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Validation, verification, and benchmarking of crystal growth simulations

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Abstract

The variety of physical phenomena in crystal growth processes requires various software tools for the numerical simulations. Both, dedicated 2D or 3D ready-to-use software for coupled simulations of a crystallization furnace and general-purpose 3D simulation packages have been used in the literature. This work proposes a general strategy for model development: validation of the physical model using model experiments; verification of the numerical model using analytical or high-accuracy solutions; testing of the computational efficiency using complex benchmark cases. The application of these steps is demonstrated for various models in directional solidification of silicon showing the capabilities of various open source or commercial software packages.

Keywords: A1. Computer simulation; A1. Heat transfer; A1. Fluid flows; A1. Magnetic fields; A1. Stresses; A2. Growth from melt

1. Introduction

Crystal growth processes are distinguished by a complex interaction between a variety of physical phenomena on multiple length scales. This is exemplary illustrated in Fig. 1 for the directional solidification of silicon. The heat transfer by high-temperature radiation and gas convection takes place globally in the entire crystallization furnace. The local convection in the silicon melt resulting from buoyancy and electromagnetic forces has a crucial influence on the processes at the solid-liquid interface on both, macroscopic (interface shape, impurity concentration) and microscopic (interface stability, nucleation, striations) scales. In the silicon crystal, macroscopic thermal stresses interact with dislocations on the atomic scale. Both, qualitative and quantitative understandings of these complex, interacting phenomena can be greatly improved by using numerical simulations as it has been reviewed in [1–4].

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