CONVECTIVE HEAT AND MASS TRANSPORT IN NOVEL BRIDGMAN CONFIGURATIONS FOR CADMIUM ZINC TELLURIDE GROWTH

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Summary We present transport models of two novel vertical Bridgman (VB) configurations used to grow cadmium zinc telluride. A top-seeded configuration has a destabilizing temperature gradient in the melt. The flows in this configuration are far more intense than occur in the stabilized bottom-seeded VB configuration, with better mixing and reduced radial segregation. An alternative is a bottom-seeded VB system with submerged heater, which gives superior control of interface shape, but which has poor lateral mixing.

INTRODUCTION

High-quality, crystalline cadmium zinc telluride ($\mathrm{Cd_{1-x}Zn_xTe}$, hereafter referred to as CZT) will enable the continued development of sensitive, portable gamma radiation detectors [1]. A major obstacle to the mass production of such detectors at moderate cost is the lack of availability of high-quality CZT crystals. The application of conventional crystal growth technology has thus far been unable to reliably produce such material in a quantity sufficient to meet demand; current growth processes based on the vertical Bridgman technique have been plagued by low yields due to crystalline defects, crack formation, compositional inhomogeneity, and inclusion formation [2]. These materials problems might be overcome by the development of different growth processes, but the incentive for crystal growers to make radical changes in growth equipment and methods using experimental trial and error is low, due to a combination of high cost and high risk. Under these circumstances, high-fidelity computer modeling provides an ideal tool to explore the feasibility and benefits of new crystal growth processes.

Problems in CZT growth can be attributed to unfavorable interface shape (concave rather than convex [3]), thermal stresses (CZT has a low critical-resolved shear stress [4]), and morphological instability (small deviations from stoichiometry have a large effect on the melting temperature of CZT [2]). Convective heat and mass transfer play a defining role in all these areas, and thus are intimately linked to growth morphology and crystal structure in growth of CZT. We are presently investigating two novel systems for vertical Bridgman growth of CZT that operate in substantially different heat and mass transport regimes to determine whether these systems can be used to improve mixing and interface shape control. The systems are a top-seeded configuration which has a destabilizing temperature gradient in the melt, and a bottom-seeded configuration with a supplementary heater submerged into the melt. The top-seeded configuration is characterized by excellent mixing due to intense buoyant flow, but has no active means of interface shape control. The submerged heater system is characterized by improved interface shape control, but has less intense mixing. We have constructed transport models of these configurations that account for fluid flow, heat and mass transport, and that use a self-consistent approach to calculate interface shape and velocity.

DESTABILIZED VERTICAL BRIDGMAN CONFIGURATION

In the conventional bottom-seeded Bridgman configuration, the crystal is situated so that it lies below the melt. In this configuration, cooler, more dense portions of the melt underlie warmer, less dense regions resulting in an inherently stable configuration. In the top-seeded approach shown in Fig. 1a, the situation is the opposite, with less-dense, warm fluid tending to displace the overlying denser, cool liquid adjacent to the crystal, resulting in an overturning flow. This destabilizing characteristic of the top-seeded configuration results in intense buoyant flows that can significantly improve mixing within the melt and reduce radial segregation. Fig. 1b compares radial segregation in stabilizing vs. destabilizing configurations [5]. Radial segregation, expressed as the percentage $(c_{max} - c_{min})/c_{max}$ along a radial slice, is decreased by a factor of 5 or more in the destabilizing configurations. This result is explained by strong flows which exist near the melt-crystal interface in the destabilizing configurations. These results are computed for a doped-semiconductor system (tellurium-doped indium antimonide) but we expect similar convective effects to occur in CZT growth.

STABILIZED VERTICAL BRIDGMAN CONFIGURATION WITH SUBMERGED HEATER

The submerged heater method (SHM) [6], a variation on the Bridgman method in which a supplementary heater is submerged into the melt, is illustrated in Fig. 2a. The heater provides increased control over the thermal environment, allowing manipulation of the melt-crystal interface shape to achieve a slightly convex interface, which reduces thermal stresses and suppresses propagation of crystalline defects. Zone-leveling, in which the regions of melt above and below the heater are loaded with different chemical compositions of starting materials, can be used to achieve more uniform chemical composition, but only if the gap width between interface and heater can be held nearly constant. Fig. 2b and c show results for thermal profiles, flow, and interface shape in quartz vs. graphite ampoules. The different ampoule materials have a dramatic effect on heat transfer, particularly the time-evolution of the heater-interface gap. Long thermal transients in this system suggest that active control of the gap width will be necessary to achieve the desired objectives. Notably, lateral

