On the effects of furnace gradients on interface shape during the growth of cadmium zinc telluride in EDG furnaces

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Abstract

Numerical simulations are performed to assess cadmium zinc telluride (CZT) interface shape dependency on thermal gradients in electrodynamic gradient (EDG) furnaces. Results explain how larger furnace gradients in these systems tend to flatten the shape of the solid–liquid interface. Convection dominates heat transfer through the melt, and mixing acts to radially homogenize the melt temperature field. These features do not significantly change with gradient conditions. In contrast, changing the rate of heat conduction through the solid, notably via changes to the furnace profile adjacent to the crystal, have an overriding influence on the interface shape. Increased gradients increase the ability for latent heat to be transported axially through the crystal and flatten the interface; however, the sensitivity of the shape of the interface to details of the furnace heating profile decreases as overall gradients increase. The engineering of the interface shape in these systems via subtle control of the furnace should be possible, but rational design changes will require the insight obtained from predictive models.

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1. Introduction

The macroscopic shape of the solid–liquid interface in vertical Bridgman systems has long been of great interest for assessing the likelihood of growing high-quality crystals. For example, an interface curved so that it is concave with respect to the melt is more likely to propagate adverse interface–ampoule interactions inward toward the crystal, potentially resulting in twinning or higher dislocation density [1]. Whereas, an interface growing convex to the melt minimizes the potential for defects or spurious crystals nucleated at the ampoule wall to propagate toward the bulk crystal [1,2]. In addition, the limit of a flat-interface shape is consistent with very low radial temperature gradients and nearly constant axial temperature gradients near the interface, thereby minimizing thermal stresses [3].

In the absence of kinetic effects, which is often the case during the melt growth of semiconductors, the interface shape is determined by the melting-point isotherm which, in turn, is set by heat transfer. The effects of heat transfer on interface shape have been studied in classical analyses of Bridgman crystal growth. Chang and Wilcox [4] developed an approximate heat transfer analysis for an idealized system with no melt convection and the same properties in both phases. Their analysis predicted that the shape of the
interface depended solely on its axial location in the furnace. They postulated that the qualitative effects of buoyant convection in the melt would tend to make the interface more concave, consistent with the action that a greater melt thermal conductivity would have on interface shape. Sen and Wilcox [5] furthered this analysis by adding an ampoule to the system, using numerical techniques to solve the resulting heat transfer problem. They showed that the ampoule conductivity should be close to the conductivities of the melt and crystal to minimize radial temperature gradients within the system. Fu and Wilcox [6] showed that adding an insulating zone (the so-called adiabatic zone) between the hot and cold zones of the furnace flattened isotherms in the interface region and decreased the sensitivity of the interface shape to perturbations. Naumann [7] developed a two-dimensional analytical model of heat transfer in Bridgman crystal growth. He studied the effects of varying different operating parameters (e.g., adiabatic zone length and ampoule pull rate) on the axial gradients in the system as well as on the melting-point isotherm shape and position. Naumann and Lehoczky [8] illustrated the effect of unequal melt and crystal thermal conductivities on the shape and position of the melt/crystal interface. Chin and Carlson [9] also showed that interface curvature was very sensitive to the ratio of crystal to melt conductivities.

The effects of conductivity mismatch near the solid–liquid interface were further investigated by Jasinski and Witt [10] in their analysis of the growth of semiconductor crystals. They demonstrated the strong influence of ampoule thermal mass on the thermal field and the interface effect, where the thermal conductivity mismatch among melt, crystal, and ampoule coupled with the release of latent heat resulted in significant interface deflection at the ampoule wall. Brandon and Derby [11] demonstrated how the effects of internal radiation in the crystal could amplify such an interface deflection by modifying the heat fluxes near the ampoule wall, terming this the radiative interface effect. Adornato and Brown [12] studied the effect of different furnace profiles and ampoule materials on interface shape and favorably compared their results to the growth experiments of Wang and Witt [13]. Dutta et al. [14,15] were able to grow GaSb crystals with a planar interface under certain ratios of furnace temperature gradient to ampoule pull rate. Similarly, Udayashankar et al. [16] calculated the critical ratio for flat-interface growth of GaInSb from their growth experiments. Arafune et al. [17] found that decreasing the thermal gradient decreased interface concavity over the growth run of InSb grown in an horizontal Bridgman furnace.

