Numerical Simulation of Transport Processes during Growth of Single Crystal using Czochralski Crystal Growth Technique

Ph.D. Synopsis

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1. Title of thesis and abstract

Title:Numerical Simulation of Transport Processes during Growth of Single Crystal using Czochralski Crystal Growth Technique.

Abstract

A numerical simulation approach has been adopted to simulate melt flow inside a Czochralski (CZ) setup crucible. Conservation equations of mass, momentum, energy and oxygen species have been solved using finite volume method approach. Effect of location of zero Gauss plane (ZGP) on oxygen concentration at crystal melt interface for growth of silicon single crystal, for laminar flow inside the crucible has been investigated. ZGP location for the CUSP magnetic field has been moved above and below the melt free surface by 10% of the melt height. Crucible melt of aspect ratio 1, 0.5 and 0.25 corresponding to high, moderate and low melt height inside the crucible have been taken into consideration. Oxygen concentration at crystal melt interface reduces with reduction of melt aspect ratio, irrespective of the ZGP location. Melt flow structure for low aspect ratio breaks down into two toroidal cells as compared to single cell structure for higher melt aspect ratio. Oxygen concentration at crystal melt interface varies along the radius of the crystal for high aspect ratio melt. Effect of change of location of ZGP on oxygen species incorporated into growing crystal depends on the melt aspect ratio.

Flow inside an industrial scale CZ setup used to grow 450 mm silicon crystal is turbulent in nature. Reynolds Average Navier Stoke's equation have been solved numerically to simulate melt motion and resulting oxygen concentration in an industrial scale CZ crucible. Low Reynolds number formulation two equation model by Launder and Jones has been used for resolving near wall flow. Effect of location of ZGP in relation to the crystal melt interface has been investigated for magnetic field of 0.04 T and 0.2 T. Melt aspect ratio 0.5 show higher oxygen concentration for magnetic field of 0.2 T where as melt aspect ratio of 0.25 has higher oxygen concentration at melt crystal interface for 0.04 T magnetic field. There exist radial variation of oxygen species at the melt crystal interface for melt aspect ratio of 1, where as it is uniform for melt aspect ratio of 0.5 and 0.25.

Type of thermal boundary condition imposed at the crucible surface greatly effects the temperature and there by the melt flow inside the CZ crucible. Numerical investigation has been carried out to study the effect of thermal boundary condition on turbulent melt flow and oxygen transfer inside a crucible used to grow 450mm diameter silicon single crystal using CZ method. Two types of thermal boundary conditions, namely, isothermal crucible surface and experimentally measured temperatures on the crucible surface have been imposed on the crucible wall and crucible bottom. Melt motion owing to buoyancy, surface tension variation at the free melt surface as well as crystal and crucible rotation has been considered. Effect of externally imposed CUSP magnetic field has also been investigated. Melt having aspect ratio of 1 and 0.5, representing high, and moderate level of melt inside the crucible have been considered. Melt motion governed by natural convection, Marangoni convection and crystal as well as crucible rotation shows higher oxygen concentration at melt crystal interface for aspect ratio of 1, when experimental temperature profile is imposed at the crucible wall. Maximum turbulent viscosity values for aspect ratio of 1, in case of experimental temperature at the crucible

are higher compared to isothermal case, which is just the opposite of the trend for aspect ratio of 0.5. Imposing a CUSP magnetic field leads to similar distribution of turbulent viscosity for both types of thermal boundary conditions. Oxygen concentration at the melt crystal interface is found to be higher in presence of CUSP magnetic field. Value of maximum turbulent viscosity for the two boundary conditions is similar for melt aspect ratio of 1. Crucible surface temperature profile for aspect ratio of 1, on actual melt aspect ratio of 0.5 predicts lower oxygen concentration at melt crystal interface. Values and distribution of turbulent viscosity are however the same for both temperature profiles.

2. Brief description on the state of the art of the research topic

Single crystal that form the backbone of semiconductor industry are grown using Czochralski (CZ) crystal growth technique. Over the years many researchers have investigated the problems related to CZ crystal growth system and number of studies related to different aspects of CZ crystal growth are available in open literature. The original method of crystal growth developed by Jana Czochralski in 1917 has undergone many modifications leading to the present day state of the art growth facilities capable of growing 350-400 mm diameter crystal [1].

Flow inside a CZ melt is essentially driven by combination of: (1) Natural convection (NC) arising out of temperature dependent density variations, (2) Forced convection owing to crystal and crucible rotation and (3) Surface tension variation at the free surface owing to variation of temperature, i.e. Marangoni convection (MC). Strength of these flow mechanism is denoted by the dimensionless numbers **Ra (Rayleigh number)**, **Re (Reynolds number**) due to crystal/crucible rotation and **Ma (Marangoni number)**. The forces driving convection are not present to the same extent in each melt growth system and their magnitude varies depending on the melt configuration and crystal growth conditions.

Understanding the effect of combination of all of the above three on heat and species transport phenomena in the melt pool is essential to grow high quality semiconductor crystal. Flow situation is further complicated under the influence of an externally applied magnetic field, which is a norm for the present day large diameter crystal growth system. Three types of magnetic field, namely, axial, transverse and inhomogeneous (CUSP) are tradionally imposed to control and manipulate flow inside the crucible melt.

