporated into the solid. Oxygen related defects, like thermal and new donors, can reduce the minority carrier lifetime in solar cells [3]. Carbon precipitates can be responsible for the nucleation of new grains, the formation of locally induced stresses, wire-sawing defects [4] and can cause ohmic shunts in solar cells [5].

The final impurity distribution in the solidified ingot strongly depends on the melt [6] and the gas flow [1,2] velocity fields. Controlling the melt flow by external force fields [7,8] is a well acknowledged tool in crystal growth. Great effort has been drawn for investigating the effects of gas flow on heat and impurity transport in Czochralski [9,10] single crystal growth and directional solidification of mc-silicon [1,2,11,12]. In latter case, little attention has been drawn on tailoring the gas flow fields with the purpose on affecting chemical reactions and the distribution of impurities to the benefit of silicon crystal properties. Variations of the argon gas flow rate and the furnace pressure and their impact on the impurity distribution have been studied in [2]. Positive effects were reported on the implementation of a gas guidance device above the melt-free surface [11,12].

In this paper we present for the first time a method for controlling primarily the gas flow pattern, and secondary, chemical reactions and the distribution of impurities in the gas phase. Based on a simplified local model derived from a semi-industrial crystallization furnace the impact of argon gas injected through a valve based on a dual nozzle on the flow pattern, chemical reactions and impurity distribution is investigated numerically. Such a specially designed valve allows one to control the flow direction independently in the vertical and horizontal directions or as a combination of the two. Details of the furnace and of the numerical model are described in Section 2. In Section 3, numerical results are presented and discussed, while concluding remarks are given in Section 4.

2. Model description

2.1. Numerical approach

The numerical study presented in this work was carried out for a semi-industrial vertical Bridgman furnace as shown in Fig. 2A.

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* Corresponding author. Tel.: +47 934 98619.
E-mail address: martin.bellmann@sintef.no (M.P. Bellmann).

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The induction heated furnace holds 120 kg of silicon, producing squared ingots of 55 × 55 cm and 16.5 cm in height. The furnace is equipped with two independently controlled susceptors which are placed above and underneath the silica crucible, each powered by a 100 kW generator. Heat is transferred to the ingot by radiation from the inductive heating of the upper and conduction by the lower susceptor. More details about the furnace, the global model and the crystallization process can be found in [13,14]. A special feature of the furnace consists in the design of the argon gas injector valve which is equipped with a dual nozzle allowing for independent flow control in the vertical and horizontal directions, as illustrated in Fig. 2C.

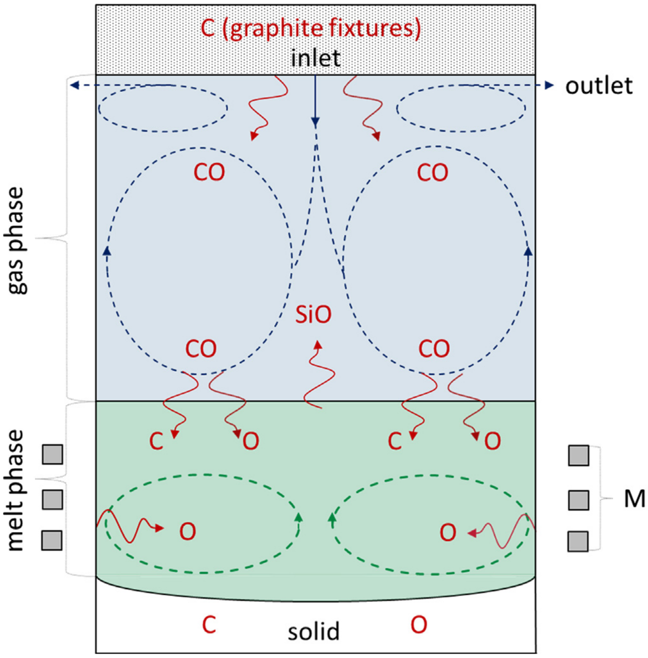

Fig. 1. Typical pathways of oxygen and carbon impurities in a silicon crystallization furnace and possible melt flow control by external force fields, e.g. magnetic fields (MF).