Nearly all of the preceding theoretical and experimental works studied the growth of semiconductor materials whose melts exhibit large thermal conductivities. Such materials are characterized by dimensionless Prandtl numbers much less than unity, typically $Pr \sim \mathcal{O}(10^{-3})$, where $Pr \equiv \nu/\alpha$, with $\nu$ representing the melt kinematic viscosity and $\alpha$ its thermal diffusivity. In such systems, the effect of melt convection on heat transfer is relatively minor, so the balance of heat flows that determines the shape of the solid–liquid interface primarily involves latent heat release and conductive fluxes in both the melt and crystal.

Here, we are interested in how the solid–liquid interface can be effectively modified during the vertical Bridgman growth of cadmium zinc telluride (CZT), a II–VI semiconductor ternary alloy with properties that make it desirable for radiation detection applications [18]. Cadmium telluride and its alloys have unusual thermophysical properties which make their growth very different from other semiconductor crystals [19]. Notably, cadmium telluride has a high melt viscosity and a low melt thermal conductivity, leading to a Prandtl number of $Pr \approx 0.4$, much higher than typical. This behavior results from a liquid phase that is semiconducting [20], rather than metallic, as are the melts of more common electronic materials such as silicon and gallium arsenide. What this means is that convective heat transfer through the molten phase of CZT is much more important than conduction heat transfer under typical growth conditions. In such systems, the conditions affecting interface shape are a balance among latent heat, conduction in the solid, and convection in the melt. Strategies known to modify interface shape for classical semiconductor crystal growth may be rendered ineffectual for CZT growth because of this importance of convective heat transfer in the melt.

Prior analyses have shed some light on interface shape during CZT grown via Bridgman processes. Kupparao et al. [21,22] analyzed a 75 mm diameter vertical Bridgman system for CZT and found that convection levels in the melt were intense enough to result in a relatively flat interface away from the ampoule. Later computations [23] showed that furnace design could control the interface shape, even made convex toward the melt, during early growth through the cone region of the ampoule, when convective effects were not strong. Yeckel and Derby [24,25] showed how transient flows driven by the accelerated crucible rotation technique (ACRT) affected mass transfer and interface shape in both large- and small-scale CZT Bridgman systems. Yeckel et al. [26] considered three-dimensional effects during small-scale, low-gradient CZT growth and found that interface shape could be affected by asymmetric heating by the furnace. Yeckel and Derby [27] also considered the effects of a submerged heater on shaping the interface during CZT growth. Pandy et al. [28] developed a sophisticated model of CZT grown via a low-pressure, electrodynamic gradient (EDG) freeze furnace used by eV Products, Inc. This approach employed a global furnace model coupled with a local model of the growing crystal to achieve a self-consistent solution of the entire growth system.

A general goal of this study is to examine how furnace gradients affect the solid–liquid interface of CZT grown in a vertical Bridgman system. We also seek to reconcile the difference in interface shapes predicted for the low-pressure
EDG system and the high-pressure EDG process (HP-EDG), also being developed by eV Products, Inc., by Szeles et al. [18]. For the nominal growth conditions in the low-pressure system considered by Pandy et al. [28], significant interface deflection is predicted, while modeling of the HP-EDG system by Reed et al. [29] predicts a relatively flat interface. The computational approach taken here aims to connect these seemingly disparate results and investigate more general phenomena affecting interface shape during CZT growth.

2. Model formulation

Our approach endeavors to assess the effects of modifying the furnace design on CZT interface shape in the EDG systems used by eV Products, Inc. We first employ the multi-scale, coupled model discussed by Pandy et al. [28] to obtain a base case corresponding to conditions employed in the low-pressure EDG system. The challenge is then to sensibly stretch the base case model to represent conditions present in the larger-diameter and higher-gradient HP-EDG system modeled by Reed et al. [29]. While efforts to improve the robustness and efficiency of the coupled approach are underway [30,31], its utilization remains rather involved and computationally expensive. Here, we employ a simpler modeling strategy for assessing changes in behavior from the low-gradient EDG system to the higher-gradient HP-EDG system. We start from the base state, then we transform the furnace temperature profile using simple scaling factors and solve for the resulting changes in heat transfer, melt convection, and interface shape in the system. More details are provided below.

