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Numerical analysis of influence of crucible shape on interface shape in a unidirectional solidification process

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Abstract

We carried out calculations to investigate the melt–crystal (m–c) interface shape with cylindrical and square crucibles and the influence of crucible shape on m–c interface shape using two-dimensional and three-dimensional global analyses. It was found that maximum deformation of the m–c interface occurs near the corner of the square crucible because outgoing heat flux, which has a significant influence on the m–c interface shape, has three-dimensionality. It was also found that shape and dimensions of the crucible have significant influence on the amount of outgoing heat flux. The results indicate that we should control not only heater power, growth ratio and melt flow but also shape and dimensions of crucibles in order to reduce deformation of the m–c interface.

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1. Introduction

Dislocations generated during the growth of multi-crystalline silicon by the unidirectional solidification method are one of the important causes of degradation of the quality of silicon ingot such as minority carrier lifetime and open-circuit voltage [1]. The presence of dislocations has been attributed to thermal stress in the solidification process [2–4]. Therefore, reduction of thermal stress is necessary to improve the quality of silicon ingots. It is important to optimize the melt–crystal (m–c) interface shape in order to reduce the thermal stress in the solidification process since the m–c interface shape has a great effect on the magnitude of thermal stress [2,5]. Since the shape of a silicon wafer used in a photovoltaic cell is square, the shape of the crucible used in the unidirectional solidification process is also square [6]. Therefore, investigation of the m–c interface shape in a solidification process with square crucibles is necessary to estimate the quality of silicon ingots.

Due to recent developments in computer technology and computation techniques, numerical simulation has become a powerful tool for investigation of m–c interface shape in a solidification process [3,7]. Since convection in the melt and radiative heat transfer have effects on m–c interface shape [8], global modeling that takes into account radiative, conductive, and convective heat transfer in a furnace is necessary for investigation of m–c interface shape. There have been some works on two-dimensional (2D) global analyses of a unidirectional solidification process with cylindrical crucibles [9,10]. When square crucibles are used, the configuration of the furnace becomes asymmetric, and heat transfer in the furnace consequently becomes

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three-dimensional (3D). Three-dimensional global modeling is therefore necessary for investigation of m–c interface shape with square crucibles.

There have been no works using global analysis to investigate the effect of crucible shape on m–c interface shape. We developed a steady code with 2D and 3D global models for the unidirectional solidification process used for cylindrical and square crucibles, respectively. In this study, we carried out calculations to investigate the m–c interface shapes with cylindrical and square crucibles and to investigate the influence of crucible shape on m–c interface shape using 2D and 3D global analyses.

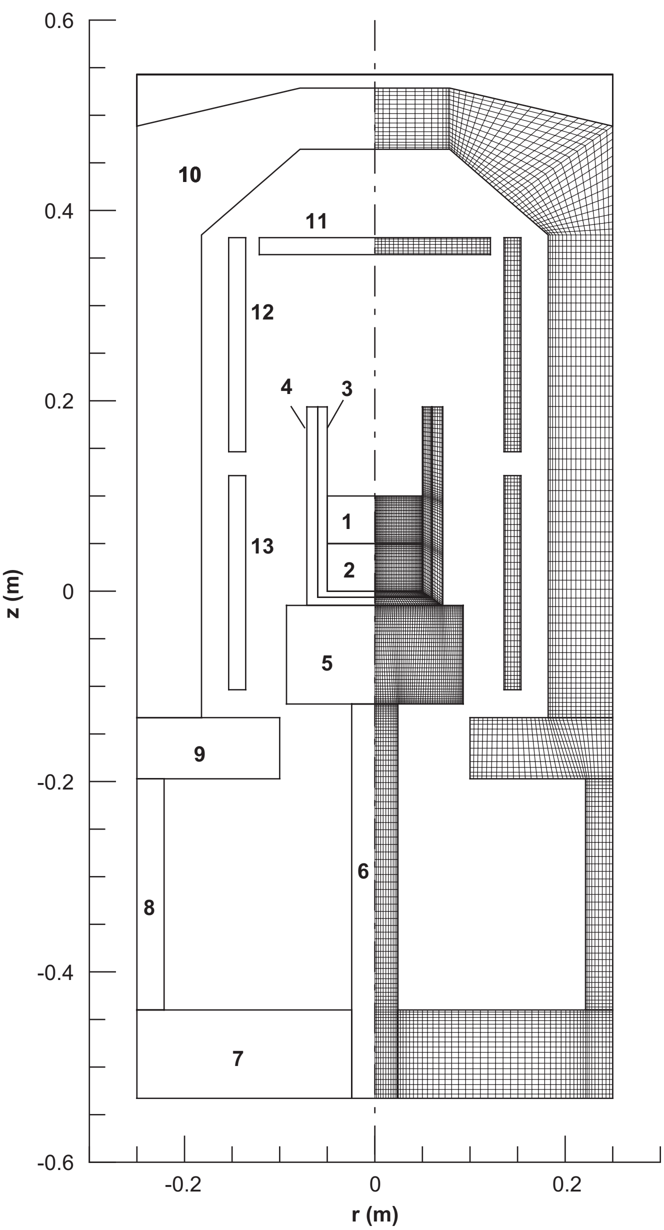

Fig. 1. Configuration and computation grid of a unidirectional solidification furnace with cylindrical crucibles.

2. Model description and computation method

Fig. 1 shows the configuration and dimensions of the unidirectional solidification furnace used for 2D global analysis with cylindrical 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 following assumptions are made for the 2D global analysis: (1) the geometry of the furnace configuration is axisymmetric, (2) radiative heat transfer is modeled as diffuse-gray surface radiation, (3) the melt flow in the crucible is laminar and incompressible, and (4) 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 the 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 [11].

Three-dimensional global analysis with square 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

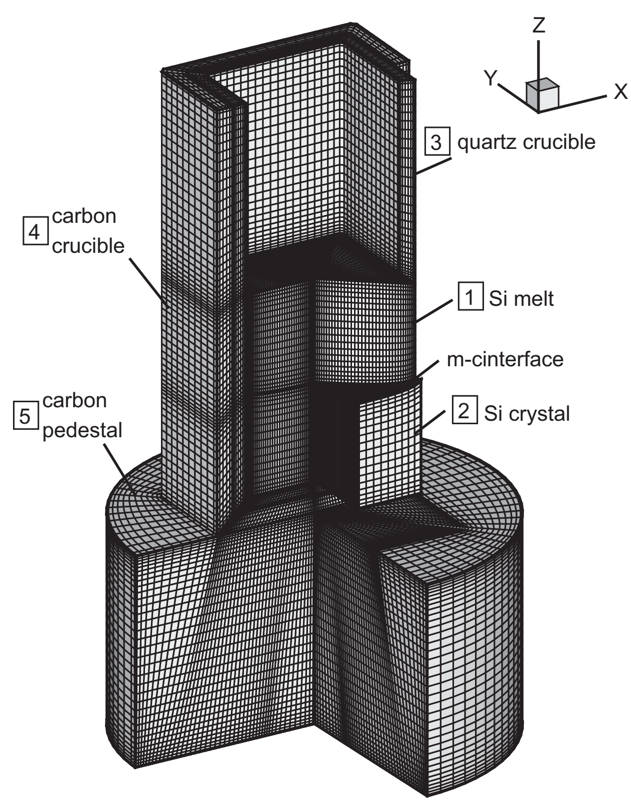

Fig. 2. Three-dimensional computation grid used for the 3D global model.