Single crystal using Czochralski (CZ) technique are generally grown using silica or quartz crucible. Impurities arising out of crucible wall are transferred to melt interface by melt convection, where they may be incorporated into the growing crystal, thus deteriorating the crystal quality. Oxygen is one of the most important impurities in commercial silicon crystal grown using CZ technique. Oxygen releases from crucible surface and its incorporation into the growing crystal is one of the major concerns in CZ growth of silicon crystal. Silicon in melt form attacks the silica crucible surface which results in release of oxygen from the crucible surface. Oxygen released at the crucible surface is picked up by the bulk melt flow and is transferred to melt free surface and melt crystal interface. Transfer of oxygen by diffusion is small compared to that by melt convection as the value of Schmidt (Sc) number for oxygen in silicon melt is around 10 [2]. At the melt free surface, silicon combines with oxygen to form SiO which is volatile in nature. The SiO thus formed evaporates from the free surface. Precise control of oxygen along the radial and axial direction of the crystal is paramount for growing crystal with necessary electronic properties.

In actual practice, with growth of solid crystal, the melt height in the crucible reduces which in turn reduces the strength of buoyant convection. Also enforcing the zero gauss plane (ZGP) for a CUSP magnetic field to coincide exactly with the melt free surface calls for stringent control of movement of crucible along the axis or movement of current carrying coils. This might lead to misalignment of the ZGP in relation to melt free surface and thus alter the magnitude and direction of Lorentz force acting on the melt fluid.

3. Definition of the problem

Investigation of melt motion and and transport of oxygen species inside a CZ crucible for growth of silicon single crystal, via numerical simulation has been done. Height of liquid melt inside the crucible drops with growth of solid crystal owing to solidification of liquid. Melt height characterized by aspect ratio of 1, 0.5 and 0.25 representing high, moderate and low level of melt inside the crucible have been taken into consideration. Crystal radius is taken to be 450 mm, which reflects the actual trend of demand of large size crystal by the semiconductor industry. A CUSP magnetic field is imposed to control the melt motion inside the crucible via the action of Lorentz force. Location of ZGP in changed with respect to the melt free surface. Effect of isothermal crucible and experimental temperature at the crucible surface on melt flow has been studied.

4. Objective and scope of work

Objectives of the present numerical investigation are to:

- Simulate laminar as well as turbulent flow owing to combined effect of natural convection, Marangoni convection and rotation of crystal as well as crucible rotation, inside a CZ melt crucible used for growth of silicon crystal.

- Investigate the effect of location of zero Gauss plane in relation to the melt free surface, on laminar as well as turbulent melt flow and the resulting oxygen concentration at the melt crystal interface.

- Investigate the effect of the type of temperature profile imposed on the crucible inner surface on the resulting turbulent melt flow and oxygen incorporated into the growing crystal.

5. Original contribution by the thesis

Owing to growth of the solid crystal from the melt inside the crucible, height of fluid column reduces, which in turn effects the melt motion inside the crucible. Effort has been made to bring out the effect of location of ZGP in relation to the crystal melt interface on oxygen concentration at the melt crystal interface, for melt characterized by different aspect ratio. Growth parameters relating to 450 mm diameter crystal, which reflects the size of the crystal grown in today's CZ industrial growth set up have been used for simulation.

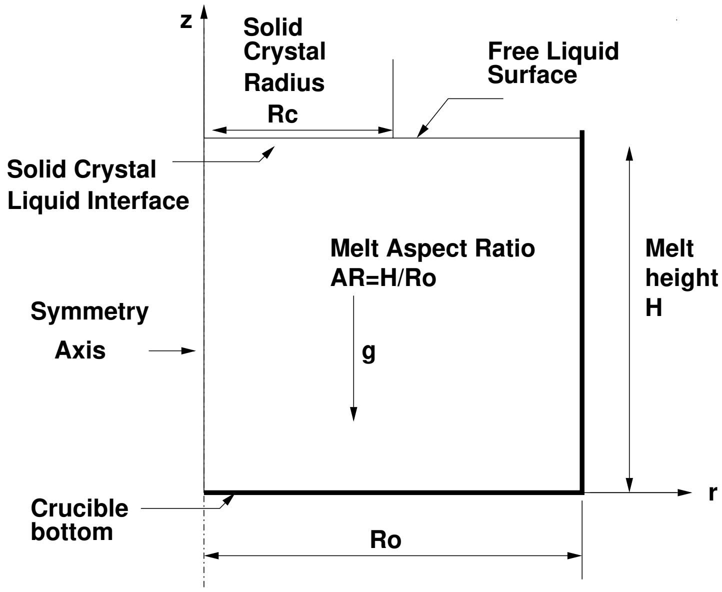
Numerical simulation related to CZ system often use experimental temperature profile measured along the crucible, as a boundary condition. The data of such type is however limited and hence simulations are also carried out considering crucible to be an isothermal surface. Effect of the above two approach on melt flow and oxygen transfer in growth of silicon crystal has been discussed. Comparison has been made for melt characterized by aspect ratio of 1 and 0.5.

Often, owing to lack of experimental data, temperature profile measured at crucible surface on melt having a given aspect ratio is used as boundary information on crucible characterized by a different melt aspect ratio all togather. Effect of imposing experimental temperature at crucible surface for melt aspect ratio 1, on a CZ crucible having aspect ratio of 0.5 has been discussed.