2.1. Base-case model

The process model for our base case is made up of two parts, the global model comprised of the furnace, and the local model consisting of the melt, crystal, and the solid–liquid interface. A schematic diagram of the meridional views of the two-dimensional, axisymmetric model is shown in Fig. 1. The global model is CrysVUN, a code developed by Müller et al. [32,33] at the Crystal Growth Laboratory of the Fraunhofer Institute IISB. CrysVUN readily depicts radiation heat transfer in high-temperature systems. It employs the finite volume method on an unstructured grid to discretize the furnace heat transfer equations, solved via a quasi-Newton iterative method. For the local model, we use our own code, Cats2D [34], a finite element model that computes heat transfer (conductive and convective), melt flow, and interface shape and location using Newton’s method. In Cats2D, elliptic mesh generation is used to discretize the problem domain, with a mixed basis of biquadratic elements with a linear pressure basis. The mesh deforms to track the location of the solid–liquid interface along a prescribed set of element edges.

The global and local models share a common boundary as seen in Fig. 1. Energy is conserved along the boundary via strict continuity of the temperature field and normal heat fluxes,

\[ T_{\text{global}}(x) = T_{\text{local}}(x), \quad (1) \]

\[ q_{\text{global}}(x) = q_{\text{local}}(x), \quad (2) \]

where \( x \) denotes the boundary coordinates, \( T \) is temperature, and \( q \) is the heat flux normal to the boundary. Obtaining a self-consistent solution of these coupled models that rigorously satisfies both Eqs. (1) and (2) is not an easy task and is dependent upon the details of how iterations are conducted between the two models. Our current implementation employs a Block Gauss–Seidel iterative approach to solve for quasi-steady-state solutions and is described in Refs. [28,30].

2.2. Furnace design

We desire to stretch the conditions of the base case to represent different furnace configurations under higher gradients. We also wish to assess the sensitivity of interface
shape to furnace changes. To do this, we take the self-consistent solution computed by the coupled model described above as our base case and assume that changes to the design of the furnace can be represented by slight modifications of the base-case temperature along the coupling boundary, namely the exterior domain boundary indicated in Fig. 1(b). With this approach, we are able to solve the local model, Cats2D, independently, and different scenarios are computed quickly and efficiently.

The temperature boundary conditions are applied to the local model via the following algebraic stretching of the self-consistent, base-case temperature profile:

\[ T(x) = \alpha (T_o(x) - T_i) + T_i, \]

where \( \alpha \) is the gradient magnification factor, \( T_o \) is the temperature along the shared boundary calculated by the coupled model, \( T \) is the new temperature, and \( T_i \) is the interfacial temperature. This approach generates a family of temperature profiles that exhibit increasing axial gradients as the gradient magnification factor, \( \alpha \), is increased from unity. The profile of the temperature along the outer vertical boundary of the local model is shown in Fig. 2 for a number of different values of \( \alpha \). The axial temperature gradient near the interface is approximately \( 2 \) K/cm for the base case; the axial gradients for the other cases then correspond to approximately \( 2\alpha \) K/cm. As \( \alpha \) is increased from the base case, corresponding to a solution for the low-pressure EDG system, the model solutions are expected to approach those of the larger, larger-gradient HP-EDG system.

We also desire to assess the general idea of how the interface shape may be affected by changing the furnace heating profile. This is accomplished by adding the following perturbation to the furnace profile:

\[ dT = \beta \left( \frac{(z_i/2)^2 - (z - z_i/2)^2}{(z_i/2)^2} \right), \]

where \( \beta \) is the perturbation maxima, \( z \) is the axial position with respect to the bottom of the crystal, and \( z_i \) is axial position of the interface along the boundary. We add this perturbation to the temperature profile only below the melting-point temperature, so that the new boundary condition around the domain is

at \( z > z_i \): \( T = T \),

at \( z \leq z_i \): \( T = T + dT \),

where \( T \) is the temperature from Eq. (3). Therefore, the temperatures along the melt are unaffected. A positive value of \( \beta \) corresponds to additional heating supplied to the crystal. Fig. 3 shows a representation of how the perturbation \( \beta \) affects the temperature boundary condition.

