



University
of Victoria

Graduate Studies

Notice of the Final Oral Examination
for the Degree of Doctor of Philosophy

of

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MASc (University of Victoria, 2009)

BEng (University of Victoria, 2006)

“Simulation and Growth of Cadmium Zinc Telluride from Small Seeds by the Travelling Heater Method”

Department of Mechanical Engineering

Wednesday, June 8, 2016

10:00 A.M.

Engineering Office Wing

Room 430

Supervisory Committee:

Dr. Sadik Dost, Department of Mechanical Engineering, University of Victoria (Supervisor)

Dr. Peter Oshkai, Department of Mechanical Engineering, UVic (Member)

Dr. Tom Tiedje, Department of Electrical and Computer Engineering, UVic (Outside Member)

External Examiner:

Dr. Ziad Saghir, Department of Mechanical Engineering, Ryerson Polytechnic University

Chair of Oral Examination:

Dr. Joan Warf-Higgins, School of Exercise, Science, Physical and Health Education, UVic

Abstract

The semiconducting compounds CdTe and CdZnTe have important applications in high-energy radiation detectors and as substrates for infrared devices. The materials offer large band gaps, high resistivity, and excellent charge transport properties; however all of these properties rely on very precise control of the material composition. Growing bulk crystals by the travelling heater method (THM) offers excellent compositional control and fewer defects compared to gradient freezing, but it is also much slower and more expensive. A particular challenge is the current need to grow new crystals onto existing seeds of similar size and quality. Simulations and experiments are used in this work to investigate the feasibility of growing these materials by THM without the use of large seed crystals. A new fixedgrid, multiphase finite element model was developed based on the level set method and used to calculate the mass transport regime and interface shapes inside the growth ampoule. The diffusivity of CdTe in liquid tellurium was measured through dissolution experiments, which also served to validate the model. Simulations of tapered THM growth find conditions similar to untapered growth with interface shapes that are sensitive to strong thermosolutal convection. Favourable growth conditions are achievable only if convection can be controlled.

In preliminary experiments, tapered GaSb crystals were successfully grown by THM and large CdTe grains were produced by gradient freezing. Beginning with this seed material, 25mm diameter CdTe and CdZnTe crystals were grown on 10mm diameter seeds, and 65mm diameter CdTe on 25mm seeds. Unseeded THM growth was also investigated, as well as ampoule rotation and a range of thermal conditions and ampoule surface coatings. Outward growth beyond one or two centimeters was achieved only at small diameters and included secondary grains and twin defects; however, limited outward growth of larger seeds and agreement between experimental and numerical results suggest that tapered growth may be achievable in the future. This would require active temperature control at the base of the crystal and reduction of convection through thermal design or by rotation of the ampoule or applied magnetic fields.