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Review

Solidification of silicon in a one-dimensional slab and a two-dimensional wedge

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ABSTRACT

We have developed mathematical models in both one and two spatial dimensions for the solidification of silicon. The one-dimensional model describes slab casting related to a set of thin-casting experiments. The model is fitted to thermocouple data and accounts for various heat transfer mechanisms as well as the latent heat. The model can be used to predict the time taken for the material to completely solidify and the solidification distance (the point where solidification fronts meet which can be observed as a discontinuity in the grain microstructure). Simple approximate analytical results, which agree very well with the full-scale numerical solutions on Matlab and COMSOL, are provided. The two-dimensional model relates to a wedge casting experiment where, again, various heat transfer mechanisms and latent heat need to be accounted for. Experimental data from thermocouples is used to quantify the heat transfer coefficients by fitting to two-dimensional COMSOL simulations. A very simple analytical "Triangle model" is derived by assuming that the solidification fronts move as flat surfaces from each of the two wedge walls and the air surface, independently of each other, as three separate one-dimensional quasi-steady approximations. This model predicts that the area of liquid silicon will diminish as shrinking self-similar triangles. This simplified model provides analytical results for the solidification time and distances which agree very well with the COMSOL simulations.

Contents

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Nomenclature

c_{p_i}	$i = l, s$. The specific heat capacity of liquid (l) and solid (s) silicon
d	the depth of the silicon melt
D	the solidification distance
h_c	the conductive heat transfer coefficient
h_a	the convective heat transfer coefficient
k_i	$i = l, s$. The thermal diffusivity of liquid (l) and solid (s) silicon
K	the ratio of solid to liquid thermal diffusivities
κ	K multiplied by the ratio of solid to liquid specific heat capacities
L	the latent heat of silicon
$\mathbf{n}$	the outward facing unit normal to an interface
N_c	the Nusselt number for conductive heat transfer to the mould
N_a	the Nusselt number for convective heat transfer to the air
N_r	the Nusselt number for radiative heat transfer to the air
q_i	$i = l, s$. The heat flux in the liquid (l) and solid (s) silicon
ρ	the density of silicon
s_i	$i = 1, 2$. The positions of the solidification fronts
σ	the Stefan–Boltzmann constant
St	the Stefan number
t^*	the solidification time
T_m	the melting temperature of pure silicon
T_0	the initial temperature of the liquid silicon before cooling
T_∞	room temperature
T_{init}	the non-dimensional initial temperature of the silicon melt
T_A	the non-dimensional room temperature
θ	the enthalpy
Θ	the non-dimensional enthalpy
V_n	the speed of the solidification front in the normal direction
ω	the position of the solidification front in two dimensions
ϕ	the wedge angle coordinate
α	the wedge angle

1. Introduction

New markets demand high yield silicon of a more homogeneous consistency. It is well known that the cooling rates and mould size affect the microstructure and homogeneity of silicon during casting. The aim of this paper is to gain insight into the cooling rates that occur in two casting geometries. Typically, when cooling rates are too fast the silicon grains are very small (see Fig. 1), causing dust, or 'fines', losses in the post-casting stage when the silicon is re-crushed. Although the yield is reduced, the small grains allow for a homogeneous distribution of impurities, which is an advantage in the silicon alloy industry. In contrast, when the silicon is cooled too slowly, the grains which form are much longer and hold impurities in the grain boundaries. These impurities are therefore distributed in a less homogeneous manner and, in fact, when the silicon is re-crushed, a large portion of them drop out from the long grain boundaries and are lost. For more specific details on the microstructure of silicon, see [1,2].

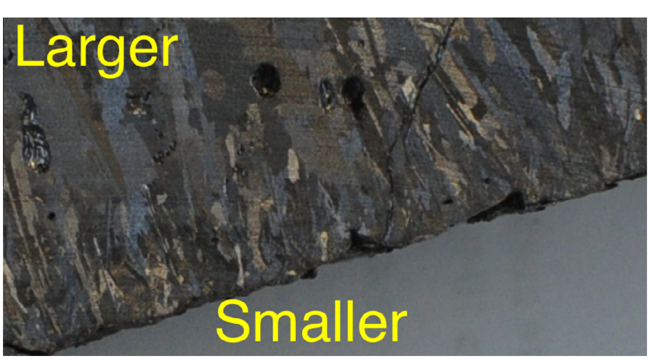

Fig. 1. Fast solidification leads to small grains and a homogeneous distribution of impurities but large loss of yield due to wasted dust (fines) when material is re-crushed. Slow solidification leads to large grains and an inhomogeneous distribution of impurities, large-scale segregation in grain boundaries but high yield. We can see here that solidification occurred more quickly at the bottom edge of this sample due to the smaller grains. (Taken from experiment at Elkem on 04/06/15.)

Recent experiments have shown that the casting of silicon in small, thin containers shows promise for creating materials with good homogeneity. Hence the emerging interest in the silicon industry of the so-called 'thin-casting' technique. One dimensional solidification models are appropriate in thin casts where the aspect ratio is small. There has been extensive work on the mathematical modelling of these types of 'Stefan problems' where there is a solidification front which moves like the square root of time [3–9]. In these examples, similarity solutions only exist in the case of Dirichlet (constant temperature) or Neumann (no heat flux) boundary conditions and are therefore limited. In the case of small Stefan number, quasi-steady approximations can be made, rendering the problem considerably easier to solve [10,11]. The existence of moving boundaries tend to make these problems difficult for numerical simulation yet many approaches have been examined [12–16]. This paper provides an analysis of the advantages and disadvantages of some of these analytical solutions for the purpose of direct comparison with silicon solidification experiments at Elkem and numerical simulations generated using COMSOL [17] and Matlab [18]. In particular, we find that the quasi-steady solution with linearised boundary conditions performs very well whilst providing simple analytical expressions for the temperature profile and position of the moving boundary. The application of the quasi-steady approximation to the domains and boundary conditions in this paper has not been explored in the literature. Furthermore, they are novel applications of mathematical modelling within the silicon manufacturing industry. The quasi steady solution, together with the parameter estimations given by the numerical simulations, will be useful for silicon manufacturers to predict the thermal history of the silicon and give approximate results for the solidification time and distance. The results will also apply to other solidification industries where the Stefan number is relatively small.

We will consider the case where the solidification of 100% pure silicon takes place due to cooling from both the metal mould and the surrounding air. The importance of different cooling mechanisms and cast depths will be investigated. We will use thermal data taken from these experiments to estimate the parameter values. The pure silicon case will give insight into the expected cooling rates that will be encountered even when impurities are present and is much simpler to analyse.