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THREE DIMENSIONAL EFFECT OF AXIAL MAGNETIC FIELD TO SUPPRESS CONVECTION IN THE SOLVENT OF Ge_{0.98}Si_{0.02} GROWN BY THE TRAVELING SOLVENT METHOD

by

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A thesis

presented to Ryerson University

in partial fulfillment of the requirement for the degree of

Master of Applied Science

in the Program of

Mechanical Engineering

Toronto, Ontario, Canada, 2004

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ABSTRACT

THREE DIMENSIONAL EFFECT OF AXIAL MAGNETIC FIELD TO SUPPRESS CONVECTION IN THE SOLVENT OF Ge0.98Si0.02 GROWN BY

THE TRAVELING SOLVENT METHOD

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A three dimensional numerical simulation of the effect of an axial magnetic field on the fluid flow, heat and mass transfer within the solvent of $Ge_{0.98}Si_{0.02}$ grown by the traveling solvent method is presented. The full steady state Navier-Stokes equations, as well as the energy, continuity and the mass transport equations, were solved numerically using the finite element technique. It is found that a strong convective flow exists in the solvent, which is known to be undesirable to achieve a uniform crystal. An external axial magnetic field is applied to suppress this convection. By increasing the magnetic induction, it is observed that the intensity of the flow at the centre of the crucible reduces at a faster rate than near the wall. This phenomenon creates a stable and flat growth interface and the silicon distribution in the horizontal plane becomes relatively homocentric. The maximum velocity is found to obey a power law with respect to the Hartmann number: $U_{max} \propto Hc^{-7/4}$.

ACKNOWLEDGEMENTS

I would like to present my sincerely thankful feelings to Dr. M. Z. Saghir, for his invaluable support, guidance and encouragement, and for many valuable suggestions in improving the course of study. Also, I acknowledge the financial support of the Canadian Space Agency (CSA), and the CRESTech.

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DEDICATION

I would like to dedicate this thesis to my husband, Farzad Azizi. His unfailing support and continuous words of encouragement throughout these years will always be remembered...

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NOMENCLATURE

E.

) B	temporal variation of magnetic field induction (Gauss/s)
B *	non-dimensionalized magnetic field induction
B	magnetic field induction (Gauss)
Bo	reference magnetic field induction (Gauss)
B_1	radial component of magnetic field induction (Gauss)
B_2	circumferential component of magnetic field induction (Gauss)
<i>B</i> ₃	axial component of magnetic field induction (Gauss)
С	non-dimensionalized concentration (atomic %)
С	solute concentration (atomic %)
Co	reference solute concentration (atomic %)
∆c	change in concentration (atomic %)
c_p	specific heat at constant pressure (cal/g·K)
D	reference length (cm)
e_z	axial unit vector
E	electric field (volt/cm)
Gr	Grashof number
g	gravity (cm/s ²)
go	earth gravity (cm/s ²)
Ha	Hartmann number: $Ha = B_0 D \sqrt{\frac{\sigma}{\mu}}$
H	magnetic field (A/m)
J	current density (A/cm 2)

- L Lorentz force (N)
- L_f latent heat (cal/g)
- *l* length of the solvent(cm)

 \overline{Nu} average Nusselt number: $\overline{Nu} = \frac{1}{l} \int_{0}^{l} \frac{\partial \theta}{\partial R} \Big|_{R=0} dz$

- p pressure (g/cm².s²)
- Pr Prandtl number
- *r* radial direction(cm)

Re Reynolds number

- Re_m magnetic Reynolds number: $Re_m = \mu_o \sigma u_0 D$
- *R* non-dimensionalized radial direction
- Sc Schmidt number
- T temperature (°C)
- T_o reference temperature (°C)
- ΔT change in temperature (°C)
- U non-dimensionalized radial velocity
- *u* radial velocity (cm/s)
- U speed: $\sqrt{u^2 + v^2 + w^2}$ (cm/s)
- \underline{V} velocity vector (cm/s)
- v circumferential velocity (cm/s)
- w axial velocity (cm/s)
- W non-dimensionalized axial velocity
- z axial direction (cm)

Z non-dimensionalized axial direction

Greek Symbols

α_T	thermal diffusivity of the species (cm ² /s)
α. _c	solutal diffusivity of the species (cm ² /s)
β_c	solutal expansion coefficient (1/at %Si))
β_T	thermal expansion coefficient (1/°C)
θ^{+}	non-dimensionalized temperature
к	thermal conductivity (cal/s.cm.K)
μ	dynamic viscosity (g/cm.s)
μο	permeability (N/A ²)
ν	kinematic viscosity (cm ² /s)
ρ	density (g/cm ³)
σ	electric conductivity (S/cm)
φ	circumferential direction
${\it \Phi}$	electric potential (volt)
Subse	ripts
0	reference

s solid phase

Superscripts

M Magnetic Field

CHAPTER 1

INTRODUCTION AND LITERATURE REVIEW

1.1 Introduction

Semiconductors are a group of materials having intermediate electric conductivities between metals and insulators. Conductivity of these materials can be varied over orders of magnitude by changes in temperature or impurity content. The electric properties of semiconductor materials are strongly affected by impurities. This variability of their electric properties makes semiconductors a wise choice for electronic devices [1]. Computer microchips, optoelectronic sensors, lasers, X-ray detectors, transistors in pocket radios and solar cells that provide electric power in artificial satellites are just some of the examples of semiconductor devices [3], [4]. The advantages of semiconductors are that they use much less power, they last longer and they can be built significantly smaller [3].

Today, the largest made single crystals are for the semiconductor industry. Silicon is used in nearly all semiconductor materials. On their own, single crystals of silicon cannot compete with other materials in areas such as mobile phones, global positioning systems (GPS) and optoelectronics. The fact that integrated circuits can be made today is the result of a considerable progress in the growth of pure, single crystals of Si [1]. The performance of silicon transistors and circuits can be improved upon by the additions of other semiconductor materials like germanium, which opens up the material to numerous new applications. Silicon germanium (SiGe) technology has given rise into low-cost, lightweight, personal communication devices such as digital wireless handsets. SiGe uses minimum power so that it extends the life of wireless phone batteries. SiGe plays a significant role in the development of other entertainment and information technologies such as digital set-top boxes, Direct Broadcast Satellites (DBS), automobile radar systems, and personal digital assistants. SiGe characteristically carries smaller and more efficient devices into communication technologies [5]. Also, Silicon Germanium is used in the automotive industry in sensors for collision avoidance radars, road speed monitors and electronic tolls and traffic management systems [6].

1.2 What is a Single Crystal?

A crystal is a solid material that has a regular internal arrangement of atoms, ions or molecules, known as a 3D crystal structure [4]. A crystalline solid is defined by arrangement of atoms in a periodic fashion. There is some basic arrangement of atoms that is repeated through the entire solid [1]. Since the periodicity is revealed, the crystal appears exactly the same at one point as at other points. In single crystals, atoms are arranged following specific patterns throughout the entire piece of material; i.e., long-range order exists throughout all single crystal materials. However, not all solids are crystals (Figure 1); some that have no periodic structure at all are called amorphous solids and some that are composed of many small regions of single crystal materials, are called polycrystalline solids. The periodic array of atoms in a single crystal is called a lattice. There are many ways of placing atoms in a volume; the difference in distances between atoms form different lattices. The lattice contains a volume, which is called unit cell; it is representative of the entire lattice and is regularly repeated through the crystal [1].



Figure 1 Three types of solids, a) crystalline, b) amorphous materials and c) polycrystalline structure [1].

A whole range of useful substances have crystalline structures, including metals (e.g., aluminium, iron, titanium, copper), inorganic compounds (e.g., silicongermanium, cadmium telluride, gallium antimonide) and biological macromolecules (e.g., proteins, lipids, nucleic acids and carbohydrates).

In nature, there are seven generic types of unit cells; namely cubic, tetragonal, rhombic, hexagonal, triagonal, monoclinic and triclinic (their differences are in the edge lengths and angles). The three simplest 3D lattices are shown in the following picture. Imagine millions of these cubes arranged next to each other in 3D; that is the concept of a crystal.



Figure 2 Three different arrangements of cubic crystal systems [4].

For the semiconductors of today's technological aspects, it is required to have the highest crystalline order as is possible in order to get the best performance out of a material. For example, if it were possible to get a large enough pure single crystal for night vision, it would be possible to see at night just as clear as in the day. Figure 2 shows the uniformity and order that exists in a single crystal.

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Figure 3 two-dimensional lattice showing translation of a unit cell [7].

Single crystals are used in electrical and optical devices, solid-state lasers, infrared detectors and a wide range of medical and industrial applications.

Single crystals of silicon play an important role in industry. As mentioned above, all-modern electronics from telecommunications to consumer electronics, from gaming consoles to life-saving medical equipment, are built from silicon.

1.3 What is Crystal Growth?

Semiconducting single crystals are vital to the electronic industry [8]. Unfortunately they are full of defects and impurities. A number of methods have been developed to grow these materials. These materials, such as silicon, first have to be produced with an acceptable purity and then grown as single crystals under very specific conditions. The properties of a material are extremely fluctuating with these imperfections in the crystalline lattice. Therefore, the crystal has to be produced with a high level of purity and homogeneity with these methods. Defections lead to a reduction in the quality of the crystal. There could be a missing atom or an extra atom in the lattice or there could be dislocations. Although the ideal condition is provided in the form of pure crystal with no such dislocations or impurities, it is essential for semiconductor materials to be provided with the right amount of impurities added to perform their best function regarding the fact that there is a connection between the resulting crystal quality, its physical properties and the growth parameters.

The very common process that has been used in industry is crystallization from the melt. Growing a solid crystal from the liquid is a technique which produces crystals from their solution, in relative^{1,1} low temperature.

Gravity also plays a role in the crystallization process and it contributes in the mass and heat transport. Because of the buoyancy, there is a convective fluid flow which results in causing an uneven concentration distribution in the melt,

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as well as reducing the perfection of the growth.

1.4 Methods of Suppressing Convection in the Melt

1.4.1 Microgravity Condition

An alternative method for reducing buoyancy-driven convection is growing the crystals in a reduced gravity environment. This has been observed in many space experiments. Under reduced gravity conditions, scientists can grow crystal that is not affected by buoyancy convection and hydrostatic pressure. These materials will have different applications such as in computer microchips, optoelectronic sensors, lasers, and X-ray detectors [4]. It should be mentioned that even the attainable space environment does not provide zero gravity.

1.4.2 Use of Magnetic Field in the Melt Growth

Metals and semiconductor melts have a relatively high electrical conductivity. By applying a magnetic field, this characteristic can be used to suppress natural convective fluid flows in the melt [8]. It is therefore useful to observe the effect of magnetic field damping as against gravity reduction.

The application of an external magnetic field to suppress convection has been found to be very beneficial and efficient. The applied magnetic field could be static or dynamic (with rotation), vertical or transverse.

This section focuses on the effects of applying a steady (static) magnetic field (transverse and axial) to a crystal growth melt. The objective is to minimize the effect of convection in the solution. The weaker the convection in the solution, the higher the growth rate will be. The level of the magnetic field has a significant effect on the intensity of the convective flow in the solution and the shape of the growth interface. The shape of growth interface becomes more uniform at a specific amount of magnetic field. Therefore the magnetic field intensity must be optimized. It should be mentioned that magnetic field damping is dependent on the Lorentz force, which is proportional to the vector product of the flow velocity and the magnetic field intensity. It therefore has an increasing effect with decreasing the flow velocity.

A magnetic field is a region of space near a magnetized body where magnetic forces can be detected. It should be mentioned that the magnetic field induction vector, B, also called the magnetic flux density, is the intensity of a magnetic field and indicates the direction of magnetic lines at any point in the domain (Figures 4 and 5). The magnetic field induction vectors are tangent to the field lines. Magnetic flux density (magnetic field induction) is measured in Webbers per square meter [Wb/m²]. A Webber is equivalent to a volt-second. The unit of Webber per square meter is also called a tesla (in the Metric system or gauss in the cgs system) [9].

Experimental studies indicate that the effective field magnitudes are in the range of 0.05 to 0.5 tesla (T). These fields have to be generated in a large volume and the bore must be large enough to embrace the crucible, the heater and the heat shields (if any). Therefore, for a small field value of only a few tenths of a tesla a large amount of the power supplied is needed. The magnetic field also imposes stresses on the crucible heater. In order to avoid resonance of periodic

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Figure 4 A bar with local magnetic field induction vectors tangent to the field lines [9].



Figure 5 Magnetic field lines and magnetic field induction vectors produced by a current carrying conductor [9].

currents and fatigue failure, the heater current must be DC [8].

The simplest examples of field that can be applied are those provided between the pole pieces of a conventional electromagnet, (figure 6) and that of a simple, wire-wound solenoid (figure7). These are the two configurations which have been studied the most. These equipments can provide axial and transverse magnetic fields, respectively. It was found that the wire-wound solenoids are easier to operate and easier to fabricate. Also, it is easy to modify them. By adding some windings to the latter it would be possible to change its characteristic. The power that is usually needed for crystal growth is somewhat about 100 kW (in order to obtain tenths of tesla), therefore the windings have to have as low resistance as possible with high conductivity such as copper [8].



Figure 6 Axial field configuration: the schematic representation of field lines [8].

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Figure 7 Transverse field configuration using an electromagnetic: the schematic representation [8].

1.5 Literature Review

Different techniques have been used in industry for crystal growth with different sizes. New methods of crystal growth, such as the Traveling Solvent Method (TSM) [2], also known as the Traveling Heater Method (THM), the Bridgman method [10-16], the Floating Zone method [17-19], the Czchralski method [20] and the Liquid Phase Electroepitaxy (LPEE) method [21] are being used in order to provide good quality crystals. Among different growth techniques, the TSM is particularly useful for the growth of bulk crystals [2] due to their characteristically large segregation effect between solid and liquid [22]. Another advantage of the TSM for crystal growth is that the process takes place at a relatively low temperature compared to the melting point of the crystal. Therefore, the pressure and the contamination from quartz as well as the

probability of the ampoule fracture reduces and crystal grows with less thermal stresses and more purity [23, 25].

Ye *et al.* [26] studied natural convection and its effects on the growth rate and uniformity as well as its effect on temperature distribution and solute distribution by the Traveling Heater Method (THM) of CdTe single crystal. Temperature, solute concentration and fluid flow fields in the growth ampoule were numerically simulated. They also showed, experimentally and numerically, that the concentration distributions, as well as growth interface, are substantially affected by convective mass transport. They realized that in order to achieve a uniform growth interface the natural convection should be as weak as possible. The influence of natural convection on the growth rate along the interface for different heater thermal profiles, with different positions of maximum temperature in the solvent (different offsets) was also investigated. They found that a smaller thermal gradient and larger offset lead to a more uniform growth.

Numerical simulation for the growth of GaInSb by the THM method was presented by Meric *et al.* [24]. It was found that the behaviour of the growth and its stability were significantly influenced by the thermal and solutal convection in the solution zone. The THM technique was also used for studies of the effects of thermal conditions for the growth of HgTe [27]. The study showed the reduction in heat transfer between the furnace and the ampoule increased the length of the liquid zone and also increased the growth rate significantly. The numerical simulation of concentration distribution showed a uniform

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concentration in the solvent region and a small concentration gradient along the growth interface indicated the importance of the convection.

Matasumoto *et al.* [28] carried out a numerical simulation of InP crystal growth by the traveling heater method. The transient crystal growth process was simulated without heater movement until the process reached a steady state. They found that in the case of strong buoyancy convection, constitutional supercooling took place near the interface, since the case of weak buoyancy convection doesn't show the same behaviour.

Okano *et al.* [25] focused on controlling the interface shape by numerically simulating the THM growth process. This report examines how this crystal interface shape is affected by the crucible temperature, crucible rotation and crucible material. This model employed actual temperature profiles obtained from an experimental process. They found that by increasing the temperature, the interface curvature became larger. The application of rotation was successful in suppressing the natural convection in the solution, and they achieved an interface with less curvature for both the higher and lower temperature cases.

They also considered two crucibles made of pBN and SiO_2 . With pBN at low temperatures no crystal growth was achieved. This was because the thermal conductivity of pBN slowed down the radial heat conduction into the solution. Consequently, they realized that a higher growth temperature is required for use of pBN crucible compared with a system using SiO_2 crucible. This study showed that the higher the temperature, the more curvature forms along the

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growth interface and rotation is useful in decreasing the curvature along the interface.