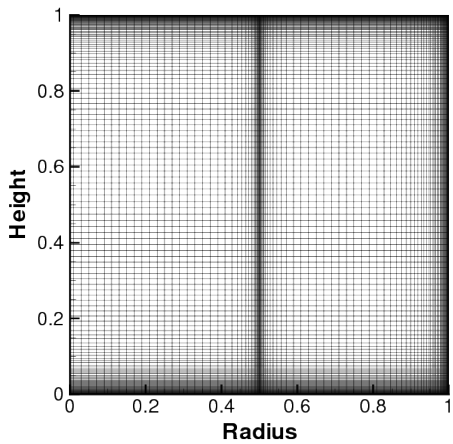
6. Methodology of research and results

6.1 Laminar Flow inside Czochralski setup crucible - Validation

Laminar flow inside an idealized Czochralski setup crucible show in Fig. 1(a) has been simulated by solving equation of conservation of mass, conservation of momentum, conservation of energy and conservation of species. Finite volume method based approach described by Ferziger and Peric [3] has been adopted with use of SIMPLE algorithm by Patankar [4] for pressure velocity coupling. The mesh used for numerical simulation is shown in Fig. 1(b). Care has been taken to refine the mesh near the solid boundaries to resolve the boundary layer gradients, as well as in the zone near intersection of free melt surface and the solid crystal.



(a)



(b)

Figure 1: Schematic of a Czochralski crystal growth system crucible and computation mesh.

Actual flow inside a CZ crucible is a result of complex interaction of buoyancy driven natural convention (NC), surface tension variation driven Marangoni convection (MC) and rotation of crystal as well as crucible. However, for sake of validation of numerical simulation, at a time the flow inside the crucible has been considered to be governed by one of the above three governing mechanisms. Validation of simulation results has been done by comparison with benchmark results published in the literature.

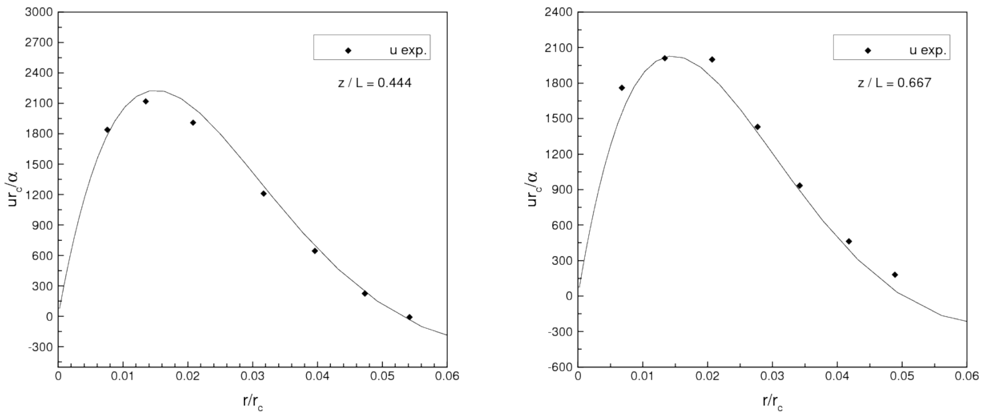


Figure 2: Axial velocity in zone near the cylinder vertical surface - comparison of numerical results with experimental observation of Hess and Miller.

Laminar natural convection inside a vertical cylindrical geometry has been investigated by Hess and Miller [5]. Variation of axial component of velocity near the solid vertical surface of the cylinder at different planes characterized by constant height from the bottom of the cylinder is shown in Fig. 2.

Owing to variation of temperature at the free surface of the fluid, there is a variation of surface tension. The resulting imbalance of force along the free surface leads to flow of fluid from hot surface toward the cold surface (when surface tension drops with rise in temperature). This is known as Marangoni convection. Experimental investigation of surface tension driven flow inside a 2-D cavity has been carried out by Schwabe and Metzger [6]. Numerical simulation of flow inside a similar geometry has been studied by Buckle and Peric [7]. Variation of velocity along the vertical plane, obtained from numerical simulation has been compared with the results published by Buckle and Peric [7] and shown in Fig. 3.

Benchmark results for four test problems of flow inside a CZ crucible proposed by A. A. Wheeler [8] have been provided by Buckle and Schafer [9]. Streamline contours for rotation of crucible alone as well as rotation of crystal and crucible simultaneously are shown in Fig. 4. Values of maximum and minimum stream function for different flow cases are shown in Table 1.

