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Multiscale Modeling of Crystal Growth and Microstructural Evolution of CdZnTe[1]

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Crystal growth models and modeling tools for CdTe and CZT along with experimental melt-growth data will be presented and discussed. The emphasis will be on creating a multiscale-modeling framework that can be applied to solve portions of the crystal quality and reproducibility problem of CZT crystals grown for high-resolution radiation detectors. The growth models and methods include ab initio models of CdTe, ab initio molecular dynamics (MD) models CdTe, MD of solidification of CdTe, equilibrium growth defects in CdTe, and development of coarser-scale microstructural evolution models using phase field methods. These model and theory results will be discussed in terms of designing a multiscale approach to two relevant problems in CZT crystal growth, namely solid-liquid interface (SLI) stability and concurrent defect generation in the hot but cooling CZT solid. This dovetails with recent experimental research focused on the growth of CdTe from Te-rich melts with an emphasis on SLI instability. Experimental data on SLI instabilities will be featured as well as results of transmitted IR data on Te-particle distributions in as-grown CZT. A new mechanism of Te-particle genesis and spatial arrangement in CdTe and CZT is discussed in terms of a Rayleigh instability mechanism coupled with crystallographic SLI instabilities during growth. However, there are gaps in our capabilities at every length and time scale, plus gaps in building coarse-grained models from fine-scale models, in statistical representations of complex equilibria, and in understanding the complexities of solidification in ternary alloy systems where coupled thermal, concentration, stress, liquid flow, and SLI morphological fields exist. The talk concludes with an assessment of methods and approaches to address desired models and simulations of CZT solidification from the melt.

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