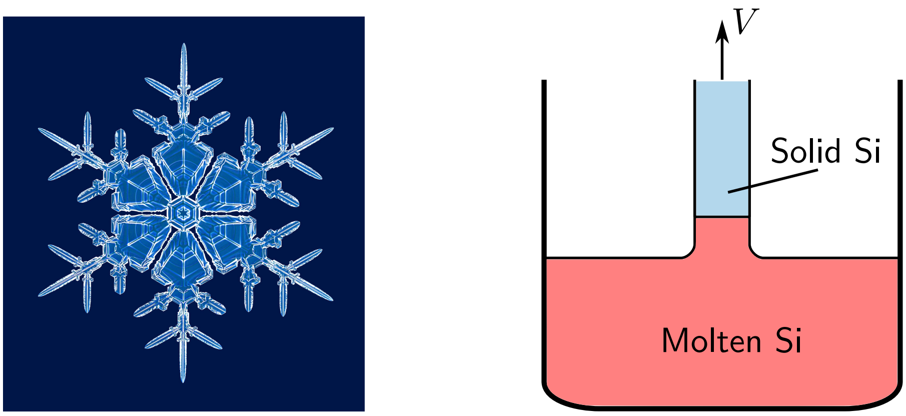
Understanding phase change through the Stefan problem

Introduction

Phase change is the transformation of a material between gas, solid, and liquid states. It is a naturally occurring phenomenon that gives rise to remarkable structures such as snowflakes (by freezing water) and clouds (by condensation of water vapour). Phase change is also an important process that takes place in industrial and technological settings, where it can have beneficial or disastrous consequences. For instance, the Czochralski process is a common method for producing large crystals of semiconducting material such as silicon by carefully freezing a molten bath and continuously extracting the solid. Excess heating in electric components can lead to melting and device failure. Better understanding of phase change is therefore not only practical but can also provide new insights into the natural world around us.



(a) (b)

Figure 1: (a) A lab-made snowflake. (b) Production of solid silicon (Si) using the Czochralski process.

Project

The general theme of this project will be to study mathematical models of phase change. These are commonly called Stefan problems, named after Josef Stefan who studied how lakes freeze in the winter. One of the most interesting features of Stefan problems is that they involve solving the heat equation on a moving domain that must be determined as part of the solution. The evolution of this domain reflects the fact that the boundary between the two phases of a material will change in time as these phases grow or shrink. There are a number of potential topics for this project, including:

- Derivation of models of phase change, calculating exact and approximation solutions, analysing their stability
- Numerical solutions of one-dimensional Stefan problems
- Practical applications such as snowflake formation, drying of deodorant, melting of nanoparticles, crystal growth using the Czochralski process

Prerequisites

Ability to solve differential equations (ordinary and partial) and use Matlab will be important. The solution techniques used in these projects will build on those covered during Michaelmas Term in B5.2 Applied Partial Differential Equations and B6.1 Numerical Solution of Differential Equations I. However, all methods could be independently learned during the project as needed.

Reading

Chapters 1 and 2 of the textbook "Theory of Solidification" by Stephen H. Davis (Cambridge University Press, 2001) provide an excellent introduction to the topic of phase change including the mathematical theory. The following research papers focus on specific issues involving phase change and may serve as useful starting points:

- F. Font, T. G. Myers, S. L. Mitchell. A mathematical model for nanoparticle melting with density change. *Microfluidics and Nanofluidics*, vol. 18, pg. 233–243, 2015.
  `https://doi.org/10.1007/s10404-014-1423-x`

- H. Kopetsch. A numerical method for the time-dependent Stefan problem in Czochralski crystal growth. *Journal of Crystal Growth*, vol. 88, pg. 71–86, 1988.
  `https://doi.org/10.1016/S0022-0248(98)90009-4`

- J. S. Langer. Instabilities and pattern formation in crystal growth. *Reviews of Modern Physics*, vol. 52, 1980.
  `https://doi.org/10.1103/RevModPhys.52.1`

- S. L. Mitchell and M. Vynnycky. Finite-difference methods with increased accuracy and correct initialization for one-dimensional Stefan problems. *Applied Mathematics and Computation*, vol. 215, pg. 1609–1621, 2009.
  `https://doi.org/10.1016/j.amc.2009.07.054`