6.2 Effect of change of zero Gauss plane location on oxygen concentration at melt crystal interface - Laminar flow

Effect of change in melt aspect ratio for buoyancy driven flow inside a CZ crucible with the zero Gauss plane (ZGP) at the melt crystal interface is shown in Fig. 5. Oxygen concentration is found

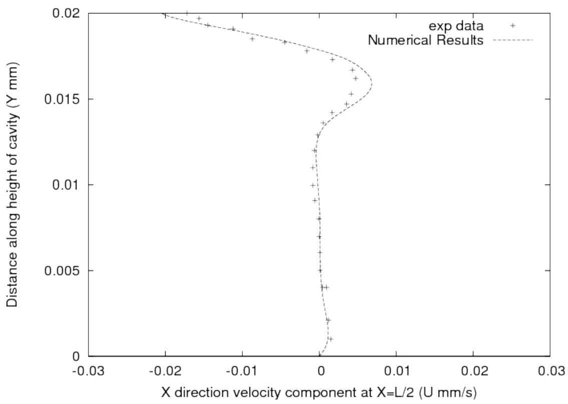
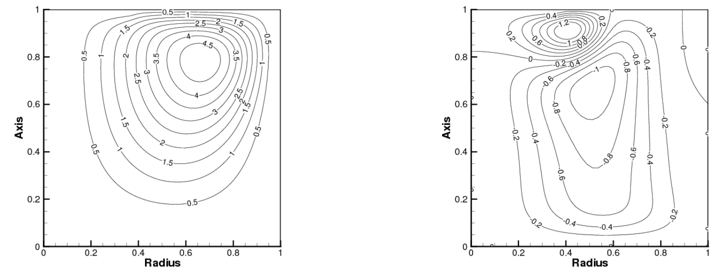


Figure 3: Variation of x direction velocity along the mid vertical plane for a surface tension driven flow



(a) Crystal rotation, Re = 1.0e03.

(b) Crystal rotation, Re = 1.0e03 and crucible rotation, Re=-2.5e02.

Figure 4: Streamline contours for flow driven by crystal and crucible.

to decrease with reduction in melt height characterized by lower aspect ratio. Also, the lower aspect ratio melt shows a remarkable uniform distribution of oxygen species at the crystal melt interface, a characteristic vital for growth of good quality single crystal. On the other hand, significant variation of radial oxygen concentration exists, nearer to the crystal surface for a large melt height.

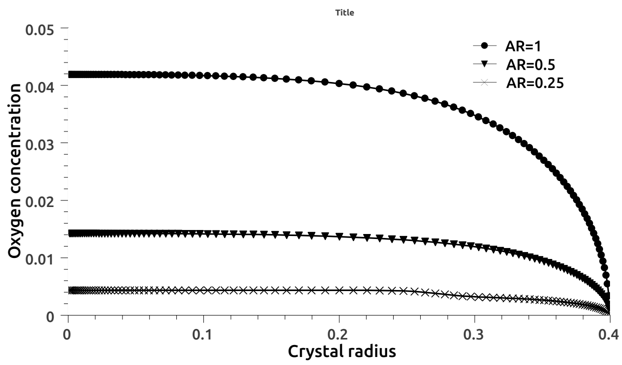


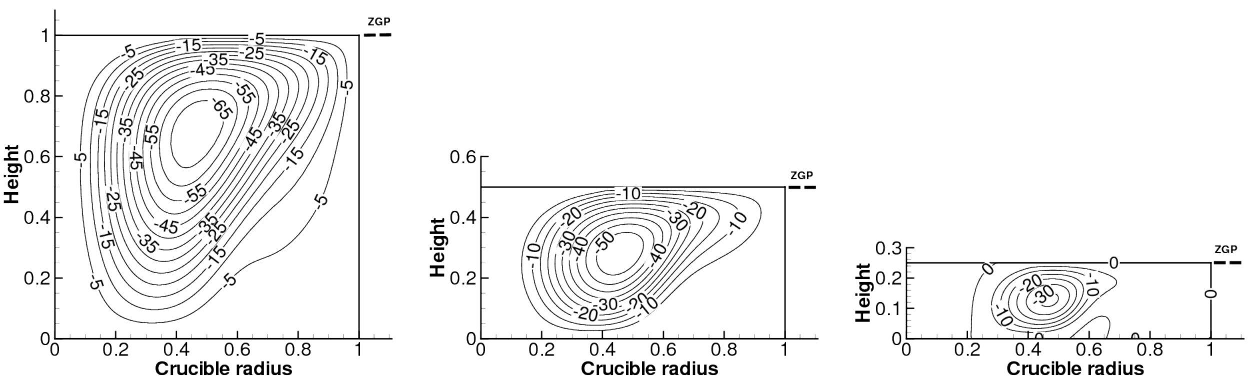
Figure 5: Oxygen concentration at crystal melt interface with ZGP at crystal melt interface

Streamline contours inside the melt for all three aspect ratio is shown in Fig. 6. Strength of buoyancy driven flow reduces with reduction in melt height inside the crucible. Flow strength near the crucible bottom in zone adjacent to wall is significantly slower owing to action of Lorentz force. Crucible base and wall wetted by melt acts as source of oxygen which is then advected by bulk flow. Single cell rotating in anticlockwise direction for melt AR of 1 carries oxygen to the growing crystal melt interface. Owing to relatively strong flow coupled with larger wetted area at the crucible wall,

Table 1: Laminar flow inside CZ crucible, comparison of numerical data with those published in literature [9]

