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The effect of surface tension and kinetic undercooling on a radially-symmetric melting problem

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ABSTRACT

The addition of surface tension to the classical Stefan problem for melting a sphere causes the solution to blow up at a finite time before complete melting takes place. This singular behaviour is characterised by the speed of the solid-melt interface and the flux of heat at the interface both becoming unbounded in the blow-up limit. In this paper, we use numerical simulation for a particular energy-conserving one-phase version of the problem to show that kinetic undercooling regularises this blow-up, so that the model with both surface tension and kinetic undercooling has solutions that are regular right up to complete melting. By examining the regime in which the dimensionless kinetic undercooling parameter is small, our results demonstrate how physically realistic solutions to this Stefan problem are consistent with observations of abrupt melting of nanoscaled particles.

1. Introduction

Solidification processes are modelled by moving boundary problems, called Stefan problems, which in their most simple form involve solving the heat equation in both the solid and liquid domains subject to a so-called Stefan condition on the solid-melt interface. This condition is an energy balance that describes the manner in which latent heat is released at the interface. For classical well-posed solidification problems, we have the additional condition that the temperature u^* on the solid-melt interface is fixed to be the freezing temperature. Problems of this sort have been dealt with extensively in the literature, the results of which are reported in books such as Gupta [39] and others [6,18,22,46]. There is the analytic 'Neumann' solution in one Cartesian coordinate [6,18,22,39,46], but otherwise practically useful exact solutions are extremely rare. Of particular interest to the present study, we note that the classical radially-symmetric Stefan problem has no known exact solution, but turns out to have a rather interesting asymptotic structure in the limit of complete freezing (we shall refer to this limit as the extinction limit) [43,59,78,79]. Further formal results for this radially-symmetric problem have been generated using a variety of numerical and analytical techniques [7,21,23,32,45,64,71]. Asymptotic studies of classical Stefan problems in more than one spatial variable exist, but are less common [49,57,58,86]. From a more rigorous perspective, much attention has been devoted to proving existence and uniqueness in one dimension (see [5,36,72], for example) and higher dimensions [35,40].

An interesting and very well studied class of Stefan problems, which in their most basic form are ill-posed, arises from modelling solidification of pure substances from an undercooled melt. One-dimensional problems of this sort have solutions in which the speed of the solid-melt interface becomes infinite at some finite time [42,50,52]; in higher dimensions, the solutions can exhibit more complicated forms of finite-time blow-up, for example via the birth of cusps or corners [44,84,85]. In order to provide a physical regularisation for such ill-posed problems, we may apply the Gibbs–Thomson condition

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$$u^* = u_m^*(1 - \sigma^* \mathcal{K}^*) - \epsilon^* v_n^*, \tag{1}$$

on the interface. Here the freezing temperature (the right-hand side of (1)) is not assumed to be simply equal to the constant bulk freezing temperature, u_m^*, but instead is corrected by two regularising terms. The first, and most studied, involves surface tension σ^*, which acts to penalise regions of the interface with high mean curvature $\mathcal{K}^*$. This term can be derived using thermodynamic arguments by considering a system in equilibrium [55]. To take into account the departure from equilibrium due to the moving solid-melt interface, a kinetic correction term is required. This kinetic correction is the second regularising term in (1) and involves a parameter ϵ^*, referred to here as the kinetic undercooling parameter, multiplied by the interface's normal velocity v_n^*. The relationship between the melting temperature and the solidification rate represents an additional driving force generated by undercooled liquid near the interface [1]. Condition (1) has also been considered as a linearised version of a more complicated kinetic relationship [22,30,33]. In the past decade there have been numerous numerical studies of crystal formation using (1) with either $\epsilon^* > 0$ or $\epsilon^* = 0$, with intricate descriptions of pattern and finger formation [13,37,48,82]. Some details of existence and uniqueness for this class of Stefan problem are provided in [14,28,56].

The stability of Stefan problems with the Gibbs–Thomson condition have been examined by several authors by tracking small perturbations of solutions for problems in one spatial dimension. Results for the surface-tension only case ($\epsilon^* = 0, \sigma^* > 0$ in (1)) include the melting and freezing of a planar solid [8,90], propagation of a planar front into a supercooled liquid [54,73] and the growth of a spherical crystals [9,65]. Less attention has been paid to the kinetic undercooling only case ($\epsilon^* > 0, \sigma^* = 0$) but there exists results for planar solidification [16,17]. Lastly, for Stefan problems with the full Gibbs–Thomson condition ($\epsilon^* > 0$ and $\sigma^* > 0$), we have stability results for planar problems [25,83] and spherical problems [68,74].

The above studies on solidification also apply to melting problems since mathematically both melting and freezing problems are equivalent, the only difference arising from switching the sign of the temperature throughout. For example, the asymptotic results for the classical well posed problem of freezing a spherical ball of liquid also describe the melting of a spherical particle. Further, the results for the ill-posed crystal formation problem also apply for the ill-posed problem of melting a superheated solid (for which there are fewer examples in nature). In the present paper we shall use the language of melting, not freezing, for reasons that should become apparent, with the understanding that results hold for both cases. Furthermore, we shall continue to use the term "kinetic undercooling parameter" for ϵ^*, even though the "undercooling" arises from freezing problems, not melting problems.

It has been observed that adding surface tension (via the Gibbs–Thomson condition with $\sigma^* > 0$ and $\epsilon^* = 0$) to the classical well-posed problem of melting a spherical particle has the unexpected result of *introducing* a singularity, with the resulting problem exhibiting finite-time blow up [38,60,63]. The full two-phase problem takes into account temperature variations in both the two phases, as depicted in the schematic in Fig. 1. The problem develops an infinite temperature gradient in the inner solid phase [60,89] shortly after this inner phase becomes locally superheated (here we use the term "locally superheated" in the sense that the temperature in the solid phase is everywhere greater than the melting temperature; this feature has also been noted in [34]). Similar observations have been made for a special class of initial conditions for which the temperature profile of the outer phase is held at the spatially-dependent melting temperature $u^* = u_m^*(1 - \sigma^*/r^*)$ for all time, resulting in a one-phase problem which focuses on the inner phase [3,63]. This type of blow up, characterised by an infinite temperature gradient in the inner phase and an unbounded moving front speed, appears to be of the same nature as the finite-time blow-up of the one-dimensional Stefan problem for the freezing of a supercooled liquid [3,24,42,50].

In the present paper we are concerned with extending a particular energy-conserving one-phase version of the radially-symmetric melting problem with surface tension (i.e., with $\sigma^* > 0$ and $\epsilon^* = 0$), treated by Wu et al. [88], which also exhibits an unbounded phase boundary speed at some finite time before the particle has completely melted. Our goal is to generalise the work of Wu et al. [88] to include the full Gibbs–Thomson condition (1), with both nonzero surface tension $\sigma^* > 0$ and

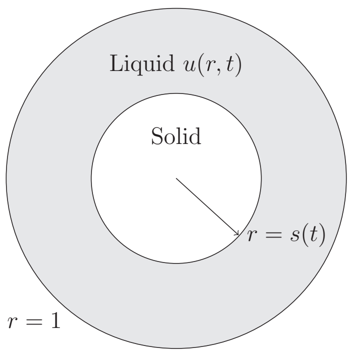

Fig. 1. A schematic of a melting particle with the dimensionless variables used in Section 2.1. The outer region (shaded) is the liquid melt layer which surrounds the inner phase: the solid core. These two phases are separated by the moving front $r = s(t)$, which propagates inwards during the melting process. It is the temperature $u(r,t)$ in the outer liquid phase that we are interested in here.