3. Results and discussion

Physical properties employed to represent CZT are listed in Table 1 along with the base-case operating parameters. The accuracy of the numerical solution was tested by comparing the solution for steady-state flow at \( \alpha = 10 \), the strongest flow case, for different mesh discretizations of the melt phase. Three meshes comprising 1400 elements, 2400 elements, and 4000 elements were employed. When the finest mesh solution was used as a benchmark, the worst-case error in predicting the magnitude of the velocity along a radial line through the melt near the solid–liquid interface was 2.1% for the 1400-element solution and 1.1% for the 2400-element solution. The worst-case error for computing the velocity along a vertical line drawn midway between the centerline and ampoule wall was 39.4% for the 1400-element solution and 4.1% for the 2400-element solution. For the purposes of this study, we concluded that the 2400-element mesh (representing a total of 28,765 degrees of freedom) was of sufficient accuracy. A full Newton step, dominated by the cost of a single factorization of the
Table 1
Physical properties (from Ref. [21]), system dimensions, and operating parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Phase</th>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal conductivity</td>
<td>Melt</td>
<td>(k_m)</td>
<td>(1.085 \times 10^{-2})</td>
<td>W/cm K</td>
</tr>
<tr>
<td></td>
<td>Solid</td>
<td>(k_s)</td>
<td>(9.07 \times 10^{-3})</td>
<td>W/cm K</td>
</tr>
<tr>
<td>Density</td>
<td>Melt</td>
<td>(\rho_m)</td>
<td>5.68</td>
<td>g/cm(^3)</td>
</tr>
<tr>
<td></td>
<td>Solid</td>
<td>(\rho_s)</td>
<td>5.68</td>
<td>g/cm(^3)</td>
</tr>
<tr>
<td>Heat capacity</td>
<td>Melt</td>
<td>(C_{pm})</td>
<td>0.187</td>
<td>J/g K</td>
</tr>
<tr>
<td></td>
<td>Solid</td>
<td>(C_{ps})</td>
<td>0.160</td>
<td>J/g K</td>
</tr>
<tr>
<td>Heat of fusion</td>
<td></td>
<td>(\Delta H_i)</td>
<td>209.2</td>
<td>J/g</td>
</tr>
<tr>
<td>Melting point</td>
<td></td>
<td>(T_{mp})</td>
<td>1365</td>
<td>K</td>
</tr>
<tr>
<td>Thermal expansivity</td>
<td>Melt</td>
<td>(\beta_T)</td>
<td>(5.0 \times 10^{-4})</td>
<td>K</td>
</tr>
<tr>
<td>Kinematic viscosity</td>
<td>Melt</td>
<td>(\nu)</td>
<td>(4.15 \times 10^{-3})</td>
<td>cm(^2)/s</td>
</tr>
<tr>
<td>Inner ampoule radius</td>
<td></td>
<td>(R)</td>
<td>4.625</td>
<td>cm</td>
</tr>
<tr>
<td>Domain height</td>
<td></td>
<td>(H)</td>
<td>8.85</td>
<td>cm</td>
</tr>
<tr>
<td>Ampoule translation rate</td>
<td>(V)</td>
<td>0.6336</td>
<td>cm/s</td>
<td></td>
</tr>
</tbody>
</table>

Jacobian matrix, took approximately 19 s on a PC with a 2.0 GHz processor speed. Typically, four to six Newton iterations were needed to obtain a fully converged solution.

3.1. Effect of axial gradients on melt flow and interface shape

We consider the response of heat transfer in the melt and crystal, flow in the melt, and interface shape as the axial gradient is increased in this system. The quasi-steady-state model solutions correspond to a point approximately halfway through the growth run. Fig. 4 shows melt streamlines, temperature isotherms, and interface shapes for the different cases with the system centerline along the left-hand side. Dashed streamline contours indicate clockwise rotation, and solid contours indicate anti-clockwise rotation. The base case for \(\alpha = 1\) shows a clockwise circulation enclosing two vortices, one near the solid–liquid interface and one near the free surface. This flow is driven by two dominant effects. First, the release of latent heat from solidification causes the center of the melt to be warmer than the solid–liquid interface, driving a clockwise circulation. In the melt away from the solid–liquid interface, the flow is strong enough to effectively flatten the temperature isotherms, leading to a temperature field that is almost one dimensional (only a thin boundary layer is present along the ampoule wall). The solid–liquid interface bows significantly to allow for radial conduction of heat through the solid.