				Values from literature		Simulation values	
Case	**Grashoff Number**	**Crystal Reynolds number**	**Crucible Reynolds number**	ψ_{min}	ψ_{max}	ψ_{min}	ψ_{max}
A1	0	1.0e02	0	-2.3447e01	1.5632e-06	-2.2342e01	1.427e-06
A2	0	1.0e03	0	-5.3642	1.5257e-04	-5.1954	1.4476e-04
A3	0	1.0e04	0	-4.0443e01	1.9320e-01	-4.1206e01	1.9290e-01
B1	0	1.0e02	-2.5e01	-5.0203e-01	1.11796e-01	-4.9823e-01	1.1931e-01
B2	0	1.0e03	-2.5e02	-1.6835	1.2414	-1.6872	1.3052
D1	1.0e05	1.0e01	0	-4.7092e-04	2.8420e01	-4.532e-04	2.8252e01
D2	1.0e05	1.0e02	0	-4.7057e-04	2.8393e01	-4.634e-04	2.7936e01
D3	1.0e05	1.0e03	0	-6.5631e-01	2.4829e01	-6.3631e-01	2.5499e01

the oxygen concentration at the crystal melt interface is found to be higher. Oxygen free melt flowing along the melt free surface meets the crystal surface resulting in low oxygen concentration at crystal periphery. Bulk flow carries and transfers oxygen from crucible wall and bottom to zone below crystal melt interface near the axis, resulting in a higher oxygen species concentration for AR of 1.

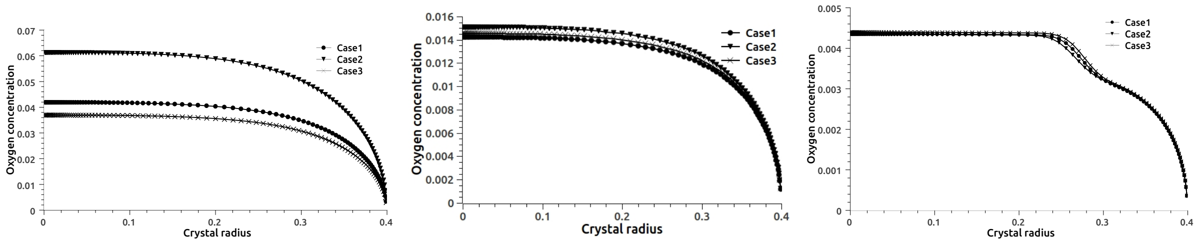


(a) AR=1 (b) AR=0.5 (c) AR=0.25

Figure 6: Streamline contours for laminar flow inside buoyancy driven CZ melt with ZGP at the melt crystal interface.

Effect of change of ZGP location in relation to the melt free surface, on oxygen incorporated in the growing crystal is shown in Fig. 7. **Case 1** corresponds to ZGP at melt crystal interface. ZGP below and above the melt free surface by 10% of the melt height is characterized as **case 2** and **case 3** respectively. It can be seen that for melt aspect ratio of 1, the oxygen concentration at crystal melt interface increases when ZGP moves into the melt and decreases if ZGP is above the melt free surface. For lower melt height characterized by AR of 0.25, the effect is opposite to that for AR of 1.

The flow strength inside the melt, for AR value of 1 is found to increase for case 2 and decrease for case 3 as seen in Fig. 8. This is owing to fact that size of melt zone under effect of Lorentz force increases when ZGP moves above the melt free surface. Movement of ZGP above or below the melt free surface, for AR of 0.25 has no significant change in flow situation below the crystal melt interface. Thus the radial variation of oxygen species in bulk crystal for AR of 0.25 with change in



(a) AR=1 (b) AR=0.5 (c) AR=0.25

Figure 7: Oxygen concentration variation at crystal melt interface for laminar flow inside the melt.

ZGP location is insignificant when compared to that for AR of 1 as seen in Fig. 7. For melt aspect ratio of 0.5, oxygen concentration at crystal melt interface is found to increase for case 2 as well as case 3. However the increase in concentration as well as distribution of oxygen species does not show a significant variation.

