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Numerical analysis of the influence of tilt of crucibles on interface shape and fields of temperature and velocity in the unidirectional solidification process

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Abstract

We carried out calculations to investigate the influence of tilt of crucibles on the melt–crystal interface shape and fields of temperature and velocity of the melt and/or crystal by three-dimensional global and melt–crystal analyses. It was found that flow velocity was larger in the case of a fixed boundary condition of edge of the interface than that in the case of a relaxed condition. Furthermore, deflection of the interface with a fixed boundary condition was smaller than that without the fixed boundary condition. These results indicate that we should use three-dimensional global analysis with a relaxed boundary condition to investigate the influence of tilt of crucibles on the interface shape and flow velocity.

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1. Introduction

The unidirectional solidification method is a key method to produce multicrystalline silicon (mc-Si) for use in highly efficient solar cells. The shortage of raw materials of silicon is now becoming a key issue in photovoltaic fields, because there is a large demand for solar cells all over the world [1]. Therefore, the challenge of photovoltaic fields is to increase the yield of silicon ingots with low manufacturing costs. In order to improve the productivity, square-shaped crucibles have been used in the unidirectional solidification process to fit the square shape of solar cells [1]. Homogenization of the distribution of minority carrier lifetime in mc-Si ingots increases the yield; however, the distribution has been reported to be of asymmetric pattern, accidentally, which may be due to unintentionally introduced tilt of crucibles [2]. It can be estimated that the tilt of crucibles has an influence not only on the melt–crystal (m–c) interface shape and fields of temperature and velocity of the melt and/or crystal but also on stress and impurity distribution in the solidified crystal [3–8]. Therefore, it is important to investigate the influence of tilt of square-shaped crucibles in a solidification process on the m–c interface shape and fields of temperature and velocity of the melt and/or crystal.

Due to the recent developments in computer technology and computation techniques, numerical simulation has become a powerful tool for the investigation of m–c interface shape, and heat and mass transfer in a solidification process [9–11]. When square-shaped crucibles are used, the configuration of the furnace becomes asymmetric.

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Heat and mass transfer in the furnace consequently becomes three-dimensional. Three-dimensional (3D) modeling is therefore necessary for the investigation of m–c interface shape, and heat and mass transfer with square-shaped crucibles. There have been some works on the influence of tilt of crucibles on the m–c interface shape using 3D melt–crystal analysis, taking into account only the melt and the crystal [3]. In 3D melt–crystal analysis [3], not only temperature distribution of the surface of the melt and/or crystal, but also m–c interface position along the vertical walls of crucible are fixed as boundary conditions. However, such temperature distribution of the surface and m–c interface shape, in fact, changes three-dimensionally due to the tilt of the crucibles. Therefore, in order to consider the above three-dimensionality, 3D global analysis in which the boundary conditions on the surface of the melt and crystal are relaxed is necessary. In this paper, we carried out calculations to investigate the influence of tilt of crucibles on the m–c interface shape and fields of temperature and velocity of the melt and crystal using 3D melt–crystal and 3D global analyses.

2. Model description and computation method

Initial conditions used for 3D melt–crystal and 3D global analyses for investigating the influence of crucible tilt on the m–c interface shape and fields of temperature and velocity are obtained by 3D global analysis without tilt of crucibles [12]. Fig. 1 shows the configuration and dimensions of a unidirectional solidification furnace used for 3D global analysis with square-shaped crucibles. The domains of all components in the furnace are subdivided into a number of block regions, as shown in the left part of Fig. 1. The melt, a crystal, crucibles and pedestals are denoted as 1, 2, 3–4 and 5–6, respectively. Thermal shields are labeled 7–10. Three heaters marked by 11–13 are set in the furnace. Each block is then discretized by structured grids as shown in the right part of Fig. 1. The 3D global analysis with square-shaped crucibles requires large computational resources because of the huge number of 3D structured grids. To overcome this difficulty, a 2D/3D mixed discretization scheme is employed to reduce the requirement of computational resources [12,13]. The domains in the central area of the furnace, in which the configuration and heat and mass transfer are non-axisymmetric, are discretized in a 3D way. A local 3D computational grid in the domains in the central area of the furnace is established as shown in Fig. 2. The other block regions that are away from the central area of the furnace, in which the configuration and heat transfer are axisymmetric, are discretized in a 2D way. The following assumptions are made for the 3D global analysis: (1) radiative heat transfer is modeled as diffuse-gray surface radiation, (2) melt flow in the crucible is laminar and incompressible, and (3) the effect of gas flow in the furnace is negligible. Conductive heat transfer in all solid components, radiative heat exchange between all diffusive surfaces in the furnace and the Navier–Stokes equations for melt flow in the crucible are coupled and solved iteratively by a finite volume method in a steady condition. The shape of an m–c interface is obtained by using a dynamic interface tracking method [13].

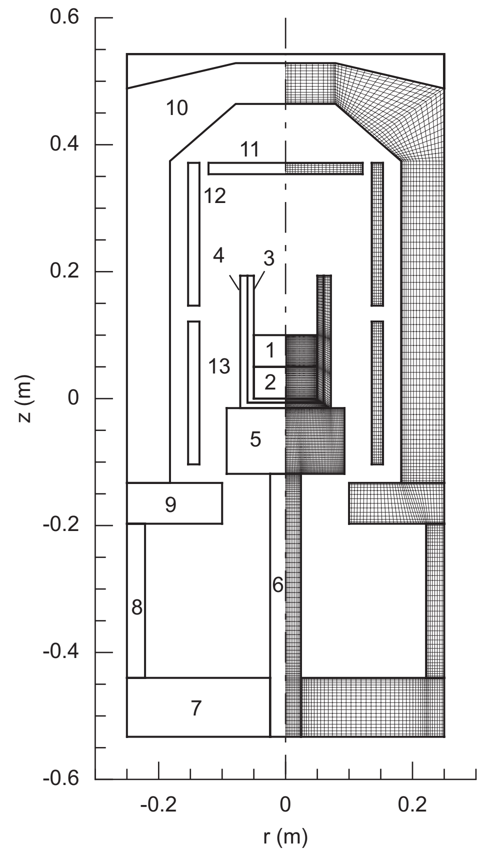

Fig. 1. Configuration and computation grid of a unidirectional solidification furnace with square-shaped crucibles.

Since no fixed boundary condition of temperature is adopted on the surface of the melt and crystal, we can relax temperature distribution on the surface due to the tilt of crucibles in the 3D global analysis (global model) by taking into account radiative heat transfer. Furthermore, deformation of the m–c interface along the vertical walls due to the tilt of crucibles is considered because the m–c interface is not fixed along the vertical walls. Only the center point of the m–c interface is fixed as shown in Fig. 3(a). In order to investigate the influence of tilt of crucibles on the m–c interface shape and fields of temperature and velocity, the gravitational acceleration vector $\mathbf{g}$ included in Navier–Stokes equations is modified as follows:

$$\mathbf{g} = \mathbf{g}(\sin\theta \cdot \mathbf{e}_x - \cos\theta \cdot \mathbf{e}_z),$$

where θ is the tilted angle of crucibles in the X-o-Z plane as shown in Fig. 3(a), and $\mathbf{e}_x$ and $\mathbf{e}_z$ are unit vectors of x and z directions, respectively.

In 3D melt–crystal analysis (m–c model), we take into account only the melt and crystal as shown in Fig. 2. The temperatures T_{wall} on the surfaces of crucible walls, heat