Potential Flow Interactions with Directional Solidification

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Introduction

The effect of convective melt motion on the growth of morphological instabilities in crystal growth has been the focus of many studies in the past decade. While most of the efforts have been directed towards investigating the linear stability aspects, relatively little attention has been devoted to experimental and numerical studies. Comprehensive reviews are provided by Langer (1980), Glicksman *et al.* (1988), and Davis (1990, 1992, 1993). In a pure morphological case, when there is no flow, morphological changes in the solid-liquid interface are governed by heat conduction and solute distribution. Under the influence of a convective motion, both heat and solute are redistributed, thereby affecting the intrinsic morphological phenomenon. The overall effect of the convective motion could be either stabilizing or destabilizing.

Recent investigations by Coriell *et al.* (1984), Forth and Wheeler (1989) have predicted stabilization by a flow parallel to the interface. In the case of non-parallel flows, e.g., stagnation point flow, Brattkus and Davis (1988) have found a new flow-induced morphological instability that occurs at long wavelengths and also consists of waves propagating against the flow. Other studies have addressed the nonlinear aspects (Konstantinos and Brown (1994), Wollkind and Segel (1970)).

In contrast to the earlier studies, our present investigation focuses on the effects of the potential flow fields typically encountered in Hele-Shaw cells. Such a Hele-Shaw cell can simulate a gravity-free environment in the sense that buoyancy-driven convection is largely suppressed, and hence negligible. Our interest lies both in analyzing the linear stability of the solidification process in the presence of potential flow fields, as well as in performing high-accuracy nonlinear simulations.

Linear stability analysis can be performed for the flow configuration mentioned above. It is observed that a parallel potential flow is stabilizing and gives rise to waves traveling downstream.

We have built a highly accurate numerical scheme which is validated at small amplitudes by comparing with the analytically predicted results for the pure morphological case. We have been able to observe nonlinear effects at larger times.

Preliminary results for the case when flow is imposed also provide good validation at small amplitudes.

Linear Stability Analysis

Based on the governing equations for directional solidification, as reviewed by Davis (1992), a linear stability analysis is performed for the fully transient equations. Our results agree well with the quasistationary results predicted by Mullins and Sekerka (1962).

We then consider a uniform Hele-Shaw flow parallel to the solid/liquid interface. The analysis is similar in concept to the pure morphological case as mentioned earlier, with one additional dimensionless parameter measuring the ratio of fluid velocity to the pulling speed. We arrive at a complex algebraic equation, which is solved using a Newton iteration method. This yields the instabilty growth rates and the wave propagation velocities.

Results indicate that the effect of the uniform flow is stabilizing. This agrees with the experimental findings currently being carried out by Zhang and Maxworthy at the University of Southern California. Figure 1 indicates that the larger the uniform flow (U), the smaller the bandwidth of instability. In principle, it is possible to stabilize all wavenumbers by imposing an appropriate U over the solid/liquid interface. Results also indicate that the parallel potential flow gives rise to traveling interfacial waves. These waves travel downstream and are usually on the order of one percent of the freestream velocity. Figure 2 shows the propagation velocity for different wavenumbers.

As expected, increasing values of the Sekerka number (M) destabilize the interface by increasing the bandwidth of instability. Furthermore, higher values of the surface energy parameter (R) lead to a stabilization of the higher wavenumbers.

It is worth taking a look at the underlying physics of the process. It is well known that the driving force in the instability is the concentration gradient. In the pure morphological case, steep concentration gradients exist over the crests and flat concentration gradients in the troughs. This gives rise to an intrinsically unstable situation where the crests grow faster than the troughs, thus leading into a runaway condition.

However, when a parallel potential flow is imposed on the interface, the horizontal component of the perturbation velocity plays a major role in solute redistribution. Solute is transferred from solute-rich regions over the crests to solute-impoverished regions over the troughs. This re-arrangement evens out the differences in concentration gradients and thus brings about stability. Similarly, the vertical component of the perturbation velocity picks up solute from the windward side of the interface and dumps it on the leeward side of the interface. This generates a small downstream propagation of the interface.