The effect of the supply of Si solute elements on the concentration distribution in the Si-rich SiGe bulk crystals was studied by Nakajima *et al.* [30]. It was done by using the multi-component zone melting method. They concluded that by controlling the pulling rate, Si-rich $Si_{1-x}Ge_x$ bulk crystals with a uniform composition of x= 0.1 would be obtained. This is because with this method they could keep the position and temperature of the interface constant.

Azuma *et al.* [10] developed an automatic feedback control system from the crystal-melt interface position in order to keep the interface growth temperature constant during the process. They could monitor the position of the interface. Thereby, the position of the pulling rod was corrected according to the position of the interface and they obtained uniform concentration distribution. They also realized that with the feedback control system they could achieve uniform composition for SiGe crystal with different composition such as Si-rich SiGe.

 $Hg_{1,x}Mn_{x}Te$ bulk crystals were produced by Reig *et al.* [30] by using the cold traveling heater method. They attained crystals with homogeneous concentration and they could reduce the high pressure of Hg vapour during the production of the alloy.

Lent *et al.* [31] presented a numerical simulation of $Ga_{1-x}In_xSb$ bulk single crystals grown by the traveling heater method. They found that the temperature profile has a significant influence on stability and the behaviour of the crystal

growth. They realized that convective fluid flow, which is caused by gravity, plays an important role in this process. Therefore, in order to suppress the convective fluid flow in the solvent they applied different levels of magnetic induction. They also considered the misalignment of the magnetic field. The convective flow due to small misalignment was found being useful for the growth process. They realized that a limitation of the amount of misalignment exists and any higher than that would make the process unstable. They also reported that a stationary magnetic field of 2 tesla (T) is sufficient to suppress the gravity effects.

A theoretical analysis of the InP crystal growth experiment by the traveling heater method was performed by Senchenkov *et al.* [32]. They observed the effectiveness of controlling heat and mass transport in the solvent by applying Rotating Magnetic Field (RMF). They produced the crystal with RMF, with the intensities of 1 and 2 mT. They found that the convective fluid flow in the melt and growth rate are significantly influenced by these amounts of field intensity. They also found that the concentration distribution along the crystals in the microgravity condition with and without RMF showed that the mass transfer would be nearly diffusive in the absence of RMF and would become convective with RMF.

Dost *et al.* [20] presented the continuum model for the liquid phase electroepitaxial (LPEE) growth process of GaAs semiconductor under stationary magnetic field. They observed the effect of the applied electric field and the electric field which was produced by the applied magnetic field, on the

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fluid flow and concentration distribution for different intensities of magnetic field. They found that the three dimensional results are more complex than two dimensional results. Simulation results showed three distinct characteristics depending on the magnetic field intensity. For weak magnetic induction a significant reduction in the flow intensity was observed, which is desirable for a crystal growth. By increasing magnetic field induction the two strong convective cells were shifted to the vertical wall of the crucible and created a Hartmann layer. At higher magnetic induction in the stable region, the Hartman layer became thinner and the flow became homocentric and axisymmetric. They found that the applied magnetic field suppressed the flow in the growth process. They also showed that for Hartmann (Ha) number higher than 150, the flow velocity increases and loses its axisymmetry. For Ha number between 150 and 220 they obtained a transient region and higher than 220 they obtained a completely unstable region and the flow structure changed over time. They also observed non-uniformity near the interface. Therefore, the effect of magnetic field would not be useful anymore. They also investigated that in the stable region the maximum velocity ($U_{\rm max}$) obeys a power law of $U_{\rm max} \propto Ha^{-5/4}$, whereas in the unstable region the velocity obeys approximately a power law of $U_{\rm max} \propto H a^{5/2}$.

The influence of a magnetic field on the melt-growth process of $Yba_2Cu_3O_x$ was studied by Awaji *et al.* [33]. They observed that the applied magnetic field influenced the crystal formation during the cooling process. Also, they observed a reduction in the growth rate by applying more magnetic field intensity. They concluded that magnetic field is a feasible option to control the crystal growth of $Yba_2Cu_3O_x$.

Single CdHgTe crystals have been grown by Senchenkov and his coworkers [34] using the traveling heater method. They applied rotating magnetic field with intensities between 2 and 6 mT. They found radial concentration homogeneity by applying a rotating magnetic field and they obtained an axisymmetric growth condition. They realized that, by applying the proper magnetic field intensity, they can control the growth interface with the desired shape and large diameter crystals with appropriate concentration.

Liu *et al.* [22] presented the 3D numerical simulation for the growth of CdTe single crystals under an applied axial static magnetic field by the traveling heater method. The effect of different magnetic field intensities on the flow, concentration distribution and the temperature fields in the solvent were examined. They found that an external stationary magnetic field is beneficial to suppress the convective fluid flow in the solvent. They have also shown that by applying relatively higher field intensities they obtain weaker convection in the solvent. This results in a homogeneous concentration distribution and uniform temperature distributions, with better growth interface for certain specific magnetic field intensities. They also showed that the flow fields exhibit three distinct regions of magnetic field induction. A stable flow which is found to be beneficial for the growth, a transitional flow in which the flow showing unstable behaviour. The flow patterns were found significantly different from each other.

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The influence of rotating magnetic field (RMF) on the flow pattern and compositional uniformity in the solution zone of the traveling heater method (THM) system for the growth of CdTe is numerically investigated by Ghaddar *et al.* [35]. They presented the simulation results for low gravity and high gravity levels. They found that under the microgravity condition, the application of RMF can be beneficial to overwhelm the residual buoyancy-induced convection and to obtain more uniformity of the solvent zone composition without changing the growth interface shape. At high-gravity levels, RMF is found unable to completely overwhelm the convective flow field. For relatively high magnetic field induction, RMF was found to result a complex flow structure in the melt and non-uniformities at the growth interface, and was also found to increase convexity of the growth interface.

Gelfat [36] showed experimental results on semiconductor single crystal growth under microgravity and the other techniques in order to obtain better materials. He realized that the electromagnetic fields are the most effective technique to suppress the convective flows of a non-gravity condition. He also presented that steady magnetic field is useful to suppress the convective fluid flow but he mentioned that the applied static magnetic field intensity should not exceed over the stable region otherwise asymmetric behaviors would be obtained. He also realized that an alternating magnetic field needs less power and the equipment of an alternating magnetic field is smaller and easier to be fabricated. This type of magnetic field also stabilizes the flow in the melt. He mentioned that in order to get the optimum condition for semiconductor single crystal growth, applying a magnetic field under the microgravity condition is a promising technique.

3D numerical simulation of the melt flow in the presence of a rotating magnetic field was studied by Vizman *et al.* [37]. They found that by rotating magnetic field they can obtain a stable melt flow.

1.6 Research Objectives

The attempt is to use the TSM technique to grow $Ge_{0.98}Si_{0.02}$ high quality bulk single crystals with uniform composition, high purity and homogeneity i.e with flat growth interface.

All this is achieved by suppressing the buoyancy convection in the $Ge_{0.98}Si_{0.02}$ solution zone. Applying an axial, steady uniform magnetic field and also growing the crystal in microgravity condition are two methods used in this thesis to suppress the convective fluid flow.

1.7 Thesis organization

This thesis is organized as follows: Chapter two presents in detail the differential equations used to solve the problem. The non-dimensionalized equations are presented as well. (The step-by-step non-dimensionalization of the three components of the Navier-Stokes equations, continuity, heat and mass transfer equations are presented in appendix B.) The full model, the furnace and the externally applied temperature profile are described. The boundary conditions are considered in Chapter two. The numerical solution technique as well as the finite element analysis is explained in the chapter as well. At the end

of the chapter, the mesh sensitivity analysis for the full model is performed. In Chapter three, the results and discussions are presented and the comparison of the terrestrial and microgravity conditions, as well as the cases with different levels of magnetic field induction, are presented in different planes. Finally, Chapter 4 presents the concluding remarks and the future work.

CHAPTER 2

A THEORETICAL APPROACH

The next segment introduces the governing equations that will be used in the simulation. All the equations are set in cylindrical coordinates and are presented in steady-state form. Thereafter the governing equations are transformed into a dimensionless form. The step-by-step dimensional analysis done for all of the equations is presented in appendix B.

2.1 Dimensional Governing Equations

2.1.1 Navier-Stokes Equations

The Navier- Stokes [36, 37] equations for laminar, steady-state incompressible Newtonian magnetohydrodynamics flows with the Boussinesq buoyancy approximation can be written in the following forms:

r - component

$$u\frac{\partial u}{\partial r} + \frac{v}{r}\frac{\partial u}{\partial \varphi} + w\frac{\partial u}{\partial z} - \frac{v^2}{r} = v\left(\nabla^2 u - \frac{u}{r^2} - \frac{2}{r^2}\frac{\partial v}{\partial \varphi}\right) - \frac{1}{\rho}\frac{\partial p}{\partial r} + \frac{1}{\rho}F_r^M$$
(2.1)

 φ - component

$$u\frac{\partial v}{\partial r} + \frac{v}{r}\frac{\partial v}{\partial \varphi} + w\frac{\partial v}{\partial z} + \frac{vu}{r} = v\left(\nabla^2 v - \frac{v}{r^2} + \frac{2}{r^2}\frac{\partial v}{\partial \varphi}\right) - \frac{1}{r}\frac{1}{\rho}\frac{\partial p}{\partial \varphi} + \frac{1}{\rho}F_{\varphi}^{\ M}$$
(2.2)

20

z - component

$$u\frac{\partial w}{\partial r} + \frac{v}{r}\frac{\partial w}{\partial \varphi} + w\frac{\partial w}{\partial z} = v(\nabla^2 w) - \frac{1}{\rho}\frac{\partial p}{\partial z} + \frac{1}{\rho}F_z^M + g\beta_t(T - T_0) - g\beta_c(c - c_0)$$
(2.3)

where the Laplacian operator is given by

$$\nabla^{2} = \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^{2}}\frac{\partial^{2}}{\partial \varphi^{2}} + \frac{\partial^{2}}{\partial z^{2}}\right)$$
(2.4)

Equations (2.1) to (2.3) correspond to the momentum equations (Navier-Stokes) in the solvent region in the radial (r), angular (φ) and axial (z) directions. In these equations u, v and w are the three velocity components in the radial (r), angular (φ) and axial (z) directions, and v, p, T, T_o , c, c_o , ρ , β_t , and β_c are the kinematic viscosity, the pressure, the temperature, the melt temperature of Ge (used as the reference temperature), the silicon concentration, the reference silicon concentration, the solution density, the thermal and the solutal volume expansion coefficients, respectively. The three forces F_r^M , F_z^M and F_{φ}^M denote the magnetic body force components along the r, z, and φ -directions, respectively.

2.1.2 Energy Equation

The energy equation for the liquid phase is:

$$u\frac{\partial T}{\partial r} + \frac{v}{r}\frac{\partial T}{\partial \varphi} + w\frac{\partial T}{\partial z} = \frac{\kappa}{\rho c_p} \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 T}{\partial \varphi^2} + \frac{\partial^2 T}{\partial z^2}\right)$$
(2.5)

where ρ , κ and c_p denote the solution density, thermal conductivity, and

specific heat of the solution, respectively.

Since there are both solid and liquid phases in the process, the governing equation for the solid phases would be only in the energy equation as follow:

$$\frac{\kappa_s}{\rho_s c_{p,s}} \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 T}{\partial \varphi^2} + \frac{\partial^2 T}{\partial z^2} \right) = 0$$
(2.6)

where ρ_s, κ_s and $c_{p,s}$ denote the density, thermal conductivity, and specific heat of solid phases respectively. (Noting that subscript *s* denotes solid phase [33].)

2.1.3 Continuity Equation

The continuity equation is:

$$\frac{1}{r}\frac{\partial}{\partial r}(ru) + \frac{1}{r}\frac{\partial v}{\partial \varphi} + \frac{\partial w}{\partial z} = 0$$
(2.7)

2.1.4 Solute Equation

$$u\frac{\partial c}{\partial r} + \frac{v}{r}\frac{\partial c}{\partial \varphi} + w\frac{\partial c}{\partial z} = \alpha_c \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 c}{\partial \varphi^2} + \frac{\partial^2 c}{\partial z^2}\right)$$
(2.8)

where c and α_c denote the silicon concentration and solutal diffusivity, respectively.

2.2 The Magnetohydrodynamics (MHD) Equations

In the presence of a magnetic field, the motion of the electrically conducting fluid across magnetic lines of force generates a current. Fluid elements carrying current which traverse magnetic lines of force give rise to an additional force acting on the element [8] called the Lorentz force, which is defined as:

$$\boldsymbol{L} = \boldsymbol{J} \times \boldsymbol{B} \tag{2.9}$$

where J is current density. The current density is given from the extended Ohm's law:

$$J = \sigma(E + V \times B) \tag{2.10}$$

where σ is the electrical conductivity of the fluid (assumed isotropic), E is electric field, and \underline{V} is the vector flow velocity.

For all kinds of crystal growth, the externally imposed field can be applied into the MHD equations. Therefore, B can be replaced by B_{\circ} , the externally imposed field. By inserting equation (2.9) into Navier-Stokes equation, magnetohydrodynamics equations would be obtained. Substituting equation (2.10) into (2.9) yields:

$$L = \sigma(E + \underline{V} \times B_{\circ}) \times B_{\circ} \quad (2.11)$$

where B_{\circ} is the externally imposed field (please see appendix A for more details). The components of the Lorentz force would represent the components of magnetic force in the Navier-Stokes equations, which were presented in equations (2.1) to (2.3). In crystal growth, with a steady applied magnetic field, one can use $E=-\nabla \Phi$ for the electric field. In this study, the electric field, E, is neglected in equation (2.11). However this assumption is valid only for the case of steady two-dimensional flows as described in ref. [8]. Moreover, the effect of the electric field on the numerical results was recently discussed [15]. Based on

ref. [15] for the axial steady magnetic field case, by assuming axisymmetric flow, there is no potential build up and therefore neglecting $\nabla \Phi$ is reasonable. In addition, to justify the statement above, $E=-\nabla \Phi$ is also included in the simulation and the same result was obtained as with no electric field.

In this model an axial static magnetic field is applied and it is assumed to be perfectly aligned with the axis of the furnace. Therefore, the two components B_1 and B_2 are set equal to zero.

The applied static axial magnetic field is considered as:

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$$B_{o} = B_{3} e_{z} \tag{2.12}$$

where e_z is the unit vector in z-direction. The magnetic body force (Lorentz force) would be:

$$\boldsymbol{L} = \boldsymbol{J} \times \boldsymbol{B} \tag{2.13}$$

As discussed, the induced electric field due to the applied magnetic field and the fluid motion is neglected. Therefore:

$$J = \sigma(B_3 v e_r - B_3 u e_{\varphi}) \tag{2.14}$$

The magnetic body force would then be given as:

$$F^{M} = F_{r}^{M} + F_{\varphi}^{M} + F_{z}^{M} = -\sigma B_{3}^{2} (ue_{r} + ve_{\varphi})$$
(2.15)

Therefore the components would be:

$$F_r^M = -\sigma B_3^2 u, \ F_{\varphi}^M = -\sigma B_3^2 v \ F_z^M = 0$$
(2.16)

Therefore the magnetic body force components acting on the solvent are in the angular (circumferential) and radial directions only.

2.3 Dimensional Analysis

Dimensional analysis is a method of simplifying complex equations by reducing the amount of variables being used in a compact way by putting them in a dimensionless form in order to observe the physical effect of the phenomena. Some examples of these dimensionless parameters are the Reynolds number, Prandtl number and the Grashof number [40].

2.3.1 Non-Dimensional Variables

In order to achieve a better convergence, the differential equations will be transformed to a non-dimensional form. These are all the non-dimensionalized variables, which will be used to non-dimensionalize the equations.

$$R = \frac{r}{D}, \quad Z = \frac{z}{D}, \quad U = \frac{u}{u_o}, \quad V = \frac{v}{u_o}, \quad W = \frac{w}{u_o}, \quad P = \frac{pD}{\mu u_o}, \quad \theta = \frac{T - T_o}{\Delta T},$$
$$C = \frac{c - c_o}{\Delta c}, \text{ and } B^* = \frac{B}{|B_o|}$$

where R, Z, U, V and W are non-dimensional radial, circumferential and axial coordinates, non-dimensional radial, circumferential and axial components of velocity, respectively. P is non-dimensional hydrodynamic pressure, theta (θ) is the non-dimensional temperature, C is the non-dimensional solute concentration and B^* is non-dimensional magnetic field induction.

 u_o is the reference velocity which is defined as $u_o = \sqrt{g\beta_t \Delta TD}$, D is the reference diameter, T_o is the reference temperature, where ΔT is set equal to one. The non-dimensional parameters used to non-dimensionalize the equations are shown in Appendix C.

