

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

of

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M Tech (Indian Institute of Technology Delhi, 2008) B Tech (Punjab Technical University, 2005)

"Numerical Simulation of Growth of Silicon Germanium Single Crystals"

Department of Mechanical Engineering

Tuesday April 14, 2015 10:00 A.M. Engineering Office Wing 502

Supervisory Committee:

Dr. Sadik Dost, Department of Mechanical Engineering, University of Victoria (Supervisor)
Dr. Ben Nadler, Department of Mechanical Engineering, UVic (Member)
Dr. Peter Oshkai, Department of Mechanical Engineering, UVic (Member)
Dr. Alexandre Brolo, Department of Chemistry, UVic (Non-Unit Member)

External Examiner:

Dr. Ziad Saghir, Department of Mechanical and Industrial Engineering, Ryerson University

Chair of Oral Examination:

Dr. Lynneth Stuart-Hill, School of Exercise, Science, Physical and Health Education, UVic

Dr. David Capson, Dean, Faculty of Graduate Studies

<u>Abstract</u>

Si x Ge1-x is a promising alloy semiconductor material that is gaining importance in the semiconductor industry primarily due to the fact that silicon and germanium form a binary isomorphous system and hence its properties can be adapted to suit the needs of a particular application. Liquid phase diffusion (LPD) is a solution growth technique which has been successfully used to grow single crystals of Si x Ge 1-x. The first part of this thesis discusses the development of a fixed grid solver to simulate the LPD growth under zero gravity condition. Initial melting is modeled in order to compute the shape of the initial growth interface along with temperature and concentration distribution. This information is then used by the solidification solver which in turn predicts the onset of solidification, evolution of the growth interface, and temperature and concentration fields as the solidification proceeds. The results are compared with the previous numerical study conducted using the dynamic grid approach as well as with the earth based experimental results. The predicted results are found to be in good qualitative agreement although certain noticeable differences are also observed owing to the absence of convective effects in the fixed grid model. The second part investigates the effects of crucible translation on the LPD technique using the dynamic grid approach. The case of constant pulling is examined first and compared with the available experimental results. Then a dynamic pulling profile obtained as a part of simulation process is used to achieve the goal of nearly uniform composition crystal. The effect of crucible translation on the interface shape, growth rate, and on the transport process is investigated. Finally, the effect of magnetic field on the LPD

growth is examined.