With an increased axial gradient applied to the system, cases (b)–(f) in Fig. 4, the total amount of heat flowing through the charge increases and the axial gradients through the system increase. The intensity of the flow increases, as shown in Fig. 5, where the maximum magnitude of the streamfunction, \(\psi_{max}\), which represents the total volumetric circulation of the melt, is plotted as a function of \(\alpha\). The flow strength scales asymptotically with \(\alpha^{1/2}\), as indicated in the figure by the functional curve fit of \(\psi_{max}\). This form is consistent with a balance of dominant forces of inertia (which is proportional to the velocity squared) and buoyancy (linearly proportional to the temperature gradient) for these nonlinear melt flows.

Interestingly, and perhaps counter-intuitively, even while the overall flow strength in the melt increases with the applied thermal gradient, the strength of the flow vortex near the interface decreases as \(\alpha\) is increased. An explanation is provided by plotting the radial temperature profile near ampoule wall and slightly above the interface, as shown in Fig. 6. Here, it is evident that the temperature gradient near the wall does decrease as the applied axial gradient is increased, leading to a simultaneous reduction of the buoyant force driving the lower vortex as \(\alpha\) is increased. The profiles for \(\alpha = 5\) and 10 are not shown in Fig. 6, since the radial gradient actually reverses near the wall for these cases. This effect opposes the clockwise circulation of the lower cell, eventually leading to a weak counter-clockwise flow adjacent to the interface for the \(\alpha = 10\) case.

The same interactions responsible for the decreasing radial melt gradient and the weakening lower flow cell, discussed above, alter the relative balance of axial and radial heat fluxes along the solid–liquid interface. There is a notable flattening of the interface shape with increases in \(\alpha\). Significantly, the progression of interface shapes displayed by these calculations captures the qualitative change between the low-pressure EDG system computed by Pandy et al. [28] and the HP-EDG system modeled by Reed et al. [29]. Indeed, the interface shape of cases \(\alpha = 2\) and 3 are quite similar to that predicted in Refs. [18,29] for the HP-EDG system. For yet higher gradients, the interface becomes even flatter.

We probe the causes of the flattening of the interface with increased gradient by concentrating on the case of \(\alpha = 2\) and performing two additional computations. Fig. 7(a) shows the original base case corresponding to \(\alpha = 1\). Next to it, in Fig. 7(b), is the case of \(\alpha = 2\), showing a flatter interface and a weaker flow in the melt near the interface. Fig. 7(c) shows a new computation where the magnification factor of \(\alpha = 2\) is applied only to the melt. This is carried out by applying the boundary condition specified by Eq. (3) with \(\alpha = 2\) for \(T \geq T_i\), and for \(\alpha = 1\) for \(T < T_i\). With larger temperature gradients in the melt, the flow is everywhere increased in strength, including the vortex near the interface. This increased flow drives warmer melt toward the center of the interface and slightly increases its deflection from the base case. Fig. 7(d) displays the result when only the crystal profile is magnified, namely \(\alpha = 1\) is used for \(T > T_i\), and \(\alpha = 2\) is applied for \(T \leq T_i\). In this case, the interface is dramatically flattened and the melt flow near the interface is significantly diminished.

Clearly, the effect of changing the temperature gradient applied to the crystal is far more important than changing...
the gradient applied to the melt. This underscores the balance among heat flows in this system that are dominated by convection in the melt, conduction in the crystal, and latent heat at the interface. Changing overall system gradients, such as achieved by scaling the entire temperature profile in the cases shown in Fig. 4, does not markedly change the nature of heat transfer through the melt, since it is dominated by convective effects. However, allowing for greater temperature gradients through the crystal dramatically affects conductive heat flows, especially in the axial direction. Latent heat, released at the growing interface, can only flow down a temperature gradient. If the axial flux of heat through the crystal is insufficient, the interface must deflect to allow some of the latent heat to flow radially outward. Promoting a greater axial heat flux by larger temperature differences along the crystal more readily accommodates the axial flow of latent heat, thereby flattening the interface.