2.3.2 Non-Dimensionalized Governing Equations

For step-by-step non-dimensionalization of the equations please refer to appendix B.

2.3.2.1 Navier-Stokes Equations

The non-dimensional steady state Navier-Stokes equations for z, r and φ -directions are, respectively:

r – component:

$$\operatorname{Re}\left[U\frac{\partial U}{\partial R} + \frac{V}{R}\frac{\partial U}{\partial \varphi} + W\frac{\partial U}{\partial Z} - \frac{V^{2}}{R}\right] = -\frac{\partial P}{\partial R} + \left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial U}{\partial R}\right) + \frac{1}{R^{2}}\frac{\partial^{2}U}{\partial \varphi^{2}} + \frac{\partial^{2}U}{\partial Z^{2}} - \frac{U}{R^{2}} - \frac{2}{R^{2}}\frac{\partial U}{\partial \varphi}\right] + Ha^{2}\left(WB_{1}^{*}B_{3}^{*} - UB_{3}^{*2} - UB_{2}^{*2} + VB_{1}^{*}B_{2}^{*}\right)$$

(2.17)

 φ – component:

$$\operatorname{Re}\left[U\frac{\partial V}{\partial R} + \frac{V}{R}\frac{\partial V}{\partial \varphi} + W\frac{\partial V}{\partial Z} + \frac{UV}{R}\right] = -\frac{\partial P}{\partial \varphi} + \left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial V}{\partial R}\right) + \frac{1}{R^{2}}\frac{\partial^{2}V}{\partial \varphi^{2}} + \frac{\partial^{2}V}{\partial Z^{2}} - \frac{V}{R^{2}} + \frac{2}{R^{2}}\frac{\partial V}{\partial \varphi}\right] + Ha^{2}\left(UB_{1}^{*}B_{2}^{*} - VB_{1}^{*2} - VB_{3}^{*2} + WB_{2}^{*}B_{3}^{*}\right)$$

$$(2.18)$$

$$z$$
 – component:

$$Re\left[U\frac{\partial W}{\partial R} + \frac{V}{R}\frac{\partial W}{\partial \varphi} + W\frac{\partial W}{\partial Z}\right] = -\frac{\partial P}{\partial Z} + \left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial W}{\partial R}\right) + \frac{1}{R^{2}}\frac{\partial^{2}W}{\partial \varphi^{2}} + \frac{\partial^{2}W}{\partial Z^{2}}\right] + \frac{Gr_{T}}{Re}\theta - \frac{Gr_{c}}{Re}C + Ha^{2}\left(VB_{3}^{*}B_{2}^{*} - WB_{2}^{*2} - WB_{1}^{*2} + UB_{1}^{*}B_{3}^{*}\right)$$

$$(2.19)$$

2.3.2.2 Energy Equation

$$RePr\left[U\frac{\partial\theta}{\partial R} + \frac{V}{R}\frac{\partial\theta}{\partial\varphi} + W\frac{\partial\theta}{\partial Z}\right] = \left[\frac{1}{R}\frac{\partial}{\partial R^2}\left(R\frac{\partial\theta}{\partial R}\right) + \frac{1}{R^2}\frac{\partial^2\theta}{\partial\varphi^2} + \frac{\partial^2\theta}{\partial Z^2}\right]$$
(2.20)

Since there are both solid and liquid phases in the process, the governing equation for the solid phase in the non-dimensional form would be only the energy equation as follow:

$$\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial\theta}{\partial R}\right) + \frac{1}{R^2}\frac{\partial^2\theta}{\partial \varphi^2} + \frac{\partial^2\theta}{\partial Z^2} = 0$$
(2.21)

2.3.2.3 Continuity Equation

$$\frac{1}{R}\frac{\partial}{\partial R}(RU) + \frac{1}{R}\frac{\partial V}{\partial \varphi} + \frac{\partial W}{\partial Z} = 0$$
(2.22)

2.3.2.4 Solute Equation

$$Re\left[U\frac{\partial C}{\partial R} + \frac{V}{R}\frac{\partial C}{\partial \varphi} + W\frac{\partial C}{\partial Z}\right] = \frac{1}{Sc}\left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial C}{\partial R}\right) + \frac{1}{R^{2}}\frac{\partial^{2}C}{\partial \varphi^{2}} + \frac{\partial^{2}C}{\partial Z^{2}}\right]$$
(2.23)

2.4 The Growth Technique

Growth has been performed in the Traveling Solvent Method (TSM). In the TSM method there are three specific parts in a quartz tube; the source or the feed rod at top, melt or solution zone in the middle of the crystal (solvent) and substrate (the seed rod) which lies at the bottom of the ampoule [19]. The feed rod is usually made of a polycrystalline material with relatively constant composition. The whole sample would be placed in a furnace and the solution zone would be heated by heating elements.

Figure 8 illustrates a TSM system consisting of a furnace with a cylindrical enclosure and the ampoule (quartz tube) containing the liquid-solid materials which is obtained from the experimental set up at Dalhousie University. During the growth, because of the characteristics of the temperature profile, (higher temperature at solution zone and lower at source and substrate) two liquid-solid interfaces are created and this causes the source materials to dissolve into the solvent. The transportation then takes place by both thermosolutal and diffusion. By downward movement of the ampoule, more materials would dissolve in the solution and at the same time crystallization would take place according to the lower temperature and large temperature gradient at the growth interface [24]. The ampoule (quartz tube) is then translated downwards the axis of the furnace,







Figure 9 Description of the Traveling Solvent Method toward the crystal growth of a homogeneous Ge_{1-x}Si_x crystal

usually at a rate of around 4 mm/day, which means it usually takes 1 to 2 weeks to grow a single crystal. Figure 9 describes the stages of the TSM toward the crystal growth. The traveling solvent method is a relatively new and promising technique for the production of high quality bulk crystal of semiconductors.

For the TSM method by applying a magnetic field, it is possible to control the buoyancy driven convective flow and the uniformity of concentration distribution at the growth interface, as well as to achieve the growth interface as flat as possible and a relatively faster growth rate. All these objectives can be obtained by optimizing the mass transport throughout the system [2]. The application of the applied magnetic field goes into this category.

2.5 Model Description

The sample having a length of 6.1 cm consists of a $Ge_{0.85}Si_{0.15}$ feed rod having a diameter of 0.8 cm and length of 3.6 cm (the source rod). This rod is located on top of a $Ge_{0.98}Si_{0.02}$ rod having the same diameter and the length of 1.0 cm (i.e. solvent). At the bottom is the germanium seed with the length of 1.5 cm (the substrate). The total sample is enclosed in a quartz tube having a wall thickness of 0.1 cm. The heater is applied at the external surface of the quartz tube. The temperature profile was obtained from the experimentally set up thermo-couple [46], which is located at the inner wall of the ampoule. This temperature profile is depicted in Figure 10. The temperature is assumed to be uniform along the circumferential direction. The melting temperature of the solvent is less than the $Ge_{0.85}Si_{0.15}$ rod. Therefore Si will be segregating from the source rod toward the bottom rod.

In this model a uniform, axial static magnetic field is applied, which is perfectly aligned with the axis of the furnace. Because the magnetic Reynolds number is much smaller than unity ($Re_m <<1$), the effects of the induced magnetic field on the applied field are negligible. Thus, the induced magnetic field by the fluid motion is not considered in the equation and only the external magnetic field is taken into account for the crystal growth.



Figure 10 Temperature profile at the internal wall of the crucible.

2.6 Boundary Conditions

The boundary conditions used in the modelling are as follows:

a) At the vertical wall of the ampoule (in the source, solvent and the substrate)

as well as on the top and the bottom of the ampoule:

1)
$$u = 0, v = 0, w = 0$$
 (Non-slip condition has been considered) (2.24)

$$2) \frac{\partial C}{\partial r} = 0 \tag{2.25}$$

b) At dissolution interface:

$$C = C_1 = 0.15$$
 (2.26)

c) At the growth interface:

$$C = C_2 = 0.02 \tag{2.27}$$

where C_1 and C_2 are the concentration of the silicon in the crystal growth process at dissolution and growth interface, respectively. The value of the concentration at the growth interface is obtained from the Ge-Si phase diagram [41]. Figure 11 demonstrates the phase diagram for Ge_{1-x}Si_x alloy.



Figure 11 Phase Diagram of the Germanium - Silicon binary system [41]

In addition, the heat transfer between the solid and the liquid phases includes a latent heat release such that the temperature at the solid and the liquid are equal, and

(2.28)

$$\kappa \frac{\partial T}{\partial z} - \kappa_s \frac{\partial T_s}{\partial z} = \rho_s L_f(w_s - w_{interface})$$

where L_f is the latent heat.

2.7 Numerical Solution Technique

The formulation of the crystallization for the TSM growth of GeSi was given in the previous section. In the solution zone the non-linear Navier-Stokes equations with the Boussinesq approximation which is coupled by the convective heat and mass transfer as well as the magnetic body force are applied. As mentioned above, on the boundaries a non-slip condition for velocity is assumed and the steady- state condition has been considered. The experimental temperature field is used to calculate the temperature field in the sample.

Here are other assumptions that have been taken into account in the input file used for the simulation:

- The fluid is Newtonian
- Thermophysical properties are constant everywhere except for the density
- The solution in electrically conductive
- The flow is laminar

• The speed of the ampoule translation is very small

2.7.1 Finite Element Analysis

The Finite Element Method (FEM) has been used to solve the governing equations. The finite element method is an efficient technique for simulation of the crystal growth and it is valid for all types of linear and nonlinear partial differential equations. The objective of the finite element method is to reduce the infinite number of degrees of freedom in a problem to a finite number by a system of algebraic equations. The domain, which is to be analyzed, is divided into small regions. These regions are called elements. These elements are defined with a finite number of nodes where the field variables, e.g. temperature, velocity, pressure, and concentration are to be evaluated. An algebraic combination of local nodal values is used to approximate the solution in each element. The approximate functions of this element are then integrated over the domain and their overall error is minimized throughout the mesh. This process gives rise to a set of N algebraic equations for the N unknown nodal values. Using matrix inversion or iteration, the nodal equations are then solved simultaneously [42]. The advantages of using the Finite Element Method is that it includes the ability to easily model irregularly shaped bodies and without difficulty handle a wide range of loading conditions. FEM makes it easy to model bodies composed of several different materials as the elemental equations are evaluated individually. It also can be used to handle unlimited numbers and different kinds of boundary conditions [42].

In this model, the Galerkin finite element method approximation has been used for velocity, pressure, temperature, and concentration. This was done in order to reduce the partial differential equations and boundary conditions to a set of algebraic equations. Then, the segregated algorithm is used to solve these algebraic equations [43].

In order to model the geometry of the sample and generate the elements and the associated nodes, the commercial software, GAMBIT was used [44]. GAMBIT has a very impressive library containing an extensive selection of elements including a three-dimensional 27 node hexahedron element. After the griding of the sample is done by GAMBIT, the geometry and the mesh are exported to the commercial computational code FIDAP [43]. FIDAP is the general-purpose computer software that is used to numerically model the crystal growth of Ge_{0.98}Si_{0.02} by the traveling solvent method. FIDAP is a computational fluid dynamics package that uses the finite element method to simulate many classes of fluid flow. In each element, the partial differential equations of fluid mechanics covering the flow regions are replaced by algebraic equations. FIDAP then solves these equations by using complicated numerical techniques to determine the velocities, pressures, temperatures, species concentrations and other unknowns throughout the region at given time intervals [43].

For the presented model, eight-node hexahedron elements have been chosen. The finite element mesh for the growth is shown in Figure 12. A refined mesh has been used within the solvent due to the large temperature and velocity gradient in the interfaces. The mesh configuration for the substrate and the source was used to obtain the temperature field within the substrate and the source (solid zones) because as it was mentioned in section 2.1.2, the only governing equation for the solid zone is the equation of energy. The configuration of the grids in the solvent is demonstrated in the Figure 12b. The temperature profile was obtained from the experimental thermo-couples, which are located at the inner wall of the ampoule. In order to simplify the computation, the crucible wall is not considered in the model. As mentioned before the segregated algorithm has been chosen for the model to solve the algebraic equations. The equations are solved simultaneously and the criteria for the convergence set for the five unknowns, temperature, u, v, and w as well as the concentration. Convergence is reached when the non-dimensional primitive variables attain a difference (between two consecutive iterations) less than 10^{-4} .

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Figure 12 The finite element model.

2.7.2 Sensitivity Analysis

In order to obtain the most accurate results and at the same time the least computational storage, an optimum number of grids should be determined. For this purpose different mesh intensities are taken into consideration and an ideal mesh is selected according to an average Nusselt number across the solvent. It is found that the parameter which is the main driving force in the simulation should be used for the sensitivity analysis. In this case the problem involves heat transfer and the temperature heater profile applied to the outside of the sample, therefore the average Nusselt number across the solvent is a viable parameter to be used for mesh sensitivity:

 $\overline{Nu} = \frac{1}{l} \int_{0}^{l} \frac{\partial \theta}{\partial R} \bigg|_{R=0} dz$

where θ is the non-dimensional temperature and l is the length of the solvent.

A mesh is deemed acceptable when the value of the average Nusselt number changes by 10^{-3} from that mesh to a more coarse mesh. Initially, the number of nodes on the circumferential direction was kept constant at 20 nodes and the number of nodes in the axial direction was increased. This is then followed by increasing the circumferential nodes to 40, 60 and 80 nodes. The results show that there is a slight difference in the result between 40, 60 and 80 nodes (see Table 1 or Figure 13). 60 nodes in the circumferential direction are chosen to minimize the computational storage and to maximize accuracy. Table 1 (or Figure 13) shows the average Nusselt number versus the axial number of nodes. It is clear that the optimum mesh is 60 by 240 nodes in the circumferential and

the axial direction, respectively, which means 79200 (87723 nodes) eight-node hexahedron elements in the whole sample are used and they are expanded as 21780 elements (24187 nodes) in the source, 33000 elements (36461 nodes) in the solvent and 24420 elements (27075 nodes) in the substrate.

40 Circumferential Number of Nodes		60 Circumferential Number of Nodes	
Axial Number of Nodes	Average Nusselt Number	Axial Number of Nodes	Average Nusselt Number
40	1.653423	40	1.659502
60	1.597216	60	1.610607
80	1.560759	80	1.550888
100	1.537114	100	1.533077
140	1.512045	140	1.492088
160	1.492922	160	1.478915
180	1.472897	180	1.475208
200	1.463672	200	1.470661
220	1.454669	220	1.462937
240	1.446673	240	1.454958
260	1.445935	260	1.454123
280	1.444534	280	1.451857

 Table 1 Mesh Sensitivity Analysis and comparison of the Average Nusselt number for 60 and 40 nodes in circumferential direction.

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Figure 13 Mesh sensitivity analysis.

CHAPTER 3

RESULTS AND DISCUSSION

3.1 Introduction

Three different cases were examined for a better understanding of the fluid flow, heat and mass transfer during the TSM process of Ge_{0.98}Si_{0.02} using the values for the properties presented in Table 2[45] which is presented in Appendix D. Firstly, the effect of buoyancy convection was studied where the gravity vector g was present and equal to g_o . Secondly, the fluid, heat and mass transfer of GeSi solvent in a low gravity condition with the gravity vector g set equal to $10^{-4}g_o$ (microgravity) is examined. Finally, the importance of the magnetic field to suppress convection in the presence of a buoyancy force is studied in detail. Since the goal is to achieve a uniform distribution of silicon on the seed and because the quality of the growth process is strongly affected by the fluid flow intensity, the silicon distribution is examined at four different locations. In particular, the results were examined at cross sections at $\varphi = 0^{\circ}$ and $\varphi = 90^{\circ}$, in the vertical plane of the solvent region (r, $\varphi = 0$, z), near the growth interface (r, φ , z=1.575cm) and at the middle of the solvent region (r, φ , z=2.0cm).

3.2 Results for the terrestrial and the Microgravity Conditions

As displayed in Figure 10, a large temperature gradient exists at the growth

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interface. This is the characteristic required for the traveling solvent method. The intention is not to melt the source interface but to try to diffuse the silicon into the solvent region. The temperature gradient near the growth interface is about 170° C/cm and the maximum temperature in the solvent is 1004.6° C. With such a temperature profile one may expect a convective pattern with hot molten particles rising to the source rod near the quartz wall and the cold molten particles coming down from the centre of the solvent region.