Nonlinear Numerical Simulations

In order to represent the linear and nonlinear phenomena accurately, it is important to employ highly accurate computational procedures. Our numerical approach employs a high-order compact finite difference method (Lele 1992) in the pulling direction. In the compact finite difference

scheme, we employ discrete approximations of central kind of sixth order accuracy away from the boundaries. At the boundaries, one-sided stencils of third order accuracy are used. A Fourier spectral method (Gottlieb and Orszag 1977) is employed in the periodic direction. The combination of these two schemes allows for the evaluation of highly accurate spatial derivatives. The calculation is advanced in time by means of a low-storage third order Runge-Kutta scheme (Wray (1991)). This combination, in conjunction with an analytical mapping leads to excellent accuracy.

To validate our numerical scheme, we performed test calculations to measure the growth of small perturbations in time for a pure morphological case. With a typical choice of 8 Fourier modes in the periodic direction and 129 finite difference grid points in the pulling direction, and for a wide range of parameters such as surface energy, stability parameter, segregation co-efficient, our results agreed to within 1% of the analytically predicted growth rates obtained from the linear stability analysis.

Subsequently we carried the simulations to longer times, where nonlinearities come into effect. We have been able to follow the interfacial growth rates to times when the depth of the grooves is comparable to their wavelengths. At late times, the interface is dominated by those wavelengths for which linear theory predicts the largest growth rates. This is indicated in Figure 3.

The next step was to incorporate the flow field into the equations. The velocity distribution is calculated by employing a boundary element technique. With this technique, one can easily simulate a potential flow. Preliminary results of interfacial growth rates at small amplitudes show excellent agreement with those predicted analytically by the linear stability. Interfacial waves are observed traveling downstream, as predicted by the linear stability analysis.

The boundary element technique mentioned above gives us the opportunity to explore a wide variety of flow configurations. Various spatial distributions of sources and sinks can be made to simulate different flow fields in order to investigate opportunities for suppressing the instabilities.

Our numerical simulations have been carried out on CRAY T90 at the San Diego Super Computing facility at the University of California, San Diego.
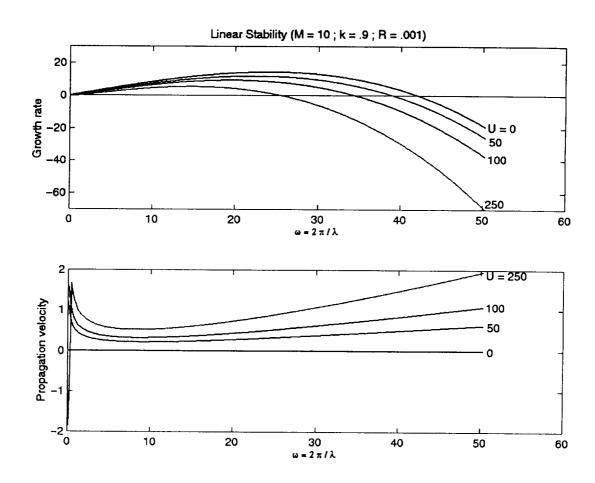
NOTE : In the following figures,

R (surface energy parameter) $= - [2T_M\gamma Vk] / [mLDc_\infty(1-k)]$

M (Stability parameter) $= [m(k-1)/k].[c_\infty V / DG] = mG_c / G$

K (Segregation co-efficient) $= c^- / c^+$

U (non-dimensional velocity) $=$ dimenstional velocity / pulling speed $= U^* / V$
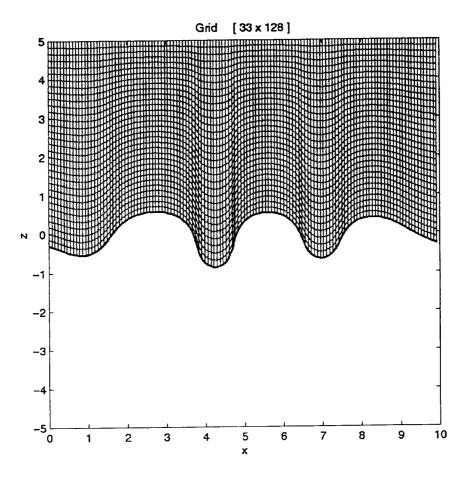
Figures 1-2

Grid [33 x 128]

Figure 3

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