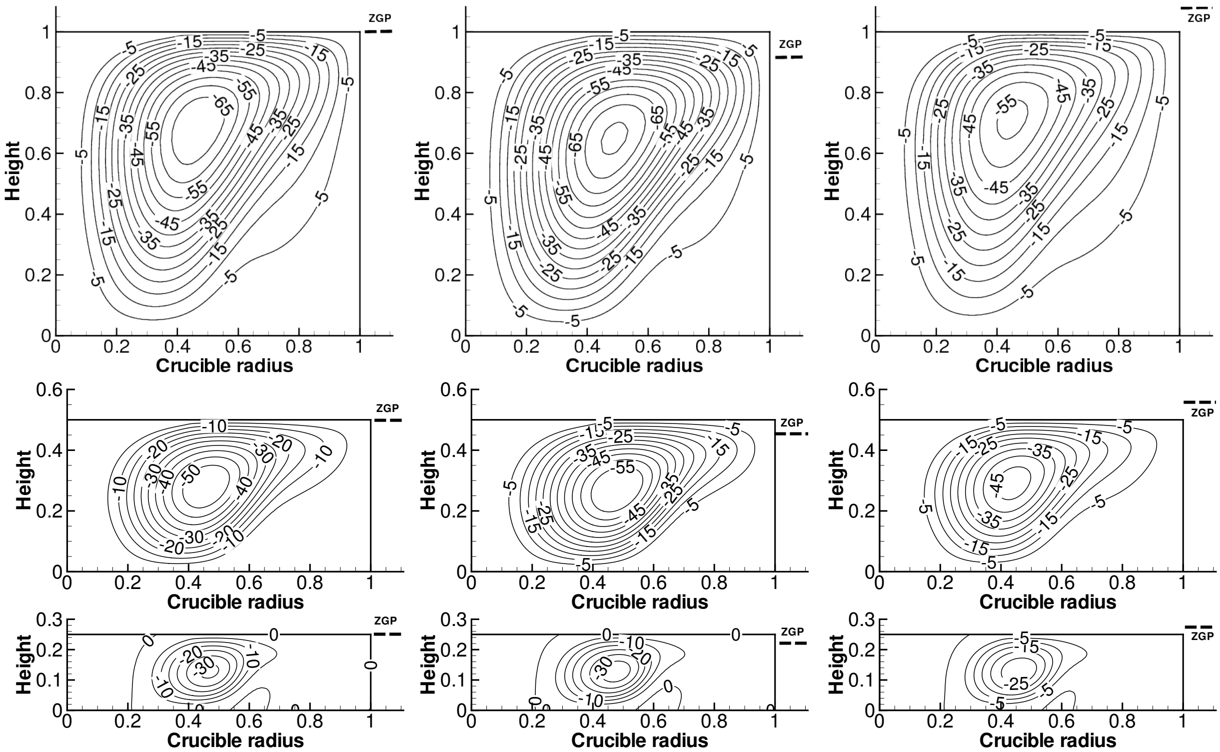


Figure 8: Streamline contours for melt aspect ratio of 1, 0.5 and 0.25. Location of ZGP show by dashed line.

6.3 Turbulent flow inside Czochralski setup crucible - Validation

Turbulent flow inside CZ crucible used to grow 450 mm diameter silicon crystal has been simulated by solving Reynolds Average Navier Stokes (RANS) equation. Low Reynolds number formulation given by Launder and Jones [10] has been adopted for resolving near wall turbulent boundary layer. Details of the mathematical model like non-dimensional form of the governing equations, boundary conditions and discretization scheme are as described by Lipchin and Brown [11]. Streamline contours and turbulent viscosity contours inside the melt of aspect ratio 1.0, for buoyancy driven flow characterized by Rayleigh number 2.0e11 is shown in Fig. 9. Comparison of numerical simulation data with those published in literature [11] is shown in Table 2.

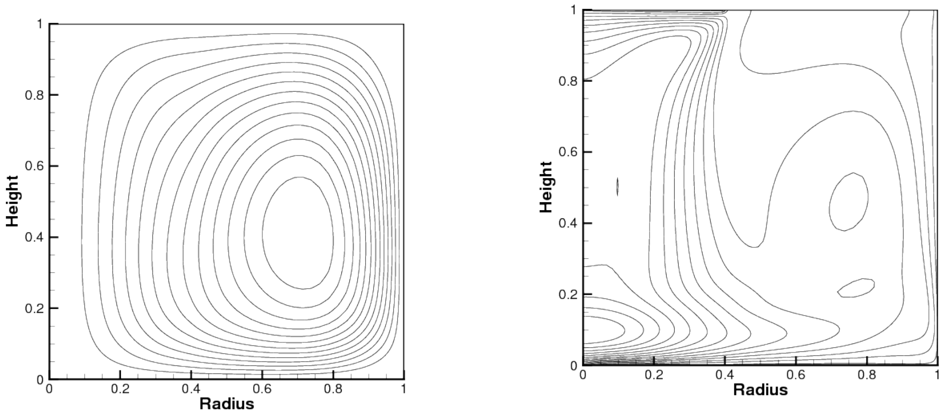


Figure 9: Streamline and isotherm contours for turbulent natural convection, Ra=2.0e11and Pr=0.11.

Table 2: Comparison of present numerical values with those reported in literature [11].

	ψ_{max}	ψ_{min}	**Nusselt number at crucible base**	**Nusselt number along side wall**	$(\nu_t)_{max}$
Values from literature - NC	6.97e-03	-0.69e-05	27.8	2.89	459
Present simulation values	6.92e-03	-7.03e-05	27.9	2.87	461.32