Figure 14 and Figure 15 present the temperature distribution for terrestrial and microgravity conditions, respectively. Figures 14b and 15b show the temperature distribution (isotherms) in the solution zone in the vertical plane (r, r) $\varphi = 0^{\circ}$, z). It can be seen that the curvature of isotherms varies from convex to concave, indicating the variation of the radial temperature gradients. However, the variation is small because the heat transfer process in semiconductor materials is dominantly conduction rather than convection [22]. As shown in Figures 14 and 15, the same behaviour of the temperature gradient is observed in both conditions. This shows that the convection in the solvent is not strong enough to deform temperature contours in the solvent. This observation is reasonable due to the fact that the material used in our simulation is GeSi, which is in the family of semiconductor materials and has a relatively low Prandtl number. For such materials, convection is not strong enough to have any effect on the temperature distribution within the solvent. Therefore one can conclude that there is the same temperature gradient for the terrestrial and microgravity cases.

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Figure 14 Temperature distribution along the TSM model for terrestrial condition (contour lines in increments of 22.44°C): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the vertical plane at central axis of the sample $(r, \varphi=0, z)$ c) in the horizontal plane in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$.

In general, for such materials with low Prandtl number, the effects of convective heat transfer on temperature distribution and on the thermally-driven buoyant convection are negligible [46].

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Figure 15 Temperature distribution along the TSM model for microgravity condition (contour lines in increments of 22.44°C): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the vertical plane at central axis of the sample $(r, \varphi=0^{\circ}, z)$ c) in the horizontal plane in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$.

The application of the temperature profile in the solution zone results in two counter-rotating flow cells. They force the flow to move upward along the crucible wall where the temperature is the highest and then push it downward along the central axis where the temperature is lower. Figure 16 shows the velocity vectors and the counter-rotating flow cells in the solvent in the vertical plane at centre axis of the sample. As shown in this figure, two buoyant convective cells are created and these two cells drive convective transport which produces non-uniformities in the concentration distribution in both the melt and the crystal.



Figure 16 Velocity vectors and counter-clockwise re-circulating cells in the solvent in the vertical plane at centre axis of the sample.

Figure 17 shows the silicon distribution in the solvent for the terrestrial condition. As shown, the silicon is following the flow pattern by moving

downward from the silicon rich concentration near the dissolution interface, towards the growth interface from the centre axis of the sample. In microgravity (Figure 18), due to the weak buoyancy convection, one observes a unoform distribution of silicon and the process is purely diffusive. A cut in the horizontal direction either in the middle of the sample or near the growth interface (Figures 18b and c) shows a uniform silicon distribution in the solvent region in microgravity and a non-linear distribution in the terrestrial case due to the influence of the buoyancy convection. If one examines the solute distribution along the radial direction in the two conditions near the interface, one may observe that in a microgravity condition, better silicon distribution does exist but still a very small non-uniformity is obtained. This is due to the residual gravity (Figure 18e), which remains in the model since one can never achieve a perfect, zero gravity. Two boundary layers are formed at the vicinity of the dissolution interface and growth interface. As mentioned before, for the case where the gravity is present, there is a relatively high concentration gradient along the wall of the crucible and at the centre axis of the sample, which is caused by the convective flow in the cell. Figure 17e shows the variation of the concentration distribution along the radial direction, and it shows a significant radial gradient in the solvent. For the microgravity condition, because of low gravity this convective flow is reduced and the flow is mostly conductive rather than convective.



Figure 17 Silicon distribution in the solvent for terrestrial condition (contour lines in increments of 1.3%): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ c) in the horizontal plane near the growth interface $(r, \varphi, z=1.575 \text{ cm})$ d) in the vertical plane at central axis of the sample $(r, \varphi=0, z)$ e) the variation of the silicon distribution along the radial direction near the growth interface $(r, \varphi=0^{\circ}, z=1.575 \text{ cm})$.





e)

Figure 18 Silicon distribution in the solvent for microgravity condition (contour lines in increments of 1.3%): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ c) in the horizontal plane near the growth interface $(r, \varphi, z=1.575 \text{ cm})$ d) in the vertical plane at central axis of the sample $(r, \varphi=0^{\circ}, z)$ e) the variation of the silicon distribution along the radial direction near the growth interface $(r, \varphi=0^{\circ}, z=1.575 \text{ cm})$.

Figures 19 and 20 show the flow field (speed contours) in terrestrial and microgravity conditions, respectively. The flow is nearly axisymmetric and also homocentric for both cases. A relatively strong flow cell is created in the middle of the solvent region near the centre axis and two weaker cells near the wall of the crucible for both cases. In the presence of the gravity (see Figure 19) the maximum speed cell has a magnitude of 0.4796 cm/s while for the microgravity condition, the same behaviour is observed but with less intensity. The maximum speed obtained for this case is 0.000168 cm/s, being much less than the previous case, is located almost in the middle of the growth cell. This indicates the existence of a weak gravity force pushing the flow downward.



Figure 19 Flow field (speed contours) in the solvent for terrestrial condition (contour lines in increments of 0.05082 cm/s): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ c) the variation of the fluid flow along the radial direction in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ d) in the horizontal plane near the growth interface $(r, \varphi, z=1.575 \text{ cm})$ e) in the vertical plane at central axis of the sample $(r, \varphi=0^{\circ}, z)$.



Figure 20 Flow field (speed contours) in the solvent for microgravity condition (contour lines in increments of 0.0001734 cm/s): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ c) the variation of the fluid flow along the radial direction in the middle of the solvent $(r, \varphi=0, z=2.0 \text{ cm})$ d) in the horizontal plane near the growth interface $(r, \varphi, z=1.575 \text{ cm})$ e) in the vertical plane at central axis of the sample $(r, \varphi=0^{\circ}, z)$.
3.3 The Effect of Applied Magnetic Field in Terrestrial Condition

In this thesis, an externally uniform, steady, axial magnetic field is applied. The purpose of the applied static axial magnetic field is that it acts as a body force, working in the opposite direction to the induced buoyancy convection in the solution zone. The application of the magnetic field is that, it prevents the sinking behaviour of the heavy particles in the melt from the centre axis of the solvent and results in less central segregation and consequently less radial concentration gradients. Different magnetic field intensities were studied. Simulation is presented for eight different levels of magnetic field. Figures 21 to 28 present the silicon distribution in the solution zone for different levels of magnetic field intensities (B=0.2, 0.4, 0.6, 0.8, 1.0, 1.5, 2.0, and 2.2 KG) at cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ (Figures 21a to 38a), in the horizontal plane in the middle of the growth cell (figures 21b to 28b), as well as the variation of the silicon concentration along the r- direction in the middle of the solvent (Figures 21c to 28c), in the horizontal plane near the growth interface (Figures 21d to 28d), and in the vertical plane at the central axis of the growth cell (Figures 21d to 28d).

Simulation results show the same behaviour for the temperature distribution as was shown for terrestrial and microgravity condition. This means that for the same reason as mentioned for the terrestrial and microgravity case, the effects of convective heat transfer on the temperature distribution and on the thermallydriven buoyant convection are negligible [46].

When the magnetic field intensity is set equal to 0.2 kilogauss (KG), the silicon distribution tends to be more axisymmetric and the silicon contours are spread more uniformly than for the case with no magnetic field. When compared with the case with no magnetic field, a more uniform concentration distribution can be observed and it becomes more evident as the magnetic field intensity is increased. When the magnetic field intensities increase, the silicon distribution becomes smoother and the silicon contours become flatter and more uniform. This represents a more uniform growth.

Figures 21e to 28e depict the concentration distribution in the vertical plane (r, $\varphi=0^{\circ}$, z). By increasing the magnetic field intensity, the radial concentration gradients decrease and the silicon contours tend to present linear behavior. As shown in Figures 27e or Figure 28e, the silicon contours are parallel and, especially near the growth interface, they are nearly flat, which is the desired condition for the growth interface.

As is observed in Figures 21a to 25a, silicon distribution does not behave the same in the $\varphi=0^{\circ}$ and the $\varphi=90^{\circ}$ planes, which means that, although the distribution is axisymmetric in one plane, it is different from plane to plane. Therefore the behaviour is changing according to the plane of view. This is because of the characteristic of the axial magnetic field intensity which results in two magnetic force components: one in the radial direction and one in the circumferential direction (see section 2.3 for more details). Despite the fact that the magnetic body force is in the opposite direction of the flow and it decreases the flow intensity, these two resulting components of magnetic force (radial and

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circumferential components) cause non-uniformities in the radial direction in the growth and the axisymmetric flow pattern is also distorted. By applying larger magnetic field intensities such as 1.5, 2.0, or 2.2 KG the convective flow would be dominantly suppressed and this asymmetric behaviour disappears.

By examining the silicon distribution at the horizontal plane near the growth interface (Figures 21d to 28d) the contours are showing that they tend to become more homocentric as the magnetic field intensity is increased. Figure 28d shows a complete homocentric silicon distribution near the growth interface. This is desirable for the crystal growth. The intensity of maximum concentration distribution near the growth interface takes place in the middle of the region (in the horizontal plane), which is slightly reduced by increasing the magnetic field intensity. The maximum silicon concentration in the horizontal plane near the growth interface is 9.99 percent for the magnetic field intensity equal to 0.2 KG while this maximum reduces to 7.48 percent when the magnetic field is increased to 0.6 KG (Figure 22c), 6.5 percent for 1.5 KG (Figure 23c) and 5.87 percent for 2.0 KG. This is reasonable due to the effect of the magnetic field in suppressing the flow field. Transport of the silicon from the dissolution interface to the growth interface is reduced accordingly. This would be continued until the magnetic field intensity reaches 2.2 KG. The maximum concentration then drops to 5.55 percent when the magnetic field intensity of 2.2 KG is applied. Compared to the case with magnetic field intensity of 2.0 KG, as is depicted in the figure, the concentration distribution doesn't change significantly, but it is homocentric.

Figures 21b to 28b show the concentration distribution in the horizontal plane in the middle of the solvent. This shows that the silicon particles are concentrated dominantly close to the centre axis of the sample in the absence of the magnetic field or small magnetic field intensity. The figures that were mentioned above show that by increasing the magnetic field intensity the silicon concentration contours are more spread out and occupy more space than the cases with no magnetic field or small magnetic field intensity, with more homocentric behaviour, which is desirable for crystal growth. Figure 28b shows complete homocentric behaviour with the magnetic field intensity equal to 2.2 KG.

Figures 21c to 28c show the variation of the silicon concentration along the *r*direction in the middle of the solvent. For low magnetic field intensities, a very large silicon distribution gradient is observed. By increasing the magnetic field intensity the behaviour tends to show linear behaviour. In Figure 27c or Figure 28c, the distribution is nearly linear and axisymmetric. The difference between the maximum and the minimum concentration percentage is much less than that of the weak magnetic field or the absence of magnetic field.





Figure 21 Silicon distribution in the solvent for magnetic field intensity of B=0.2 KG (contour lines in increments of 1.3%): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ c) the variation of the silicon distribution along the radial direction in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ d) in the horizontal plane near the growth interface $(r, \varphi, z=1.575 \text{ cm})$ e) in the vertical plane at central axis of the sample $(r, \varphi=0^{\circ}, z)$.

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Figure 22 Silicon distribution in the solvent for magnetic field intensity of B=0.4 KG (contour lines in increments of 1.3%): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in the middle of the solvent (r, φ , z=2.0 cm) c) the variation of the silicon distribution along the radial direction in the middle of the solvent (r, $\varphi=0^{\circ}$, z=2.0 cm) d) in the horizontal plane near the growth interface (r, φ , z=1.575 cm) e) in the vertical plane at central axis of the sample $(r, \varphi=0^\circ, z)$.





Figure 23 Silicon distribution in the solvent for magnetic field intensity of B=0.6 KG (contour lines in increments of 1.3%): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ c) the variation of the silicon distribution along the radial direction in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ d) in the horizontal plane near the growth interface $(r, \varphi=0^{\circ}, z=1.575 \text{ cm})$ e) in the vertical plane at central axis of the sample $(r, \varphi=0^{\circ}, z)$.





Figure 24 Silicon distribution in the solvent for magnetic field intensity of B=0.8 KG (contour lines in increments of 1.3%): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ c) the variation of the silicon distribution along the radial direction in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ d) in the horizontal plane near the growth interface $(r, \varphi, z=1.575 \text{ cm})$ e) in the vertical plane at central axis of the sample $(r, \varphi=0^{\circ}, z)$.



Figure 25 Silicon distribution in the solvent for magnetic field intensity of B=1.0 KG (contour lines in increments of 1.3%): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ c) the variation of the silicon distribution along the radial direction in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ d) in the horizontal plane near the growth interface $(r, \varphi=0^{\circ}, z=1.575 \text{ cm})$ e) in the vertical plane at central axis of the sample $(r, \varphi=0^{\circ}, z)$.







Figure 26 Silicon distribution in the solvent for magnetic field intensity of B=1.5 KG (contour lines in increments of 1.3%): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in the middle of the solvent (r, φ , z=2.0 cm) c) the variation of the silicon distribution along the radial direction in the middle of the solvent (r, $\varphi=0^{\circ}$, z=2.0 cm) d) in the horizontal plane near the growth interface (r, φ , z=1.575 cm) e) in the vertical plane at central axis of the sample (r, $\varphi=0^{\circ}$, z).





Figure 27 Silicon distribution in the solvent for magnetic field intensity of B=2.0 KG (contour lines in increments of 1.3%): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ c) the variation of the silicon distribution along the radial direction in the middle of the solvent $(r, \varphi=0^{\circ}, z=2.0 \text{ cm})$ d) in the horizontal plane near the growth interface $(r, \varphi, z=1.575 \text{ cm})$ e) in the vertical plane at central axis of the sample $(r, \varphi=0^{\circ}, z)$.





Figure 28 Silicon distribution in the solvent for magnetic field intensity of B=2.2 KG (contour lines in increments of 1.3%): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ c) the variation of the silicon distribution along the radial direction in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ d) in the horizontal plane near the growth interface $(r, \varphi, z=1.575 \text{ cm})$ e) in the vertical plane at central axis of the sample $(r, \varphi=0^{\circ}, z)$.

Figures 29 to 36 summarize the flow patterns in the solvent region for eight different levels of axial magnetic field intensities (B=0.2, 0.4, 0.6, 0.8, 1.0, 1.5,2.0, and 2.2 KG) at cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ (Figures 29a to 36a), along the radial direction in the middle of the growth cell (Figures 29b to 36b), the variation of the speed along the radial direction in the middle of the growth cell (Figures 29c to 36c), at the horizontal plane near the growth interface (Figures 29d to 36d), and in the vertical plane at the center of the growth cell (Figures 29e to 36e). It was found that the two counter-rotating velocity vectors (see Figure 16) in the solvent translated into three speed cells as shown in Figure 29: one relatively strong located in the readle of the growth cell (in vertical plane) and two weaker cells near the ampoule wall in the case with weak magnetic field intensities (see Figure 29e). The maximum speed cell is located closer to the growth interface rather than near the dissolution interface. This is because of the influence of the gravity pushing the flow downward towards the growth interface. This means that the gravity is not significantly suppressed with this field intensity. The magnitude of the maximum speed in the case with magnetic intensity of 0.2 KG was found to be equal to 0.19635 cm/s, which is less than that of the case with no magnetic field and, the other two cells close to the wall have less intensity than the middle cell (Figure 29e).

When *B* is increased to a level of 0.4 KG, the maximum speed in the middle cell has the same value as the two cells close to the crucible wall. All three cells have the maximum speed value of 0.05934 cm/s (Figure 30e). When *B* reaches a level of 0.6 KG (Figure 31e), the strong cell in the middle becomes weaker but

the flow intensity of the two cells close to the wall does not drop as significantly as the middle cell does; therefore, the behavior of the flow changes along the radial direction. The magnitude of the maximum speed for the two cells close to the wall becomes higher than the cell located in the middle. Also the two cells close to the wall are squeezed and shifted to the crucible wall. These two relatively strong cells create a layer along the crucible wall which is called the Hartmann layer. As *B* is increased beyond 0.6 KG, the Hartmann layer becomes thinner and is squeezed further. This phenomenon confirms the observations of references [11] and [16]. This behavior creates mostly a weak flow intensity in the middle of the solution zone and relatively strong flow field close to the crucible wall, which is desired and it leads to a better control of the crystal growth process, as well as creates a stable and flat growth interface. Figure 36e, shows that the cells are still closer to the growth interface rather than the dissolution interface which shows that the slight effect of the gravity in the fluid flow still exists.

Figures 29c to 36c confirm the above statements. In comparing Figure 29c with 36c, three peaks are shown in the variation of the speed along the radial direction. The maximum peak is located in the middle of the region near the centre axis of the crucible in the case with intensity of 0.2 KG while for the magnetic intensity of 2.2 KG the maximum peak is located very close to the wall rather than the centre axis.

