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Numerical study of the influence of forced melt convection on the impurities transport in a silicon directional solidification process

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ABSTRACT

Time dependent three-dimensional numerical simulations were carried out in order to understand the effects of forced convection induced by electromagnetic stirring of the melt, on the crucible dissolution rate and on the impurity distribution in multicrystalline silicon (mc-Si) melt for different values of the diffusion coefficient and electric and magnetic field parameters.

Once the electromagnetic stirring is switched on, in a relative short period of time approx. 400 s the impurities are almost homogenized in the whole melt. The dissolution rate was estimated from the total mass of impurities that was found in the silicon melt after a certain period of time. The obtained results show that enhanced convection produced by the electromagnetic stirring leads to a moderate increase of the dissolution rate and also to a uniform distribution of impurities in the melt.

1. Introduction

Nowadays, most solar cells are based on crystalline silicon, out of which over 60% is obtained through the Directional Solidification (DS) method [1]. In order to reduce costs, there are two main trends in the DS of PV silicon: the increase in ingot size and the use of a feedstock material of lesser purity. However, both these measures could lead to potential problems such as the detrimental curvature of the solid-liquid interface, the accumulation of more impurities during the longer growth time needed for larger ingots or from the lesser purity feedstock [2] leading to the morphological destabilization of the growth interface [3] or to their precipitation after the solubility limit is reached [4–6]. The solution for these problems would consist in controlling the melt flow structure. A complete homogenization is required in order to have the optimal distribution of impurities, as this will reduce the impurity diffusion boundary layer thickness at the growth interface and lead to optimal axial segregation profiles. Due to the fact that in the method of DS the solidification starts from the bottom and consequently the temperature is hotter at the top than at the bottom of the crucible, the buoyant convection in the melt occurs just because of the lateral temperature gradients and cannot generate a good mixing in the whole melt volume. This requires the employment of a forced convection.

Several studies exist for obtaining a forced convection of the melt by using travelling (TMF) [7–10], rotating (RMF) [11,12] or carousel magnetic fields [13], while others rely on mechanical [14] or ultrasound vibration stirring [15]. Magnetic fields are a powerful tool to control the convection in electrically conducting melts and, therefore, play a key role in the optimization of semiconductor bulk crystal growth processes [16]. An interesting approach proposed lately [17–19] was based on a mix between vertical magnetic field and electrical current generating an electromagnetic field stirring (EMF). However, the effect of the EMF melt mixing on the impurity distribution in a silicon DS process has not been investigated yet. It is the purpose of this paper to study the effects of the EMF mixing on an impurity distribution originating from the crucible walls.

2. Numerical model

The computational domain used in the 3D simulations consists of silicon melt and crystal as shown in Fig. 1. The square shaped crucible is $38 \times 38 \times 40$ cm^3 corresponding to a G2 standard crucible.

At the melt free surface two electrodes are placed through which an electrical current is injected into the melt. In the simulation the two electrodes were placed in an asymmetric configuration: one electrode is placed in the center of the free melt surface and the second electrode is placed on a diagonal at 1/3 of the diagonal length from the corner as seen in Fig. 1.

The melt flow and heat transfer are described by the three-dimensional equations of mass, momentum and heat conservation taking into account the Boussinesq approximation for an incompressible fluid and the Lorentz force density. The mathematical model is largely presented in [17]. The boundary conditions for temperature and

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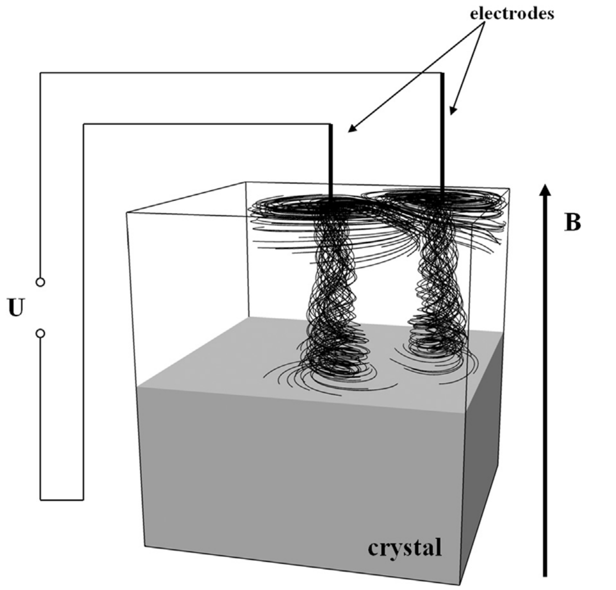


Fig. 1. Schematic representation of the computational domain.

velocity field and the material properties are also presented in [17]. The temperature is fixed along the lateral walls and at the bottom. A temperature gradient of 3 K/cm was used in the melt, and 10 K/cm in the crystal. At the free melt surface a radiative heat exchange to an ambient temperature of T_{ref}=1785 K is applied.

The impurity distribution is modeled by the diffusion equation:

$$\frac{\partial c}{\partial t}=-\frac{\partial}{\partial y_j}\left(v_j c - D\frac{\partial c}{\partial y_j}\right) \quad (1)$$

where $v_j$is the j-th component of the flow velocity in Cartesian coordinates, *c* represents the impurity concentration and D is the diffusion coefficient.