6.4 Effect of change of zero Gauss plane location on oxygen concentration at melt crystal interface - Turbulent flow

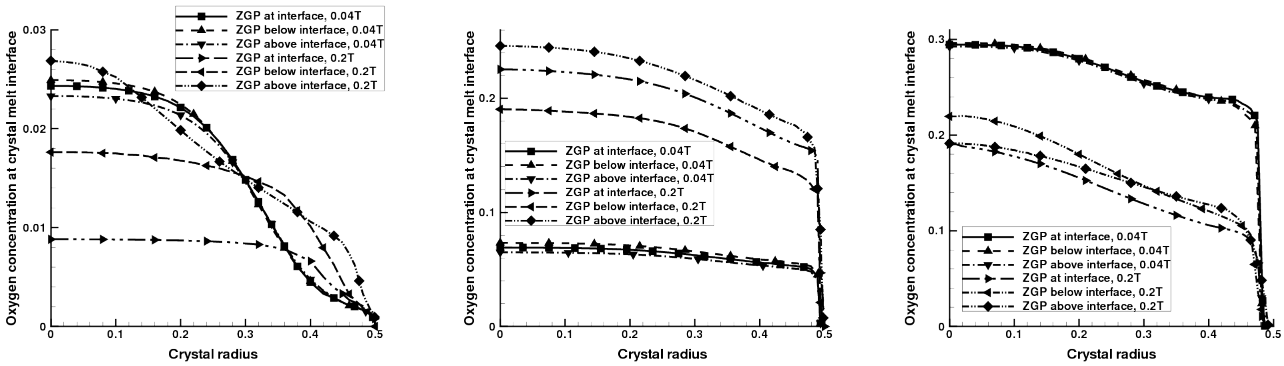
Growth of a 450 mm diameter silicon single crystal in presence of a CUSP magnetic field has been investigated via numerical simulation. Details of non dimensional form of governing equation, boundary conditions, turbulence model are listed by Lipchin and Brown [11]. Flow inside the melt is governed by natural convection, Marangoni convection coupled with crystal and crucible rotation in opposite direction. Effect of location of ZGP at the melt crystal interface, 10% above the melt crystal interface and 10% below the melt crystal interface has been taken into consideration to study the variation of oxygen incorporated into the growing crystal. Equation for scalar electric potential and boundary condition for the same are listed by S. Jana et al. [12]. Melt flow is characterized by non-dimensional parameters listed in Table 3. The values are based on reference height of 450 mm, 225 mm and 125 mm for melt aspect ratio of 1, 0.5 and 0.25 respectively. Property values for silicon are borrowed from work of A. Raufeisen et al. [13].

Oxygen variation at crystal melt interface with change in ZGP in relation to the melt free surface is shown in Fig. 10. Magnetic field of strength 0.04 T and 0.2 T have been imposed on the the melt.

Melt having aspect ratio of 1 shows higher oxygen species concentration at the melt crystal interface for 0.04 T magnetic field. However, for ZGP located at the melt free surface, 0.2 T magnetic

Table 3: Governing non dimensional parameters related to turbulent flow for melt of different aspect ratio

Aspect ratio	Grashoff number	Crucible Reynolds number	Crystal Reynolds number	Marangoni number	Hartmann number
AR = 1	2.92e10	3.11e05	-12.46e05	7.46e04	697.13 (0.04T) 3659.96 (0.2T)
AR = 0.5	3.65e09	0.78e05	-3.11e05	3.73e03	348.56 (0.04T) 1742.84 (0.2T)
AR = 0.25	4.56e08	0.19e05	-0.78e05	1.86e03	174.28 (0.04T) 871.39 (0.2T)



(a) AR=1 (b) AR=0.5 (c) AR=0.25

Figure 10: Oxygen concentration variation at the melt crystal interface for turbulent flow inside the melt.

field shows higher oxygen concentration at the melt crystal interface as compared to that for 0.04 T magnetic field strength. There exists radial oxygen concentration variation for magnetic field of 0.2 T as well as 0.04 T, irrespective of the location of ZGP.

For melt aspect ratio of 0.5, magnetic field on 0.2 T shows higher oxygen concentration at the crystal melt interface as compared to magnetic field of 0.04 T strength.The difference in concentration with change in ZGP location is negligible for 0.04 T magnetic field. For melt characterized by aspect ratio of 0.25, 0.04 T magnetic field shows higher oxygen concentration as compared to the oxygen concentration for 0.2 T magnetic field. There is radial uniformity in distribution of oxygen species for melt aspect ratio of 0.5 and 0.25, irrespective of strength of magnetic field and ZGP location.

6.5 Effect of type of thermal boundary condition at the crucible surface

Effect of two types of thermal boundary conditions namely, isothermal crucible surface and experimentally observed crucible surface temperature values, on temperature dependent melt flow inside a CZ crucible used to grow a 450 mm diameter silicon crystal has been investigated. Temperature profile at the crucible surface for aspect ratio 1.0 has been borrowed from experimental observation by Hirata and Hoshikawa [14]. For melt aspect ratio of 0.5, temperature at crucible surface have been measured by Grabner et al. [15] and is shown in Fig.11. Similar temperature profile has also been used for numerical DNS and LES simulation of turbulent flow inside a CZ crucible [13, 16].

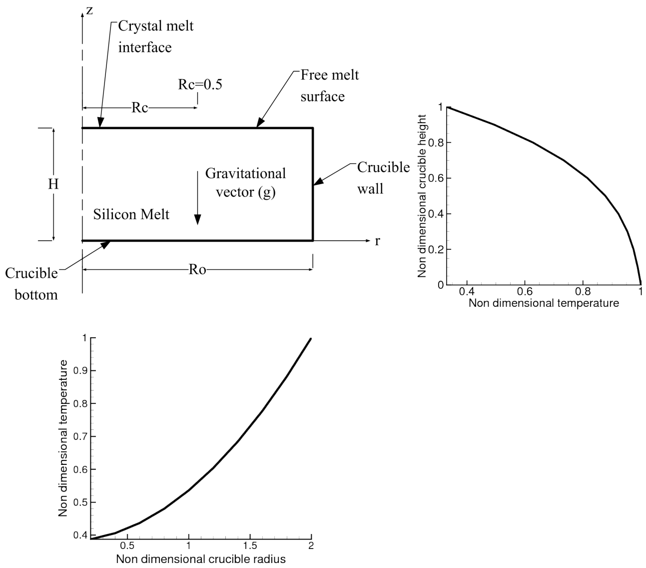


Figure 11: Temperature profile at crucible surface for melt aspect ratio of 0.5 based on experimental data [15] .