The flow field in the horizontal plane in the middle of the growth cell shows that by increasing the magnetic field intensity the core cell in the middle is

suppressed and two stronger cells are moving towards the wall. The same behavior can be observed at the growth interface (Figures 29d to 36d).

As depicted in Figures 29a to 36a, the flow field does not present the same pattern in the $(r, \varphi=0^{\circ}, z)$ plane and $(r, \varphi=90^{\circ}, z)$ plane, which means that although the distribution is axisymmetric in one plane, it is different from plane to plane. Therefore the behaviour is changing accordingly with the plane of view. This is because of the same reason that explained in section 3.3.





Figure 29 Flow field (speed contours) in the solvent for magnetic field intensity of B=0.2 KG (contour lines in increments of 0.0231 cm/s): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in middle of the solvent (r, φ , z=2.0 cm) c) the variation of the flow intensity along the radial direction in the middle of the solvent (r, $\varphi=0^{\circ}$, z=2.0 cm) d) in the horizontal plane near the growth interface (r, φ , z=1.575 cm)e) in the vertical plane at central axis of the sample (r, $\varphi=0^{\circ}$, z).

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d)

e)

Figure 30 Flow field (speed contours) in the solvent for magnetic field intensity of B=0.4 KG (contour lines in increments of 0.009156 cm/s): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in middle of the solvent (r, φ , z=2.0 cm) c) the variation of the flow intensity along the radial direction in the middle of the solvent (r, φ , z=1.575 cm) e) in the vertical plane at central axis of the sample (r, $\varphi=0^{\circ}$, z).



a)



2

e)





d)

Figure 31 Flow field (peed contours) in the solvent for magnetic field intensity of B=0.6 KG (contour lines in increments of 0.004968 cm/s): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in middle of the solvent (r, φ , z=2.0 cm) c) the variation of the flow intensity along the radial direction in the middle of the solvent (r, $\varphi=0^{\circ}$, z=2.0 cm) d) in the horizontal plane near the growth interface $(r, \varphi, z=1.575 \text{ cm})e)$ in the vertical plane at central axis of the sample ($r, \varphi=0^{\circ}, z$).





d)

Figure 32 Flow field (speed contours) in the solvent for magnetic field intensity of B=0.8 KG (contour lines in increments of 0.003053 cm/s): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in middle of the solvent (r, φ , z=2.0 cm) c) the variation of the flow intensity along the radial direction in the middle of the solvent (r, $\varphi=0^{\circ}$, z=2.0 cm) d) in the horizontal plane near the growth interface $(r, \varphi, z=1.575 \text{ cm})$ e) in the vertical plane at central axis of the sample $(r, \varphi=0^\circ, z)$.



Figure 33 Flow field (speed contours) in the solvent for magnetic field intensity of B=1.0 KG (contour lines in increments of 0.00095 cm/s): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ c) the variation of the flow intensity along the radial direction in the middle of the solvent $(r, \varphi, z=1.575 \text{ cm})$ e) in the vertical plane at central axis of the sample $(r, \varphi=0^{\circ}, z)$.

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Figure 34 Flow field (speed contours) in the solvent for magnetic field intensity of B=1.5 KG (contour lines in increments of 0.001103 cm/s): a) cross section at $\varphi=0^{\circ}$ and $\varphi=90^{\circ}$ b) in the horizontal plane in middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ c) the variation of the flow intensity along the radial direction in the middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ c) the variation of the solvent $(r, \varphi=0^{\circ}, z=2.0 \text{ cm})$ d) in the horizontal plane near the growth interface $(r, \varphi, z=1.575 \text{ cm})$ e) in the vertical plane at central axis of the sample $(r, \varphi=0^{\circ}, z)$.



a)

b)

c)



Figure 35 Flow field (speed contours) in the solvent for magnetic field intensity of B=2.0 KG (contour lines in increments of 0.0007332 cm/s): a) cross section at $\varphi=0^{\circ}$ and $\varphi=900$ b) in the horizontal plane in middle of the solvent $(r, \varphi, z=2.0 \text{ cm})$ c) the variation of the flow intensity along the radial direction in the middle of the solvent $(r, \varphi=0^{\circ}, z=2.0 \text{ cm})$ d) in the horizontal plane near the growth interface $(r, \varphi, z=1.575 \text{ cm})$ e) in the vertical plane at central axis of the sample $(r, \varphi=0^{\circ}, z)$.





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The variation of the fluid intensities along the radial direction near the growth interface for different levels of axial magnetic field as well as microgravity and terrestrial conditions with no magnetic field are depicted in Figure 37. In the absence of magnetic field two peaks can be observed. By increasing the magnetic field intensities these peaks become flatter and the flow intensity gradient along radial direction is reduced. The flow is stronger in the middle of the growth cell in the absence of the magnetic field or, weak magnetic field intensities. By increasing the applied magnetic field this strong flow in the middle becomes weaker and the flow becomes more uniform which is desirable for the crystal growth. One may conclude that the optimum magnetic field intensity is near B=2.2 KG where, a uniform flow intensity is observed, except for the area very close to the crucible wall.



Figure 37 Variation of the flow intensities along the radial direction near the growth interface for different magnetic field intensities as well as terrestrial and microgravity condition ($r, \varphi = 0^{\circ}, z = 1.575$ cm).

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Figure 37 shows a very small difference between the behaviours of the fluid flow for the case with the intensity of 2.2 KG and microgravity condition which is located near the crucible wall.

The variation of the fluid intensities along radial direction in the middle of the growth cell for the different levels of magnetic field as well as for the case in the absence of magnetic field and the microgravity condition is summarized in Figure 38. As mentioned earlier, for the case without magnetic field or for a weak magnetic intensity (i.e. 0.2 KG), the flow has two peaks of maximum speed. The strongest peak is located in the middle of the region. As the magnetic intensity increases, the flow is reduced in the middle region at a faster rate compared to near the wall. This explains the earlier observation that with



Figure 38 Variation of the flow intensities along the radial direction in the middle of the solvent for different levels of magnetic field intensities as well as terrestrial and microgravity condition $(r, \varphi=0^\circ, z=2.0 \text{ cm})$.

the increase in magnetic field, the flow becomes weak in the middle but remains relatively strong near the quartz wall. For strong applied magnetic field intensities, a slight change of fluid flow can be seen only near the wall since it is the desired environment to grow the crystal. Figure 38 shows a very small difference between the behavior of the fluid flow for the case with the intensity of 2.2 KG and microgravity condition which is located very close to the crucible wall. Therefore one can conclude that the intensity of 2.2 KG is optimum for the crystal growth in terrestrial environment.

Silicon distribution along the radial direction in the middle of the solvent for different applied magnetic field intensities (r, $\varphi=0^{\circ}$, z=2.0 cm) as well as the terrestrial and microgravity conditions are depicted in Figure 39. For weak magnetic field intensity (i.e. 0.2 KG), a very large concentration gradient is observed. By applying larger magnetic field intensity, the gradient decreases and the difference between the maximum and the minimum concentration percentage drops. The ideal condition to grow crystal is microgravity where diffusion is the only transport of silicon to the growth interface.



Figure 39 Variation of the Silicon distribution along the radial direction in the middle of the growth cell for different levels of magnetic field intensities as well as terrestrial and microgravity condition($r, \varphi=0^{\circ}, z=2.0$ cm).

Figure 40 indicates the silicon distribution near the growth interface (r, $\varphi=0^{\circ}$, z=1.575 cm) along the radial direction for different levels of magnetic field, as well as the terrestrial and microgravity conditions. Three humps are observed: one at the centre axis of the sample and two closer to the crucible wall where the maximum concentration gradients are located. As *B* increases, these humps become flatter and the growth is faced with a nearly linear concentration distribution and consequently, flat interface.



Figure 40 Variation of silicon distribution along the radial direction near the growth interface for different magnetic field intensities as well as the terrestrial and microgravity condition ($r, \varphi = 0^{\circ}, z=1.575$ cm).

Figure 41 indicates the sili on distribution closer to the growth interface $(r, \varphi=0^{\circ}, z=1.515 \text{ cm})$ along the radial direction for different levels of magnetic field, as well as the terrestrial and microgravity conditions, in order to have better observation of the growth interface. This figure confirms that the best growth is in the microgravity condition. The gradient of silicon distribution is decreased by increasing the applied magnetic field. Also, the silicon concentration percentage is reduced by applying the magnetic field, which is the consequence of suppressing the convection. As is shown in Figure 41, the radial distributions of the silicon particles tend to exhibit horizontal behaviour by increasing the magnetic field intensity and having a uniform silicon concentration. The microgravity case shows a nearly complete flat interface.

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Figure 41 Variation of silicon distribution along the radial direction very close to the growth interface for different magnetic field intensities as well as the terrestrial and microgravity condition $(r, \varphi=0^{\circ}, z=1.515 \text{ cm})$.

The variation of the maximum flow intensity with respect to the nondimensional magnetic field intensity, the Hartmann number, is summarized in Figure 42. The variation is given in the logarithmic pattern in order to find the relationship between the maximum velocity and the Hartmann number. It was found that the maximum velocity obeys a power law with respect to Hartmann number: $U_{\text{max}} \approx Ha^{-7/4}$. The observation of the logarithmic behaviour with respect to Hartmann number confirms the observation of refs [2] and [18], with different slopes.



Figure 42 Variation of the non-dimensional maximum velocity as a function of the Hartmann number

By observing Figure 42, one may conclude that the best result would be obtained by increasing the magnetic field intensities as much as possible. It should be mentioned that although the magnetic body force suppresses the gravitational body force, when the level of the magnetic field exceeds the critical value, where the magnetic body force balances the gravitational body force completely, the two magnetic force components become extra forces acting on the crystal growth and cause non-uniformities in the solvent region and the growth interface. Therefore, the magnetic field must be optimized.

CHAPTER 4

CONCLUSION AND RECOMMENDATIONS

4.1 Conclusions

A three-dimensional numerical simulation of the fluid flow, heat and mass transfer within a $Ge_{0.98}Si_{0.02}$ solvent under an axial magnetic field was carried out. The full steady-state Navier-Stokes equations as well as the continuity, energy and the mass transport equations, were solved numerically using the finite element technique. It was found that in the earth environment, there is a strong convective flow, which is undesirable for the growth uniformity in the crystal. An external axial magnetic field was applied to suppress this convection. Results revealed that with the increase in the intensity of the magnetic field, the silicon distribution in the horizontal plane became more homocentric and the distribution of the silicon became wider in the vertical plane.

The intensity of the flow at the centre of the crucible decreases at a faster rate compared to the flow near the walls. This phenomenon creates a stable and flat growth interface. It was also found that the maximum velocity obeys a power law with respect to Hartmann number ($U_{max} \sim Ha^{-7/4}$) in the stable region. One can conclude that in the absence of a magnetic field in earth gravity condition, the migration of the silicon is mostly due to convective flow. In the presence of the magnetic field, the convective flow is suppressed and the diffusion plays an

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important role in the silicon distribution in the solvent. Also, microgravity condition $(10^{-4}g)$ was numerically simulated for reducing the buoyancy convection in the solvent. A reduction in gravity represented a reduction in the driving body force in natural convection and a uniform concentration distribution would be obtained.

4.2 Future Work

The ideal results for crystal growth were obtained in the microgravity environment where the growth took place in a pure diffusion environment. It should be mentioned that even the attainable space environment does not provide zero gravity. Therefore, the best results can be obtained from combining of microgravity and a magnetic field, wherein the microgravity would reduce the slow, steady convective flows to a minimum with the magnetic field damping any residuals [8].

However, while located on the space station, one might encounter some unexpected disturbances from astronauts and from running equipment which is called G- jitter. It is for this reason that the extension of this work will be to examine how G-jitter may create some convection. And the final goal would be to apply a magnetic field to suppress this unwanted convection due to G-jitter in microgravity. This could be the long-term objective for this project.

In addition, for the simulation presented in this thesis, the temperature profile is considered uniformly distributed around the sample since a small nonuniformity exists according to the geometry of the heating elements; future

work could be to consider these non-uniformities.

Finally, applying a rotating magnetic field could be the best way of suppressing the convective fluid flow in the growth for the terrestrial condition with less curvature in the growth interface.

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APPENDIX A

MAGNETOHYDRODYNAMICS EQUATIONS

The MHD equations are obtained from Maxwell's equations coupled with the Navier- Stokes equations. Maxwell's equations can be written as:

$$\nabla \times \boldsymbol{H} = \boldsymbol{J} \tag{A.1}$$

$$\nabla \times \boldsymbol{E} = -\overset{\circ}{\boldsymbol{B}} \tag{A.2}$$

$$\nabla \cdot \boldsymbol{B} = 0 \qquad (A.3)$$

and

$$\boldsymbol{B} = \boldsymbol{\mu}_{\circ} \boldsymbol{H} \tag{A.4}$$

where E is electric field, J is the current density; H is the magnetic field and μ_o is the permeability.

The current density is given from the extended Ohm's law:

$$\boldsymbol{J} = \boldsymbol{\sigma} \left(\boldsymbol{E} + \boldsymbol{V} \times \boldsymbol{B} \right) \tag{A.5}$$

where σ is the electrical conductivity of the fluid (assumed isotropic) and \underline{V} is the vector flow velocity.

From equation (A.1) and (A.5) we J can be eliminated:

$$\nabla \times \boldsymbol{H} = \sigma \left(\boldsymbol{E} + \underline{\boldsymbol{V}} \times \boldsymbol{B} \right) \tag{A.6}$$

and from equation (A.4) we H can be eliminated:

$$H = \frac{B}{\mu_{\circ}} \tag{A.7}$$

Therefore from equation (A.6) and (A.7):

$$\nabla \times \frac{B}{\mu_{\circ}} = \sigma \left(E + \underline{V} \times B \right) \tag{A.8}$$

and

$$(\nabla \times B) = (\sigma \mu_{\circ})(E + \underline{V} \times B)$$
(A.9)

By applying $\nabla \times$ to both side of the equation above:

$$\nabla \times (\nabla \times B) = (\sigma \mu_{\circ}) \nabla \times (E + \underline{V} \times B)$$
(A.10)

and

$$(\sigma\mu_{\circ})^{-1}(\nabla \times (\nabla \times B)) = \nabla \times E + \nabla \times (\underline{V} \times B)$$
(A.11)

Substituting equation (A.2) into the equation above, the equation for the magnetic induction will be obtained:

$$\boldsymbol{B} = \nabla \times (\boldsymbol{V} \times \boldsymbol{B}) - (\boldsymbol{\mu}_{\circ} \boldsymbol{\sigma})^{-1} \nabla \times (\nabla \times \boldsymbol{B}).$$
(A.12)

which indicates the temporal variation of the B. The first term indicates the convection of the flow and the second term indicates the diffusion. The ratio of the first to the second term is of order of magnitude:

$$Re_m = \mu_o \sigma u_0 D \tag{A.13}$$

which is a non-dimensional ratio which is called the magnetic Reynolds number. u_0 and D are a characteristic (reference) flow velocity and a characteristic length, respectively.

For large flow velocities, and consequently, large magnetic Reynolds number, the second term on the right hand side of equation (A.12) (The magnetic dissipation term) can be neglected. When Re_m is very small, the first term is small and therefore the flow would not distort the magnetic field lines.

The essential incorporation of the magnetic field in the Navier-Stokes equation is the incorporation of the Lorentz force. In small magnetic Reynolds number flows, (Re_m small compared to unity), simplification of the Navier-Stokes equation is possible [8]. One can apply the externally imposed field, for all kinds of crystal growth. Therefore, we can replace **B** by B_o , the externally imposed field. By inserting the equation (A.5) into the Lorentz force equation:

$$\boldsymbol{L} = \boldsymbol{\sigma}(\boldsymbol{E} + \boldsymbol{V} \times \boldsymbol{B}_{\circ}) \times \boldsymbol{B}_{\circ} \tag{A.14}$$

Consequently dB/dt=0. Therefore, from equation (A.2) E can be simplified as $E = -\nabla \phi$.

And:

$$\boldsymbol{L} = \boldsymbol{\sigma} \left(-\nabla \phi + \underline{\boldsymbol{V}} \times \boldsymbol{B}_{\circ} \right) \times \boldsymbol{B}_{\circ} \tag{A.15}$$

The components of the Lorentz force would then represent the components of the magnetic force in the Navier-Stokes equation, which was presented in Equations (2.1) to (2.3).