The gas flow model has been implemented into the commercial CFD code ANSYS Fluent 13 running on an Intel based Linux cluster. In order to reduce the computational time of the simulations thus increasing the feasibility of advanced physical modeling, the gas domain is extracted from the global furnace model and reduced to a quarter (see Fig. 2B). Fourfold symmetry is applied at cutting planes [13–16].

For general three-dimensional problems, the dependent variables are the velocity u_i, the pressure p, the turbulent kinetic energy k, the energy dissipation rate ϵ and the species concentration Y_i. These time-dependent variables are solved from the incompressible Navier–Stokes equations including the continuity equation, the k–ϵ turbulence model and the species transport equation. Model equations for mass and momentum conservation, with u_i representing the velocity component in direction x_i, are

$$\frac{\partial u_i}{\partial x_i}=0 \tag{1}$$

$$\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}=-\frac{1}{\rho}\frac{\partial p}{\partial x_i}+g_i+\frac{\partial}{\partial x_j}\left((\nu+\nu_t)\frac{\partial u_i}{\partial x_j}\right)-\frac{2}{3}\frac{\partial k}{\partial x_i}. \tag{2}$$

In Eq. (2), t is the time, ρ is the density, g_i is the gravitational acceleration, ν is the molecular kinematic viscosity and ν_t is the turbulent kinematic viscosity. The latter, which is not a fluid property, depends on the internal friction in the flow and increases the apparent viscosity of the fluid. Argon fluid properties are considered for atmospheric pressure and at 300 K. Heat transfer is not part of the problem (isothermal flow), and model terms that account for buoyancy are therefore omitted from the momentum equations.

Turbulence in the fluid flow domain above the melt-free surface is introduced by argon gas that continuously enters the domain through an centrally positioned gas injection system. The Reynolds number Re is in the order of 2800 and a turbulence model is required. To compute turbulence the standard k–ϵ model [17] is employed. The turbulent kinetic energy, k, and its rate of dissipation, ϵ, respectively, are obtained from the two-equation model:

$$\frac{\partial k}{\partial t}+u_j\frac{\partial k}{\partial x_j}=\frac{\partial}{\partial x_j}\left[\left(\nu+\frac{\nu_t}{C_k}\right)\frac{\partial k}{\partial x_j}\right]+P_k-\epsilon \tag{3}$$

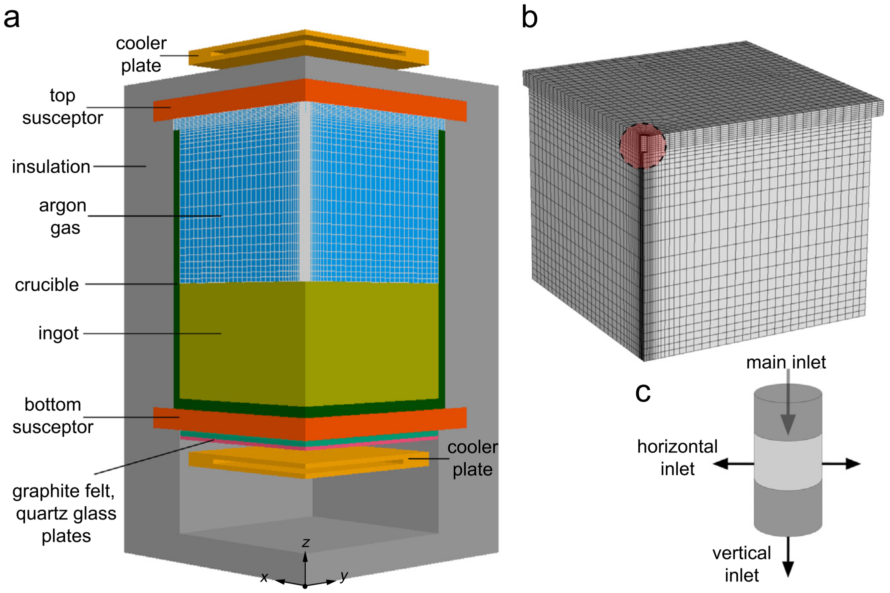

Fig. 2. Furnace model geometry and parts (A) (furnace casing excluded), extracted argon gas domain (B), argon gas injector valve with a dual nozzle for independent flow control in the vertical and horizontal directions (C).