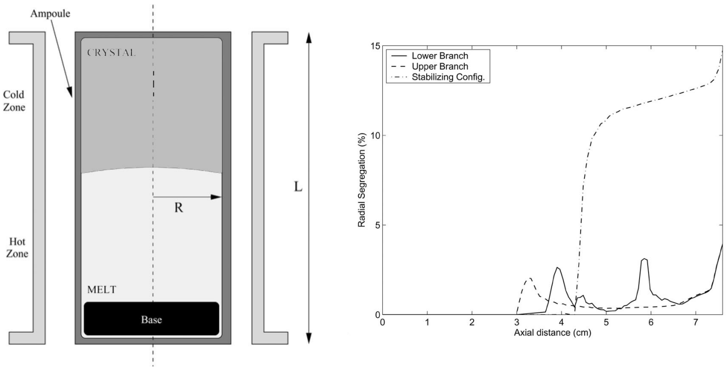

Figure 1. *Left:* Schematic diagram of the destabilizing vertical Bridgman growth configuration. *Right:* Percentage radial segregation in the grown crystal as a function of axial position; from [5]. Curves for the destabilizing configuration cases are denoted by “Lower Branch” and “Upper Branch.”

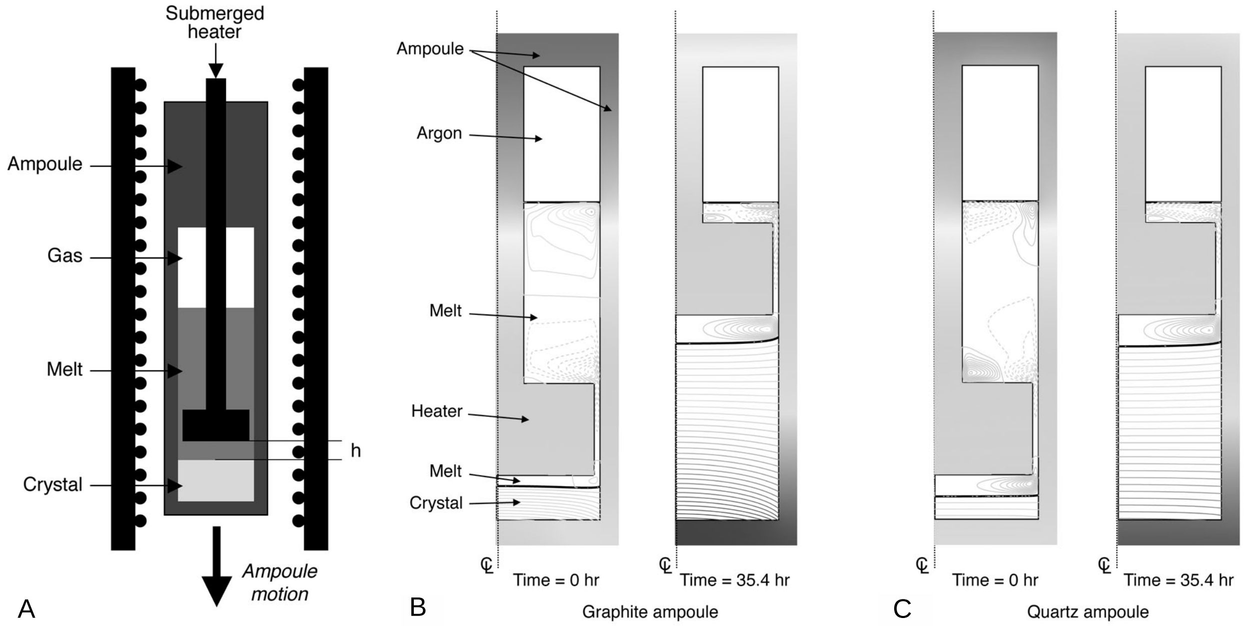

Figure 2. (a) Schematic diagram the stabilizing vertical Bridgman configuration with submerged heater. Temperature contours, streamlines, and interface shape (b) in graphite ampoule and (c) in quartz ampoule.

mixing is poor in this system; rotating the heater or ampoule to drive convection in the gap may be necessary to adequately control radial segregation.

CONCLUSIONS

Results from our computer simulations will be used to evaluate two novel vertical Bridgman designs, one a destabilized configuration, the other a submerged heater system, based on interface shape, morphological stability, segregation behavior, and thermal stresses.

References

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