Usually, the electric field due to the applied magnetic field and the motion of the fluid flow is neglected for axisymmetric flow patterns [8]. Therefore the magnetic field forces are written as follows:

$$F_{z}^{M} = \sigma \left(vB_{3}B_{2} - wB_{2}^{2} - wB_{1}^{2} + uB_{1}B_{3} \right)$$
(A.16)

$$F_r^M = \sigma \left(w B_1 B_3 - u B_3^2 - u B_2^2 + v B_1 B_2 \right)$$
(A.17)

$$F_{\varphi}^{M} = \sigma \left(u B_{1} B_{2} - \nu B_{1}^{2} - \nu B_{3}^{2} + w B_{2} B_{3} \right)$$
(A.18)

where B_1 , B_2 and B_3 represent the components of the applied magnetic field. Consequently, the magnetohydrodynamics equations can be presented as follows:

z-component:

$$\rho \left[u \frac{\partial w}{\partial r} + \frac{v}{r} \frac{\partial w}{\partial \varphi} + w \frac{\partial w}{\partial z} \right] = -\frac{\partial p}{\partial z} + \mu \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial w}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 w}{\partial \varphi^2} + \frac{\partial^2 w}{\partial z^2} \right] + \rho g \left[\beta_t (T - T_0 - \beta_c (c - c_0)) \right] + \sigma \left(v B_3 B_2 - w B_2^2 - w B_1^2 + u B_1 B_3 \right)$$
(A.19)

r-component:

$$\rho \left[u \frac{\partial u}{\partial r} + \frac{v}{r} \frac{\partial u}{\partial \varphi} + w \frac{\partial u}{\partial z} - \frac{v^2}{r} \right] = -\frac{\partial p}{\partial r} + \mu \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 u}{\partial \varphi^2} + \frac{\partial^2 u}{\partial z^2} - \frac{u}{r^2} - \frac{2}{r^2} \frac{\partial u}{\partial \varphi} \right]$$

$$+ \sigma \left(w B_1 B_3 - u B_3^2 - u B_2^2 + v B_1 B_2 \right)$$
(A.20)

 φ -component:

$$\rho \left[u \frac{\partial v}{\partial r} + \frac{v}{r} \frac{\partial v}{\partial \varphi} + w \frac{\partial v}{\partial z} + \frac{uv}{r} \right] = -\frac{1}{r} \frac{\partial p}{\partial \varphi} + \mu \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v}{\partial \varphi^2} + \frac{\partial^2 v}{\partial z^2} - \frac{v}{r^2} + \frac{2}{r} \frac{\partial v}{\partial \varphi} \right] + \sigma \left(u B_1 B_2 - v B_1^2 - v B_3^2 + w B_2 B_3 \right)$$
(A.21)

The non-dimensional steady state Navier-Stokes equations for z, r and φ -direction are, respectively:

z-component:

$$Re\left[U\frac{\partial W}{\partial R} + \frac{V}{R}\frac{\partial W}{\partial \varphi} + W\frac{\partial W}{\partial Z}\right] = -\frac{\partial P}{\partial Z} + \left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial W}{\partial R}\right) + \frac{1}{R^2}\frac{\partial^2 W}{\partial \varphi^2} + \frac{\partial^2 W}{\partial Z^2}\right] + \frac{Gr_T}{Re}\theta - \frac{Gr_c}{Re}C \quad (A.22) + Ha^2\left(VB_3^*B_2^* - WB_2^{*2} - WB_1^{*2} + UB_1^*B_3^*\right)$$

r-component:

$$Re\left[U\frac{\partial U}{\partial R} + \frac{V}{R}\frac{\partial U}{\partial \varphi} + W\frac{\partial U}{\partial Z} - \frac{V^2}{R}\right] =$$

$$-\frac{\partial P}{\partial R} + \left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial U}{\partial R}\right) + \frac{1}{R^2}\frac{\partial^2 U}{\partial \varphi^2} + \frac{\partial^2 U}{\partial Z^2} - \frac{U}{R} - \frac{2}{R^2}\frac{\partial U}{\partial \varphi}\right] \qquad (A.23)$$

$$+ Ha^2\left(WB_1^*B_3^* - UB_3^{*2} - UB_2^{*2} + VB_1^*B_2^*\right)$$

$$\varphi \text{ -component:}$$

$$Re\left[U\frac{\partial V}{\partial R} + \frac{V}{R}\frac{\partial V}{\partial \varphi} + W\frac{\partial Z}{\partial Z} + \frac{UV}{R}\right] =$$

$$-\frac{\partial P}{\partial \varphi} + \left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial V}{\partial R}\right) + \frac{1}{R^2}\frac{\partial^2 V}{\partial \varphi^2} + \frac{\partial^2 V}{\partial Z^2} - \frac{V}{R^2} + \frac{2}{R^2}\frac{\partial V}{\partial \varphi}\right]$$

+
$$Ha^{2}\left(UB_{1}^{*}B_{2}^{*}-VB_{1}^{*2}-VB_{3}^{*2}+WB_{2}^{*}B_{3}^{*}\right)$$

(A.24)

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APPENDIX B

NON-DIMENSIONALIZATION

B.1 Navier-Stokes Equations

z -Component

As mentioned before, the dimensional form of z-direction momentum equation

is:

$$\rho \left[u \frac{\partial w}{\partial r} + \frac{v}{r} \frac{\partial w}{\partial \varphi} + w \frac{\partial w}{\partial z} \right] = -\frac{\partial p}{\partial z} + \mu \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial w}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 w}{\partial \varphi^2} + \frac{\partial^2 w}{\partial z^2} \right] + \rho g \left[\beta_t (T - T_0) - \beta_c (c - c_0) \right] + \sigma \left(v B_3 B_2 - w B_2^2 - w B_1^2 + u B_1 B_3 \right)$$
(B.1)

First, all the non-dimensionalized variables are placed into the equation.

 $r = RD, \quad z = ZD, \quad u = Uu_o, \quad v = Vu_o, \quad w = Wu_o, \quad T - T_0 = \Delta T6, \quad c - c_o = \Delta cC$ $p = \frac{P\mu u_o}{D}, \quad B_1^* = \frac{B_1}{B_0}, \quad B_2^* = \frac{B_2}{B_0}, \text{ and } \quad B_3^* = \frac{B_3}{B_0}$

Therefore by substituting these variables inside the equation above:

$$\rho \left[Uu_{o} \frac{\partial (Wu_{o})}{\partial (RD)} + \frac{Vu_{o}}{RD} \frac{\partial (Wu_{o})}{\partial \varphi} + Wu_{o} \frac{\partial (Wu_{o})}{\partial (ZD)} \right] = -\frac{\partial \left(\frac{P\mu u_{o}}{D} \right)}{\partial (ZD)} + \mu \left[\frac{1}{RD} \frac{\partial}{\partial (RD)} \left(RD \frac{\partial (Wu_{o})}{\partial (RD)} \right) + \frac{1}{(RD)^{2}} \frac{\partial^{2} (Wu_{o})}{\partial \varphi^{2}} + \frac{\partial^{2} (Wu_{o})}{\partial (ZD)^{2}} \right] + \rho g \left[\beta_{\iota} \Delta T \theta \right] - \rho g \left[\beta_{c} \Delta cC \right] + \sigma \left(Vu_{o} B_{3}^{*} B_{o} B_{2}^{*} B_{o} - Wu_{o} B_{2}^{*2} B_{o}^{2} - Wu_{o} B_{1}^{*2} B_{o}^{2} + Uu_{o} B_{1}^{*} B_{o} B_{3}^{*} B_{o} \right)$$
(B.2)

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where B_1^* , B_2^* , and B_3^* are components of non-dimension magnetic field induction.

All the common variables are collected and extracted from the brackets. Then, the equations are divided by a factor chosen to simplify the equation. The equation above is divided by $\frac{\mu u_o}{D^2}$. $\frac{\rho u_o^2}{D} \left[U \frac{\partial W}{\partial R} + \frac{V}{R} \frac{\partial W}{\partial \varphi} + W \frac{\partial W}{\partial Z} \right] \frac{D^2}{\mu u_o} = -\frac{\mu u_o}{D^2} \frac{\partial P}{\partial Z} \cdot \frac{D^2}{\mu u_o} + \frac{\mu u_o}{D^2} \left[\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial W}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 W}{\partial \varphi^2} + \frac{\partial^2 W}{\partial Z^2} \right] \frac{D^2}{\mu u_o} + \frac{\rho g \left[\beta_i \Delta T \theta - \beta_c \Delta c C \right]}{\frac{\mu u_o}{D^2}} + \frac{\sigma B_o^2 u_o \left(V B_3^* B_2^* - W B_2^{*2} - W B_1^{*2} + U B_1^* B_3^* \right)}{\frac{\mu u_o}{D^2}}$ (B.3)

Now by organizing all the common factors it becomes:

$$\frac{\rho u_0 D}{\mu} \left[U \frac{\partial W}{\partial R} + \frac{V}{R} \frac{\partial W}{\partial \varphi} + W \frac{\partial W}{\partial Z} \right] = -\frac{\partial P}{\partial Z} + \left[\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial W}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 W}{\partial \varphi^2} + \frac{\partial^2 W}{\partial Z^2} \right] + \frac{\rho g D^2}{\mu u_0} \left[\beta_r \Delta T \theta - \beta_c \Delta c C \right] + \frac{\sigma B_0^2 D^2 \left(V B_3^* B_2^* - W B_2^{*2} - W B_1^{*2} + U B_1^* B_3^* \right)}{\mu}$$

(B.4)

Next the common factors are related to the non-dimensionalized terms.

This gives rise to the non-dimensionalized form of the z-component of the Navier-Stokes equation.

$$Re\left[U\frac{\partial W}{\partial R} + \frac{V}{R}\frac{\partial W}{\partial \varphi} + W\frac{\partial W}{\partial Z}\right] = -\frac{\partial P}{\partial Z} + \left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial W}{\partial R}\right) + \frac{1}{R^2}\frac{\partial^2 V}{\partial \varphi^2} + \frac{\partial^2 W}{\partial Z^2}\right] + \frac{Gr_T}{Re}\theta - \frac{Gr_c}{Re}C \qquad (B.5)$$

$$+ Ha^2\left(VB_3^*B_2^* - WB_2^{*2} - WB_1^{*2} + UB_1^*B_3^*\right)$$
r-Component

$$\rho\left[u\frac{\partial u}{\partial r} + \frac{v}{r}\frac{\partial u}{\partial \varphi} + w\frac{\partial u}{\partial z} - \frac{v^2}{r}\right] = -\frac{\partial P}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \varphi^2} + \frac{\partial^2 u}{\partial z^2} - \frac{u}{r^2} - \frac{2}{r^2}\frac{\partial u}{\partial \varphi}\right] + \sigma\left(wB_1B_3 - uB_3^2 - uB_2^2 + vB_1B_2^*\right)$$

Substituting the variables inside the equation above:

$$\rho \left[Uu_{o} \frac{\partial (Uu_{o})}{\partial (RD)} + \frac{Vu_{o}}{RD} \frac{\partial (Uu_{o})}{\partial \varphi} + Wu_{o} \frac{\partial (Uu_{o})}{\partial (ZD)} - \frac{(Vu_{o})^{2}}{(RD)} \right] = -\frac{\partial \left(\frac{P \mu u_{o}}{D}\right)}{\partial (RD)} + \mu \left[\frac{1}{RD} \frac{\partial (Uu_{o})}{\partial (RD)} \left(RD \frac{\partial (Uu_{o})}{\partial (RD)} \right) + \frac{1}{(RD)^{2}} \frac{\partial^{2} (Uu_{o})}{\partial \varphi^{2}} + \frac{\partial^{2} (Uu_{o})}{\partial (ZD)^{2}} - \frac{Uu_{o}}{R^{2}D^{2}} - \frac{2}{R^{2}D^{2}} \frac{\partial (Vu_{o})}{\partial \varphi} \right] + \sigma \left(Wu_{o}B_{1}^{*}B_{o}B_{3}^{*}B_{o} - Uu_{o}B_{3}^{*2}B_{o}^{2} - Uu_{o}B_{2}^{*2}B_{o}^{2} + Vu_{o}B_{1}^{*}B_{o}B_{3}^{*}B_{o} \right)$$
(B.7)

)

(B.6)

and then dividing by $\frac{\mu u_o}{D^2}$:

100

$$\frac{\rho u_0^2}{D} \left[U \frac{\partial U}{\partial R} + \frac{V}{R} \frac{\partial U}{\partial \varphi} + W \frac{\partial U}{\partial Z} - \frac{V^2}{R} \right] \cdot \frac{D^2}{\mu u_0} = -\frac{\mu u_0}{D^2} \frac{\partial P}{\partial R} \cdot \frac{D^2}{\mu u_0}$$
$$+ \frac{\mu u_0}{D^2} \left[\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial U}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 U}{\partial \varphi^2} + \frac{\partial^2 U}{\partial Z^2} - \frac{U}{R^2} - \frac{2}{R^2} \frac{\partial V}{\partial \varphi} \right] \cdot \frac{D^2}{\mu u_0} \quad (B.8)$$
$$+ \frac{\sigma B_0^2 u_0 \left(W B_1^* B_3^* - U B_3^{*2} - U B_2^{*2} + V B_1^* B_2^* \right)}{\frac{\mu u_0}{D^2}}$$

Now by organizing all common factors it becomes:

$$\frac{\rho u_0 D}{\mu} \left[U \frac{\partial U}{\partial R} + \frac{V}{R} \frac{\partial U}{\partial \varphi} + W \frac{\partial U}{\partial Z} \right] =$$

$$- \frac{\partial P}{\partial R} + \left[\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial U}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 U}{\partial \varphi^2} + \frac{\partial^2 U}{\partial Z^2} - \frac{U}{R^2} - \frac{2}{R^2} \frac{\partial V}{\partial \varphi} \right]$$

$$+ \frac{\sigma B_0^2 D^2 \left(V B_3^* B_2^* - W B_2^{*2} - W B_1^{*2} + U B_1^* B_3^* \right)}{\mu}$$
(B.9)

The non-dimensionalized form of the *r*- component of the Navier-Stokes equation would be:

$$Re\left[U\frac{\partial U}{\partial R} + \frac{V}{R}\frac{\partial U}{\partial \varphi} + W\frac{\partial U}{\partial Z}\right] = -\frac{\partial P}{\partial R} + \left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial U}{\partial R}\right) + \frac{1}{R^{2}}\frac{\partial^{2}U}{\partial \varphi^{2}} + \frac{\partial^{2}U}{\partial Z^{2}} - \frac{U}{R^{2}} - \frac{2}{R^{2}}\frac{\partial V}{\partial \varphi}\right] + \qquad (B.10)$$
$$Ha^{2}\left(WB_{1}^{*}B_{3}^{*} - UB_{3}^{*2} - UB_{2}^{*2} + VB_{1}^{*}B_{2}^{*}\right)$$
$$\varphi \text{-Component}$$

$$\rho \left[u \frac{\partial v}{\partial r} + \frac{v}{r} \frac{\partial v}{\partial \varphi} + w \frac{\partial v}{\partial z} + \frac{uv}{r} \right] = -\frac{1}{r} \frac{\partial p}{\partial \varphi} + \mu \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v}{\partial \varphi^2} + \frac{\partial^2 v}{\partial z^2} - \frac{v}{r^2} + \frac{2}{r^2} \frac{\partial v}{\partial \varphi} \right] + \sigma \left(u B_1 B_2 - v B_1^2 - v B_3^2 + w B_2 B_3 \right)$$
(B.11)

Substituting the variables inside the equation above:

$$\rho \left[\left(Uu_0 \right) \frac{\partial (Vu_0)}{\partial (RD)} + \frac{(Vu_0)}{(RD)} \frac{\partial (Vu_0)}{\partial \varphi} + (Wu_0) \frac{\partial (Vu_0)}{\partial (ZD)} + \frac{(Uu_0 Vu_0)}{(RD)} \right] = -\frac{1}{(RD)} \frac{\partial \left(\frac{p \mu u_0}{D} \right)}{\partial \varphi} + \mu \left[\frac{1}{(RD)} \frac{\partial (Vu_0)}{\partial (RD)} \left((RD) \frac{\partial (Vu_0)}{\partial (RD)} \right) + \frac{1}{(RD)^2} \frac{\partial^2 (Vu_0)}{\partial \varphi^2} + \frac{\partial^2 (Vu_0)}{\partial (ZD)^2} - \frac{Vu_0}{R^2 D^2} + \frac{2}{R^2 D^2} \frac{\partial (Vu_0)}{\partial \varphi} \right] + \sigma \left(Uu_0 B_1^* B_2^* - Vu_0 B_1^{*2} - Vu_0 B_3^{*2} + Wu B_2^* B_3^* \right)$$
(B.12)

and then dividing by
$$\frac{\mu u_o}{D^2}$$
:

$$\frac{\rho u_0^2}{D} \left[U \frac{\partial V}{\partial R} + \frac{V}{R} \frac{\partial V}{\partial \varphi} + W \frac{\partial V}{\partial Z} + \frac{UV}{R} \right] \frac{D^2}{\mu u_0} = -\frac{\mu u_0}{D^2} \frac{\partial P}{\partial \varphi} \frac{D^2}{\mu u_0} + \frac{\mu u_0}{D^2} \left[\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial V}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 V}{\partial \varphi^2} + \frac{\partial^2 V}{\partial Z^2} - \frac{V}{R^2} + \frac{2}{R^2} \frac{\partial V}{\partial \varphi} \right] + \frac{\sigma B_0^2 u_0}{D^2} \left(U B_1^* B_2^* - V B_1^{*2} - V B_3^{*2} + W B_2^* B_3^* \right)$$

