564e Analysis of an Industrial Electro-Dynamic Gradient Process for Czt Growth

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Cadmium zinc telluride (CZT) is a promising material for application to a new generation of portable, sensitive, room-temperature gamma-ray detection devices. However, the growth of this material is plagued by a host of problems that have thus far been difficult to address via experimentation alone. Experiments coupled with numerical models promise to advance growth technology and understanding at a much more rapid pace.

In this paper we present our efforts to model an industrial electro-dynamic gradient freeze (EDG) furnace that is used to grow large CZT crystals by eV Products, Inc. First, we present simplified, two-dimensional (planar), transient simulations to study segregation of zinc during growth under various degrees of ampoule tilting. Ampoule tilting breaks the symmetry of the underlying system and dramatically changes the nature of buoyant flows in the melt. These changes also affect the shape of the growth interface and the segregation of zinc throughout the grown crystal. Interestingly, while the tilted ampoule cases studied here show little difference in vertical segregation, they show noticeable improvement of lateral segregation for specific angles, suggesting that intentional tilting may be beneficial. Next, we present simulations from a more detailed analysis in which a global model, CrsyVUn, that computes high-temperature, furnace heat transfer, is coupled with a local model, Cats, that solves for heat transfer, incompressible melt flow, and melt-crystal interface shape. These models are solved using an iterative scheme to compute a self-consistent solution. Model results are compared with experimental measurements, and the insight gained from modeling is discussed. Of particular interest is how different growth strategies are predicted to impact the shape of the crystal interface.