At the solid-liquid the impurity segregation was considered:

$$(\rho_s D_s \nabla c|_s - \rho_l D_l \nabla c|_l)\bullet n_l = -(1 - K)u_g c_l \rho_s \quad (2)$$

with n_l the outgoing normal from the fluid, but the impurity concentration was computed only in the liquid phase and so the diffusion in the solid phase was neglected. The segregation coefficient, K, was set to the characteristic value of carbon, $7\cdot10^{-2}$ [4]. ρ_s and ρ_l are the densities of the Si crystal and the melt and u_g is the growth rate fixed at 10 mm/h for all of the simulations.

For the diffusion coefficient in the melt, D_l, four different values were used: $0.5\cdot10^{-8}$ m²/s, $2\cdot10^{-8}$ m²/s, $3\cdot10^{-8}$ m²/s and $5\cdot10^{-8}$ m²/s, which represent characteristic values for the impurities found in a directional solidified multicrystalline silicon ingot.

The impurity concentration is fixed on the lateral walls at $9\cdot10^{24}$ atoms/m³ which is the solubility limit of carbon in silicon [20].

For the diffusion equation, a no-flux boundary condition ($\frac{\partial c}{\partial n}$=0) was set at the melt free surface. The initial concentration in the melt was set to zero.

The three-dimensional numerical simulations were done using the STHAMAS3D software which has already been validated in DS processes [21] and EMF stirring experiments [18,19]. The computational domain is subdivided into two blocks with a grid refinement at the walls so that two grid points are contained in the boundary layer (estimated at 2 mm). The mesh consists of 396,000 control volumes. The simulation extended over 500 s in real time with a time step 0.1 s.

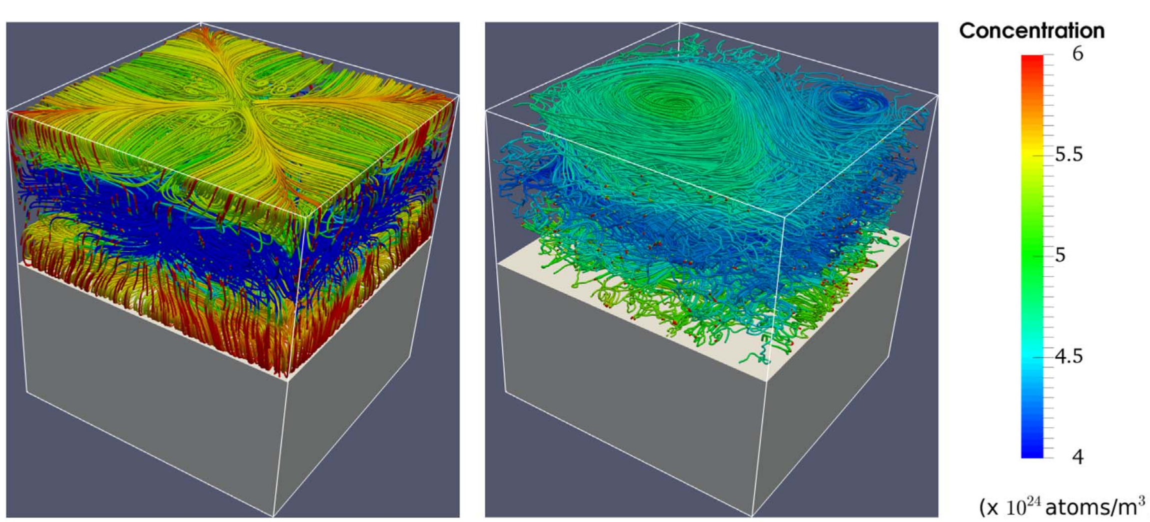
3. Results and discussions

In [17] the influence of the electromagnetic stirring on the temperature field and interface shape was presented and discussed. In the present contribution we will focus on the effect of electromagnetic stirring on the impurity distribution.

To study the influence of the electromagnetic field on the impurities transport and crucible dissolution rate for a silicon directional solidification process the transport equations were solved along with the scalar potential equation.

Two values of the magnetic induction, B, were considered, 10 mT and 20 mT, and two values for the electrical current intensity, I, 5 A and 10 A were used. These values were chosen to be easily obtained in a real growth experiment.

First, the impurity distribution in the melt was computed for a case where only natural convection was considered. In a previous study [22] it was shown that for a temperature gradient of 3 K/cm in the melt and 10 K/cm in the crystal, using a growth rate of 10 mm/h, there are two main convection areas in the melt: one at the melt free surface and one near the solid-liquid interface. Convection rolls appear in both of these areas that transport the impurities from the crucible walls into the melt. As it was previously shown, the two main areas of convection are completely separated which leads to a poor mixing in the middle part of the melt. This behavior can be seen in Fig. 2(a). The impurity concentration is high near the melt free surface and near the solid-liquid interface and between these two parts an area with low



(a) natural convection (b) EMF forced convection

Fig. 2. Impurity distribution at 200 s in the case of natural convection (a) and in the case of forced convection generated by an EMF (b).