(B.13)

Now by organizing all common factors it becomes:

$$\frac{\rho u_0 D}{\mu} \left[U \frac{\partial V}{\partial R} + \frac{V}{R} \frac{\partial V}{\partial \varphi} + W \frac{\partial V}{\partial Z} + \frac{UV}{R} \right] = \frac{1}{R} \frac{\partial P}{\partial \varphi} + \left[\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial V}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 V}{\partial \varphi^2} + \frac{\partial^2 V}{\partial Z^2} - \frac{V}{R^2} + \frac{2}{R^2} \frac{\partial V}{\partial \varphi} \right] + \frac{\partial B_0^2 D^2}{\mu} \left(U B_1^* B_2^* - V B_1^{*2} - V B_3^{*2} + W B_2^* B_3^* \right)$$
(B.14)

The non-dimensionalized form of the φ - component of the Navier-Stokes equation would be:

$$Re\left[U\frac{\partial V}{\partial R} + \frac{V}{R}\frac{\partial V}{\partial \varphi} + W\frac{\partial V}{\partial Z} + \frac{UV}{R}\right] = -\frac{1}{R}\frac{\partial P}{\partial \varphi} + \left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial V}{\partial R}\right) + \frac{1}{R^{2}}\frac{\partial^{2}V}{\partial \varphi^{2}} + \frac{\partial^{2}V}{\partial Z^{2}} - \frac{V}{R^{2}} + \frac{2}{R^{2}}\frac{\partial V}{\partial \varphi}\right]$$

$$+ Ha^{2}\left(UB_{1}^{*}B_{2}^{*} - VB_{1}^{*2} - VB_{3}^{*2}^{*2} + WB_{2}^{*}B_{3}^{*}\right)$$
(B.15)

B.2 Energy Equation

$$u\frac{\partial T}{\partial r} + \frac{v}{r}\frac{\partial T}{\partial \varphi} + w\frac{\partial T}{\partial z} = \frac{\kappa}{\rho c_p} \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 T}{\partial \varphi^2} + \frac{\partial^2 T}{\partial z^2}\right)$$
(B.16)

Substituting the variables inside the equation above:

$$\rho c_{p} \left[U u_{o} \frac{\partial (\Delta T \theta + T_{0})}{\partial (RD)} + \frac{V u_{0}}{(RD)} \frac{\partial (\Delta T + T_{0})}{\partial \varphi} + W u_{o} \frac{\partial (\Delta T \theta + T_{0})}{\partial (ZD)} \right] =$$

$$\kappa \left[\frac{1}{RD} \frac{\partial}{\partial (RD)} \left(RD \frac{\partial (\Delta T \theta + T_{o})}{\partial (RD)} \right) + \frac{1}{(RD)^{2}} \frac{\partial^{2} (\Delta T \theta + T_{0})}{\partial \varphi^{2}} + \frac{\partial^{2} (\Lambda T \theta + T_{o})}{\partial (ZD)^{2}} \right]$$
(B.17)

Now by organizing all common factors it becomes:

$$\frac{\rho c_{p} u_{0} \Delta T}{D} \left[U \frac{\partial \theta}{\partial R} + \frac{V}{R} \frac{\partial \theta}{\partial \varphi} + W \frac{\partial \theta}{\partial Z} \right] = \frac{\kappa \Delta T}{D^{2}} \left[\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial \theta}{\partial R} \right) + \frac{1}{R^{2}} \frac{\partial^{2} T}{\partial \varphi^{2}} + \frac{\partial^{2} \theta}{\partial Z^{2}} \right]$$
(B.18)

By multiplying and dividing μ to the left hand side of the equation above:

$$\frac{\rho c_{p} u_{0} D}{\kappa} \cdot \frac{\mu}{\mu} \left[U \frac{\partial \theta}{\partial R} + \frac{V}{R} \frac{\partial \theta}{\partial \varphi} + W \frac{\partial \theta}{\partial Z} \right] = \left[\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial \theta}{\partial R} \right) + \frac{1}{R^{2}} \frac{\partial^{2} T}{\partial \varphi^{2}} + \frac{\partial^{2} \theta}{\partial Z^{2}} \right]$$
(B.19)

Therefore:

$$Re Pr\left[U\frac{\partial\theta}{\partial R} + \frac{V}{R}\frac{\partial\theta}{\partial\varphi} + W\frac{\partial\theta}{\partial Z}\right] = \left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial\theta}{\partial R}\right) + \frac{1}{R^2}\frac{\partial^2 T}{\partial\varphi^2} + \frac{\partial^2 \theta}{\partial Z^2}\right]$$
(B.20)

B.3 Continuity Equation

$$\frac{1}{r}\frac{\partial}{\partial r}(ru) + \frac{1}{r}\frac{\partial v}{\partial \varphi} + \frac{\partial w}{\partial z} = 0$$
(B.21)

Substituting the variables inside the equation above:

$$\frac{1}{(RD)}\frac{\partial}{\partial(RD)}(RDUu_0) + \frac{1}{(RD)}\frac{\partial(Vu_0)}{\partial\varphi} + \frac{\partial(Wu_0)}{\partial(ZD)} = 0$$
(B.22)

and then

$$\frac{1}{R}\frac{\partial}{\partial R}(RU) + \frac{1}{R}\frac{\partial V}{\partial \varphi} + \frac{\partial W}{\partial Z} = 0$$
(B.23)

B.4 Solute Equation

$$u\frac{\partial c}{\partial r} + \frac{v}{r}\frac{\partial c}{\partial \varphi} + w\frac{\partial c}{\partial z} = \alpha_c \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 c}{\partial \varphi^2} + \frac{\partial^2 c}{\partial z^2}\right)$$
(B.24)

Substituting the variables inside the equation above:

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$$\rho \left[Uu_{o} \frac{\partial (C\Delta c + c_{o})}{\partial (RD)} + \frac{Vu_{0}}{(RD)} \frac{\partial (C\Delta c + c_{0})}{\partial \varphi} + Wu_{o} \frac{\partial (C\Delta c + c_{o})}{\partial (ZD)} \right] = \rho \alpha_{c} \left[\frac{1}{(RD)} \frac{\partial}{\partial (RD)} \left((RD) \frac{\partial (C\Delta c + c_{o})}{\partial (RD)} \right) + \frac{1}{(RD)^{2}} \frac{\partial^{2} (C\Delta c + c_{0})}{\partial \varphi} + \frac{\partial^{2} (C\Delta c + c_{o})}{\partial (ZD)^{2}} \right]$$
(B.25)

Now by organizing all common factors it becomes:

$$\frac{\rho u_0 \Delta c}{D} \left[U \frac{\partial C}{\partial R} + \frac{V}{R} \frac{\partial C}{\partial \varphi} + W \frac{\partial C}{\partial Z} \right] = \frac{\rho \alpha_c \Delta c}{D^2} \left[\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial C}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 C}{\partial \varphi} + \frac{\partial^2 C}{\partial Z^2} \right] (B.26)$$

By multiplying and dividing v to the left hand side of the equation above:

$$\frac{u_0 D}{\alpha_c} \frac{v}{v} \left[U \frac{\partial C}{\partial R} + \frac{V}{R} \frac{\partial C}{\partial \varphi} + W \frac{\partial C}{\partial Z} \right] = \left[\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial C}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 C}{\partial \varphi} + \frac{\partial^2 C}{\partial Z^2} \right]$$
(B.27)

Therefore:

$$Re\left[U\frac{\partial C}{\partial R} + \frac{V}{R}\frac{\partial C}{\partial \varphi} + W\frac{\partial C}{\partial Z}\right] = \frac{1}{Sc}\left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial C}{\partial R}\right) + \frac{1}{R^{2}}\frac{\partial^{2}C}{\partial \varphi^{2}} + \frac{\partial^{2}C}{\partial Z^{2}}\right]$$
(B.28)

APPENDIX C

DEFINITION OF NON-DIMENSIONAL

Name	Definition	Parameter	
Reynolds	inertia force viscous force	$Re = \frac{\rho u_o D}{\mu}$	
Magnetic Reynolds	<u>convection</u> diffusion	$Re_m = \mu_{\circ} \sigma u_0 D$	
Prandtl	momentum thermal diffusivities	$\Pr = \frac{c_p \mu}{\kappa}$	
Schmidt	viscous force solutal diffusivity	$S_C = \frac{v}{\alpha_c}$	
Thermal Grashof	buoyancy force viscous force	$Gr_T = \frac{\beta_T \Delta T g D^3 \rho^2}{\mu^2}$	
Solutal Grashof	buoyancy force viscous force	$Gr_c = \frac{\beta_c \Delta T g D^3 \rho^2}{\mu^2}$	
Hartmann	magnétic force viscous force	$Ha = \boldsymbol{B}_0 D \sqrt{\frac{\sigma}{\mu}}$	

PARAMETERS

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APPENDIX D

PHYSICAL PROPERTIES

Table 2 Physical properties of GeSi growth by TSM used in the simulation [45]

Physical Properties of Ge _{0.85} Si _{0.15}		Physical Properties of Ge _{0.98} Si _{0.02}		Physical Properties of Ge	
c _p	$0.04008 J/g \cdot K$	c _p	$0.04008 J/g \cdot K$	c _p	$0.0390 J/g \cdot K$
T_m	1100° <i>C</i>	L_f	39 cal/g	T _m	935°C
α _c	$2.6 \times 10^{-4} cm^2/s$		944.7° <i>C</i>	α _c	$1.0 \times 10^{-4} \ cm^2/s$
α_T	$1.43 \times 10^{-1} cm^2/s$	ac	$0.52 \times 10^{-4} \ cm^2/s$	α _T	$1.16 \times 10^{-1} \ cm^2/s$
β _c	0.005 1/at.%Si	β _c	0.005 1/at.%Si	β _c	0.005 1/at.%Si
β,	$1.1 \times 10^{-4} \ 1/^{o}C$	β _t	1.1×10 ⁻⁴ 1/°C	βι	1.1×10 ⁻⁴ 1/°C
к	$0.2905W/cm\cdot K$	ĸ	$0.2559W/cm\cdot K$	к	$0.25W/cm\cdot K$
μ	$7.4 \times 10^{-3} g/cm \cdot s$	μ	$8.3496 \times 10^{-3} g/cm \cdot s$	μ	$8.5 \times 10^{-3} g/cm \cdot s$
ν	$1.46 \times 10^{-3} \ cm^2/s$	ν	$1.53192 \times 10^{-3} \ cm^2/s$	ν	$1.5424 \times 10^{-3} cm^2/s$
ρ	$5.06785 g/cm^3$	ρ	$5.4504 g/cm^3$	ρ	$5.51 g/cm^3$
		σ	2.5×10^4 S/cm		

APPENDIX E

INPUT FILES

E.1 Input File for the Terrestrial Condition

```
/ *****
/ Disclaimer: The geometry and the grids are written by GAMBIT and contains
/ all the continuum and boundary entities and coordinate systems
/ defined in GAMBIT. Additionally, some frequently used FIPREP
/ commands are added. Modifying/Adding any necessary commands are applied in
/ FIPREP (FIDAP input file).
/ Refer to FIPREP documentation for complete listing of commands.
/ *****
1
     CONVERSION OF NEUTRAL FILE TO FIDAP Database
1
1
FICONV(NEUTRAL)
INPUT( FILE="60x240.FDNEUT" )
OUTPUT( DELETE )
END
1
TITLE
60x240- B=0.0
1
FIPREP
1
     PROBLEM SETUP
1
```

1

1

EXECUTION(NEWJOB)

PROBLEM (3-D, NONLINEAR, BUOYANCY, FREE, BUOYANCY =1)

PRINTOUT(NONE)

DATAPRINT(CONTROL)

/ CONTINUUM ENTITIES

.

```
RENUMBER( PROFILE )
```

ENTITY (NAME = "source", SOLID, PROPERTY = "source")

ENTITY (NAME = "solvent", FLUID, PROPERTY = "solvent", SPECIES = 1, MDIFF = 3, MEXP = 3)

ENTITY (NAME = "substrate", FLUID, PROPERTY = "substrate", SPECIES = 1, MDIFF = 3

```
/
```

/ BOUNDARY ENTITIES

1 -

)

```
ENTITY ( NAME = "top", PLOT, ATTACH = "source" )
```

ENTITY (NAME = "outflow", PLOT, ATTACH = "solvent")

```
ENTITY ( NAME = "inflow", MELT, ATTACH = "solvent", NATTACH = "substrate",
MSPHT = "solvent", DEPTH = -1, SPECIES = 1, M1LIQU = "solvent")
```

```
ENTITY ( NAME = "bottom", SURFACE, SPINE, STRAIGHT, DEPTH = 0, CONTINUE,
```

ATTACH = "substrate")

ENTITY (NAME = "profile1", PLOT)

ENTITY (NAME = "profile2", PLOT)

ENTITY (NAME = "profile3", PLOT)

ENTITY (NAME = "interface", PLOT, ATTACH = "solvent")

ENTITY(NAME = "inferfacedge", PLOT, ATTACH = "solvent")

LIQUIDUS(SET = "solvent", CONSTANT = 12.56, TEMPERATURE)

/ LOCAL COORDINATE SYSTEMS DEFINED

1 .

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/ SOLUTION PARAMETERS

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SOLUTION(SEGREGATED = 450)

PRESSURE(MIXED = 1.E-8, DISCONTINUOUS)

/RELAX(HYBRID)

OPTIONS(UPWINDING)

UPWIND(1STO)

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MATERIAL PROPERTIES

```
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```

/ Partial list of Material Properties data

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DENSITY(SET = "source", CONSTANT = 233, TYP2, TEMPERATURE, SPECIES = 1)

```
VISCOSITY(SET = "source", CONSTANT = 1)
```

```
CONDUCTIVITY(SET = "source", CONSTANT = 1)
```

SPECIFICHEAT(SET = "source", CONSTANT = 2.25E-2)

VOLUMEXPANSION(SET = "source", CONSTANT = 1, TEMPERATURE)

1 .

DENSITY(SET = "solvent", CONSTANT = 450, TYP2, TEMPERATURE, SPECIES = 1)

VISCOSITY(SET = "solvent", CONSTANT = 1)

CONDUCTIVITY(SET = "solvent", CONSTANT = 1)

SPECIFICHEAT(SET = "solvent", CONSTANT = 7E-3, LATENT = 2.23, TMELT = 36)

VOLUMEXPANSION(SET = "solvent", CONSTANT = 1, TEMPERATURE)

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1 VOLUMEXPANSION(SET =3, CONSTANT = 42, SPECIES = 1) DIFFUSIVITY(SET = 3, CONSTANT = 1.587E-4, SPECIES = 1) 1 /DENSITY(SET = "substrate", CONSTANT = 409, TYP2, TEMPERATURE, SPECIES = 1) VISCOSITY(SET = "substrate", CONSTANT = 1) CONDUCTIVITY(SET = "substrate", CONSTANT = 1) SPECIFICHEAT(SET = "substrate", CONSTANT = 7E-3) VOLUMEXPANSION(SET = "substrate", CONSTANT = 1, TEMPERATURE) 1 INITIAL AND BOUNDARY CONDITIONS 1 /ICNODE(, CONSTANT = 0, ALL)1 /BODYFORCE(ENTITY = "solvent", LORENTZ = 2, VXB = 1, FZ = 10) /BCNODE(SPECIES = 2, CONSTANT = 0, ENTITY = "solvent")

/BCNODE(SPECIES = 2, CONSTANT = 0, ENTITY = "source")

/BCNODE(SPECIES = 2, CONSTANT = 0, ENTITY = "substrate")

BCNODE(SURFACE,ZERO, ENTITY = "inferfacedge") BCNODE(SURFACE, ZERO, ENTITY = "bottom")

BCNODE(SPECIES = 1, CONSTANT = 0.15, ENTITY = "source") BCNODE(SPECIES = 1, CONSTANT = 0.02, ENTITY = "inflow") BCNODE(SPECIES = 1, CONSTANT = 0.15, ENTITY = "outflow")

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```
BCNODE( VELOCITY, CONSTANT = 0, ENTITY = "source" )
BCNODE( VELOCITY, CONSTANT = 0, ENTITY = "substrate" )
/
```

BCNODE(COORDINATE, ENTITY = "inferfacedge")

BCSYSTEM(SET = 1, EDGE)

1.