3.2. Effect of furnace perturbations on interface shape

Finally, we wish to address the possibility of modifying the shape of the interface by slight changes in the furnace heating profile, an action that is made feasible by the design of the furnace.
of multiple-zone EDG furnaces. We specifically consider the response of the interface shape to the furnace perturbation previously described by Eq. (4) and represented in Fig. 3. Fig. 8 shows the shape of the interface for various values of the perturbation parameter, \( \beta \), for the case of the low axial gradient, \( \alpha = 1 \), and the high axial gradient, \( \alpha = 10 \). Applying this perturbation to the temperature field scarcely changes flows and heat transfer through the melt. However, increasing the value of \( \beta \) increases the temperature in the crystal underneath the interface, thereby decreasing the ability for conduction to dissipate the latent heat through the crystal. To accommodate the reduced conductive fluxes, the interface deflects even more from its original position. Interestingly, a negative value of \( \beta \) has the converse effect. By improving the driving force for conduction out of the crystal, latent heat is more easily removed and the interface flattens.

The two cases clearly demonstrate that the interface is more sensitive to the furnace perturbation under lower gradient conditions, Fig. 8(a), than at higher gradients, Fig. 8(b). In fact, the absolute movement of the centerline interface position caused by changing the value of \( \beta \) is over 20 times greater for the low-gradient system compared to the high-gradient case.

4. Concluding remarks

We have employed a numerical model to assess how furnace design affects the growth of CZT crystals via vertical Bridgman processes. Our approach is based on the results of the multiple-scale, self-consistent model of Pandy et al. [28] and an approach devised to scale this rigorous computation in a cost-effective manner to represent a range of conditions spanning from eV Products’ low-pressure EDG system to their larger, higher-gradient HP-EDG system [18]. With this modeling approach, we also assess the effects of perturbations to the thermal profile on interface shape under low- and high-gradient growth conditions.

Our results show that the different interface shapes of the low-pressure and high-pressure growth systems is explained by a continuous evolution from a significantly deflected shape [28] to a much flatter shape [29] that is driven by the temperature gradients in the system. The physical mechanism behind this evolution is explained by the balance among heat fluxes through the melt (dominated by convection) and crystal (by conduction only) and, especially, the heat released at the solid–liquid interface by phase change (latent heat). Interestingly, changing the
Gradient in the melt had a relatively minor effect on the system, since radial heat transfer is dominated by strong, nonlinear flows and convective mixing in these high-Prandtl-number liquids. Of overriding importance in these systems is heat conduction through the crystal, which is strongly affected by the temperature profile of the furnace below the melting point. Interface flatness is primarily determined by the ability of latent heat to be conducted away from the interface, through the crystal, in the axial direction. If axial conduction is too little, as is the case when gradients are small, the interface deflects so that radial conductive fluxes can dissipate latent heat. On the other hand, a higher applied gradient promotes the axial conduction of latent heat, and the interface flattens. This result is exactly as computed by Kuppurao et al. [23], where the relative balance of axial and radial fluxes, as affected by the design of the ampoule support, was shown to affect interface shape of CZT in the cone region of the ampoule.

Consistent with these mechanisms, our results also demonstrated that small changes to the furnace profile will have a stronger effect on changing the interface shape in lower-gradient systems. Here, small perturbations to the temperature profile applied to the crystal were able to move the interface, but this effect was only significant in the low-gradient system.

The results of this study do not point to any obvious strategies to improve CZT growth in vertical Bridgman systems. On the one hand, higher-gradient conditions yield a flatter interface, which is arguably better than a more deflected shape. However, only low-gradient growth allows for the possible engineering of the interface shape by furnace design changes. Indeed, the ability to specify different furnace inner bore temperature profiles is one of the advantages of multiple-zone EDG furnaces, yet the fine tuning of such profiles will require considerable insight. We believe that the best path for improving growth conditions is via the use of rigorous, predictive models for process design and optimization. Our work to develop such approaches is ongoing [28,30,31].

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References