BCNODE(VELOCITY, CONSTANT = 0, ENTITY = "top") BCNODE(VELOCITY, CONSTANT = 0, ENTITY = "bottom") BCNODE(VELOCITY, CONSTANT = 0, ENTITY = "profile1") BCNODE(VELOCITY, CONSTANT = 0, ENTITY = "profile2") BCNODE(VELOCITY, CONSTANT = 0, ENTITY = "profile3") BCNODE(VELOCITY, CONSTANT = 0, ENTITY = "profile3") -171.491674619836000 -23.468172284192400 0 0 1 784.323802803643000 0 0 2 -

825.939526461064000 0 0 3 338.295844875043000 0 0 4 -62.326428754429800 0 0 5 4.325223592473780 0 0 6

BCNODE(TEMPERATURE, POLYNOMIAL = 6, ENTITY = "profile2")

 -171.491674619836000
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 784.323802803643000
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 825.939526461064000
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 338.295844875043000
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 4
 -62.326428754429800
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BCNODE(TEMPERATURE, POLYNOMIAL = 6, ENTITY = "profile3")

 -171.491674619836000
 -23.468172284192400
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 0
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 784.323802803643000
 0
 0
 2

 825.939526461064000
 0
 0
 3
 338.295844875043000
 0
 0
 4
 -62.326428754429800
 0
 0
 5

 4.325223592473780
 0
 0
 6
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END

1

CREATE(FIPREP, DELETE)

PARAMETER(LIST)

CREATE(FISOLV)

/RUN(FISOLV, FOREGROUND)

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E.2 Input File for the Microgravity Condition

```
/ Disclaimer: The geometry and the grids are written by GAMBIT and contains
/ all the continuum and boundary entities and coordinate systems
/ defined in GAMBIT. Additionally, some frequently used FIPREP
/ commands are added. Modifying/Adding any necessary commands are applied in
/ FIPREP (FIDAP input file).
/ Refer to FIPREP documentation for complete listing of commands.
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     CONVERSION OF NEUTRAL FILE TO FIDAP Database
FICONV(NEUTRAL)
INPUT( FILE="60x240.FDNEUT" )
OUTPUT( DELETE )
END
1
TITLE
60x240-Microgravity
1
FIPREP
1
1
    PROBLEM SETUP
```

1

PROBLEM (3-D, NONLINEAR, BUOYANCY, FREE, BUOYANCY =1)

EXECUTION(NEWJOB)

PRINTOUT(NONE)

```
DATAPRINT( CONTROL )
```

```
/ CONTINUUM ENTITIES
```

```
1
```

RENUMBER(PROFILE)

ENTITY (NAME = "source", SOLID, PROPERTY = "source")

ENTITY (NAME = "solvent", FLUID, PROPERTY = "solvent", SPECIES = 1, MDIFF = 3, MEXP = 3)

ENTITY (NAME = "substrate", FLUID, PROPERTY = "substrate", SPECIES = 1, MDIFF = 3

/ BOUNDARY ENTITIES

/

)

1

```
ENTITY (NAME = "top", PLOT, ATTACH = "source")
```

ENTITY (NAME = "outflow", PLOT, ATTACH = "solvent")

ENTITY (NAME = "inflow", MELT, ATTACH = "solvent", NATTACH = "substrate",

MSPHT = "solvent", DEPTH = -1, SPECIES = 1, M1LIQU = "solvent")

```
ENTITY (NAME = "bottom", SURFACE, SPINE, STRAIGHT, DEPTH = 0, CONTINUE,
```

```
ATTACH = "substrate" )
```

```
ENTITY (NAME = "profile1", PLOT)
```

ENTITY (NAME = "profile2", PLOT)

ENTITY (NAME = "profile3", PLOT)

ENTITY (NAME = "interface", PLOT, ATTACH = "solvent")

```
ENTITY( NAME = "inferfacedge", PLOT, ATTACH = "solvent" )
```

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LIQUIDUS(SET = "solvent", CONSTANT = 12.56, TEMPERATURE)

LOCAL COORDINATE SYSTEMS DEFINED

SOLUTION PARAMETERS

1

SOLUTION(SEGREGATED = 450)

PRESSURE(MIXED = 1.E-8, DISCONTINUOUS)

/RELAX(HYBRID)

OPTIONS(UPWINDING)

UPWIND(1STO)

1

/ MATERIAL PROPERTIES

1

/ Partial list of Material Properties data

1

DENSITY(SET = "source", CONSTANT = 233, TYP2, TEMPERATURE, SPECIES = 1)

VISCOSITY(SET = "source", CONSTANT = 1)

CONDUCTIVITY(SET = "source", CONSTANT = 1)

SPECIFICHEAT(SET = "source", CONSTANT = 2.25E-2)

VOLUMEXPANSION(SET = "source", CONSTANT = 1, TEMPERATURE)

1

1

DENSITY(SET = "solvent", CONSTANT = 450, TYP2, TEMPERATURE, SPECIES = 1)

VISCOSITY(SET = "solvent", CONSTANT = 1)

CONDUCTIVITY(SET = "solvent", CONSTANT = 1)

SPECIFICHEAT(SET = "solvent", CONSTANT = 7E-3, LATENT = 2.23, TMELT = 36)

VOLUMEXPANSION(SET = "solvent", CONSTANT = 1, TEMPERATURE)

GRAVITY(MAGNITUDE = 0.0001)

VOLUMEXPANSION(SET =3, CONSTANT = 42, SPECIES = 1) DIFFUSIVITY(SET = 3, CONSTANT = 1.587E-4, SPECIES = 1)

1

1

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1

/DENSITY(SET = "substrate", CONSTANT = 409, TYP2, TEMPERATURE, SPECIES = 1)

VISCOSITY(SET = "substrate", CONSTANT = 1)

CONDUCTIVITY(SET = "substrate", CONSTANT = 1)

SPECIFICHEAT(SET = "substrate", CONSTANT = 7E-3)

VOLUMEXPANSION(SET = "substrate", CONSTANT = 1, TEMPERATURE)

/ INITIAL AND BOUNDARY CONDITIONS

/ICNODE(, CONSTANT = 0, ALL)

/BODYFORCE(ENTITY = "solvent", LORENTZ = 2, VXB = 1, FZ = 10)
/BCNODE(SPECIES = 2, CONSTANT = 0, ENTITY = "solvent")
/BCNODE(SPECIES = 2, CONSTANT = 0, ENTITY = "source")
/BCNODE(SPECIES = 2, CONSTANT = 0, ENTITY = "substrate")

BCNODE(SURFACE, ZERO, ENTITY = "inferfacedge") BCNODE(SURFACE, ZERO, ENTITY = "bottom")

BCNODE(SPECIES = 1, CONSTANT = 0.15, ENTITY = "source") BCNODE(SPECIES = 1, CONSTANT = 0.02, ENTITY = "inflow") BCNODE(SPECIES = 1, CONSTANT = 0.15, ENTITY = "outflow")

BCNODE(VELOCITY, CONSTANT = 0, ENTITY = "source") BCNODE(VELOCITY, CONSTANT = 0, ENTITY = "substrate")

BCNODE(COORDINATE, ENTITY = "inferfacedge")

BCSYSTEM(SET = 1, EDGE)

1

BCNODE(VELOCITY, CONSTANT = 0, ENTITY = "top") BCNODE(VELOCITY, CONSTANT = 0, ENTITY = "bottom") BCNODE(VELOCITY, CONSTANT = 0, ENTITY = "profile1") BCNODE(VELOCITY, CONSTANT = 0, ENTITY = "profile2") BCNODE(VELOCITY, CONSTANT = 0, ENTITY = "profile3") BCNODE(TEMPERATURE, POLYNOMIAL = 6, ENTITY = "profile1") -171.491674619836000 -23.468172284192400 0 0 1 784.323802803643000 0 0 2 -825.939526461064000 0 0 3 338.295844875043000 0 0 4 -62.326428754429800 0 0 5 4.325223592473780 0 0 6

BCNODE(TEMPERATURE, POLYNOMIAL = 6, ENTITY = "profile2")

 -171.491674619836000
 -23.468172284192400
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 784.323802803643000
 0
 0
 2

 825.939526461064000
 0
 0
 3
 338.295844875043000
 0
 0
 4
 -62.326428754429800
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 4.325223592473780
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BCNODE(TEMPERATURE, POLYNOMIAL = 6, ENTITY = "profile3")

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 1
 784.323802803643000
 0
 0
 2

 825.939526461064000
 0
 0
 3
 338.295844875043000
 0
 0
 4
 -62.326428754429800
 0
 0
 5

 4.325223592473780
 0
 0
 6
 <td

/

END

/

CREATE(FIPREP, DELETE)

PARAMETER(LIST)

CREATE(FISOLV)

/RUN(FISOLV, FOREGROUND)

E.3 Input File for the applied Magnetic Field (B=0.2KG)

/ Disclaimer: The geometry and the grids are written by GAMBIT and contains

/ all the continuum and boundary entities and coordinate systems

/ defined in GAMBIT. Additionally, some frequently used FIPREP

/ commands are added. Modifying/Adding any necessary commands are applied in / FIPREP (FIDAP input file).

/ Refer to FIPREP documentation for complete listing of commands.

CONVERSION OF NEUTRAL FILE TO FIDAP Database

```
FICONV(NEUTRAL)
```

INPUT(FILE="60x240.FDNEUT")

OUTPUT(DELETE)

END

1

1

1

1

```
TITLE
```

60x240-B=0.3KG

/

FIPREP

1

/ PROBLEM SETUP

1

PROBLEM (3-D, NONLINEAR, BUOYANCY, FREE, BUOYANCY =1, BUOYANCY = 2) EXECUTION(NEWJOB)

PRINTOUT(NONE)

```
DATAPRINT( CONTROL )
```

```
/ CONTINUUM ENTITIES
```

1

```
RENUMBER( PROFILE )
```

```
ENTITY (NAME = "source", SOLID, PROPERTY = "source")
```

```
ENTITY (NAME = "solvent", FLUID, PROPERTY = "solvent", SPECIES = 1, MDIFF = 3,
```

```
MEXP = 3)
```

ENTITY (NAME = "substrate", FLUID, PROPERTY = "substrate", SPECIES = 1, MDIFF = 3

```
)
```

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```
/ BOUNDARY ENTITIES
```

```
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```

```
ENTITY (NAME = "top", PLOT, ATTACH = "source")
```

```
ENTITY ( NAME = "outflow", PLOT, ATTACH = "solvent" )
```

ENTITY (NAME = "inflow", MELT, ATTACH = "solvent", NATTACH = "substrate",

MSPHT = "solvent", DEPTH = -1, SPECIES = 1, M1LIQU = "solvent")

```
ENTITY ( NAME = "bottom", SURFACE, SPINE, STRAIGHT, DEPTH = 0, CONTINUE,
```

```
ATTACH = "substrate" )
```

```
ENTITY (NAME = "profile1", PLOT)
```

```
ENTITY (NAME = "profile2", PLOT)
```

```
ENTITY (NAME = "profile3", PLOT)
```

```
ENTITY (NAME = "interface", PLOT, ATTACH = "solvent")
```

```
ENTITY( NAME = "inferfacedge", PLOT, ATTACH = "solvent" )
```

```
1
```

1

```
LIQUIDUS( SET = "solvent", CONSTANT = 12.56, TEMPERATURE )
```

/ LOCAL COORDINATE SYSTEMS DEFINED

```
1
     SOLUTION PARAMETERS
1
1
SOLUTION(SEGREGATED = 450)
PRESSURE( MIXED = 1.E-8, DISCONTINUOUS )
/RELAX(HYBRID)
OPTIONS( UPWINDING )
UPWIND(1STO)
1
     MATERIAL PROPERTIES
1
1
/ Partial list of Material Properties data
1
DENSITY( SET = "source", CONSTANT = 233, TYP2, TEMPERATURE, SPECIES = 1)
VISCOSITY(SET = "source", CONSTANT = 1)
CONDUCTIVITY(SET = "source", CONSTANT = 1)
SPECIFICHEAT(SET = "source", CONSTANT = 2.25E-2)
VOLUMEXPANSION( SET = "source", CONSTANT = 1, TEMPERATURE )
1
DENSITY( SET = "solvent", CONSTANT = 450, TYP2, TEMPERATURE, SPECIES = 1)
VISCOSITY(SET = "solvent", CONSTANT = 1)
CONDUCTIVITY(SET = "solvent", CONSTANT = 1)
SPECIFICHEAT(SET = "solvent", CONSTANT = 7E-3, LATENT = 2.23, TMELT = 36)
VOLUMEXPANSION(SET = "solvent", CONSTANT = 1, TEMPERATURE)
GRAVITY(MAGNITUDE = 1)
1
VOLUMEXPANSION(SET =3, CONSTANT = 42, SPECIES = 1)
DIFFUSIVITY(SET = 3, CONSTANT = 1.587E-4, SPECIES = 1)
```

```
/
```

```
/DENSITY(SET = "substrate", CONSTANT = 409, TYP2, TEMPERATURE, SPECIES = 1)
VISCOSITY(SET = "substrate", CONSTANT = 1)
CONDUCTIVITY( SET = "substrate", CONSTANT = 1)
SPECIFICHEAT(SET = "substrate", CONSTANT = 7E-3)
VOLUMEXPANSION(SET = "substrate", CONSTANT = 1, TEMPERATURE)
1
1
     INITIAL AND BOUNDARY CONDITIONS
1
/ICNODE(, CONSTANT = 0, ALL)
1
BODYFORCE(ENTITY = "solvent", LORENTZ = 2, VXB = 1, FZC = 1.74963553)
BCNODE( SPECIES = 2, CONSTANT = 0, ENTITY = "solvent")
BCNODE( SPECIES = 2, CONSTANT = 0, ENTITY = "source")
BCNODE( SPECIES = 2, CONSTANT = 0, ENTITY = "substrate" )
1
1
1
BCNODE( SURFACE,ZERO, ENTITY = "inferfacedge" )
BCNODE( SURFACE, ZERO, ENTITY = "bottom" )
1
BCNODE( SPECIES = 1, CONSTANT = 0.15, ENTITY = "source")
BCNODE( SPECIES = 1, CONSTANT = 0.02, ENTITY = "inflow" )
BCNODE( SPECIES = 1, CONSTANT = 0.15, ENTITY = "outflow")
1
BCNODE(VELOCITY, CONSTANT = 0, ENTITY = "source")
BCNODE( VELOCITY, CONSTANT = 0, ENTITY = "substrate")
1
```

```
BCNODE( COORDINATE, ENTITY = "inferfacedge" )
```

```
BCSYSTEM(SET = 1, EDGE)
```

```
BCNODE( VELOCITY, CONSTANT = 0, ENTITY = "top" )
BCNODE( VELOCITY, CONSTANT = 0, ENTITY = "bottom")
BCNODE( VELOCITY, CONSTANT = 0, ENTITY = "profile1" )
BCNODE( VELOCITY, CONSTANT = 0, ENTITY = "profile2" )
BCNODE( VELOCITY, CONSTANT = 0, ENTITY = "profile3")
BCNODE( TEMPERATURE, POLYNOMIAL = 6, ENTITY = "profile1")
825.939526461064000 0 0 3 338.295844875043000 0 0 4 -62.326428754429800 0 0 5
4.325223592473780006
BCNODE( TEMPERATURE, POLYNOMIAL = 6, ENTITY = "profile2")
-171.491674619836000 \\ -23.468172284192400 \\ 0 \\ 0 \\ 1 \\ 784.323802803643000 \\ 0 \\ 0 \\ 2 \\ -
825.939526461064000 0 0 3 338.295844875043000 0 0 4 -62.326428754429800 0 0 5
4,325223592473780006
BCNODE( TEMPERATURE, POLYNOMIAL = 6, ENTITY = "profile3")
825.939526461064000 0 0 3 338.295844875043000 0 0 4 -62.326428754429800 0 0 5
4,325223592473780006
1
END
1
CREATE(FIPREP, DELETE)
```

PARAMETER(LIST)

CREATE(FISOLV)

/RUN(FISOLV, FOREGROUND)