Flow inside the CZ crucible has been broken into four cases to investigate the effect of type of thermal boundary condition at the crucible surface. These are namely: (1) Natural convection driven melt flow, (2) Natural convection coupled with Marangoni convection at the melt free surface, (3) Natural convection, Marangoni convection with rotation of crystal and crucible and (4) Natural convection, Marangoni convection with rotation of crystal and crucible in presence of a CUSP magnetic field.

However, results for flow governed by natural convection, Marangoni convection coupled with rotation of crystal and crucible, with and without a CUSP magnetic field are discussed, as this relates closely to the actual CZ crystal growth industrial scenario. Values of governing non dimensional parameter are similar to those listed in Table 3. Magnetic field strength is assumed to be 0.2 T. Variation of oxygen concentration at the melt crystal interface for flow governed by natural convection, Marangoni convection and crystal as well as crucible rotation is shown in Fig. 12. For melt aspect ratio of 1, experimental temperature profile at the crucible wall results in higher oxygen concentration at melt crystal interface compared to isothermal boundary condition. However, for melt aspect ratio of 0.5 the trend is just the opposite of the above.

Streamline contours shown in Fig. 13 shows flow breaking into multi cellular structure in presence of crystal and crucible rotation. In case of isothermal boundary condition, strong counter clockwise rotating cell transfers oxygen rich fluid from bottom of crucible wall to the melt crystal interface.

Turbulent viscosity contours for melt aspect ratio 1 and 0.5 shown in Fig. 14 shows presence of low turbulent viscosity intensity melt below the crystal near the axis of the crucible. However, the values of turbulent viscosity in the said zone are higher for isothermal crucible boundary condition when melt aspect ratio is 0.5.

A CUSP magnetic field imposed on the melt flow governed by natural convection, Marangoni convection and crystal as well as crucible rotation results in significant slowdown in melt flow strength owing to the presence of Lorentz force, as seen from stream lines in Fig. 15. Melt motion inside the crucible breaks down into two cells rotating in opposite directions for melt aspect ratio of 1 as well as

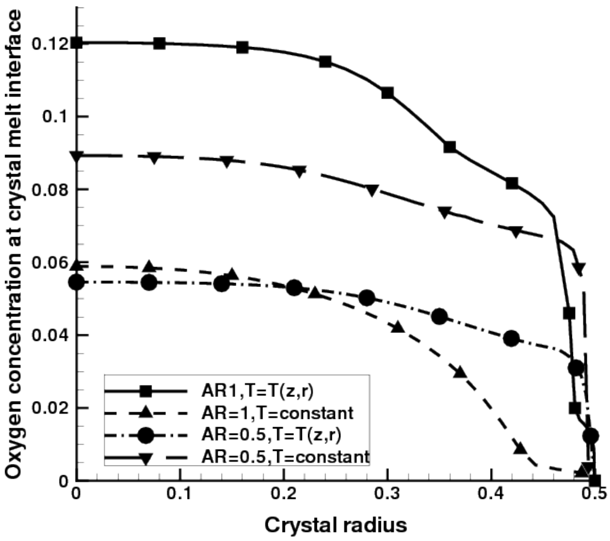
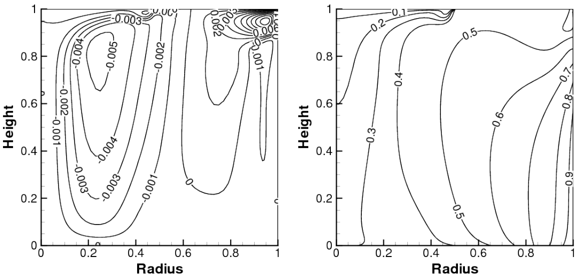
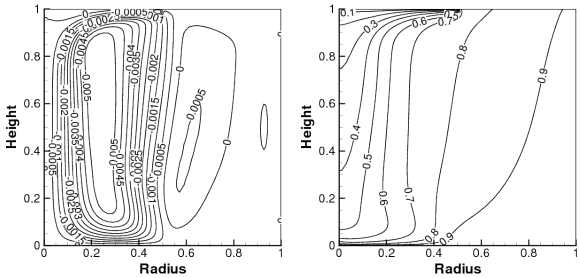


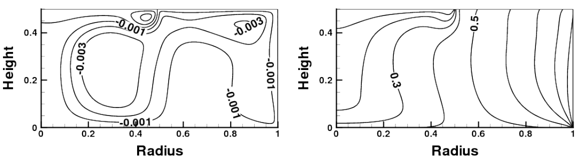
Figure 12: Oxygen variation at the crystal melt interface for natural convection combined with Marangoni convection and crystal as well as crucible rotation



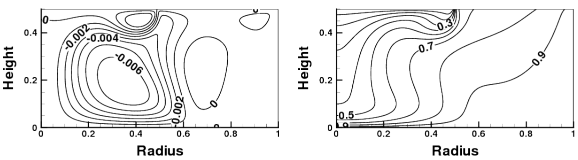
(a) Experimental temperature at crucible surface, AR=1



(b) Isothermal crucible surface, AR=1



(c) Experimental temperature at crucible, AR=0.5



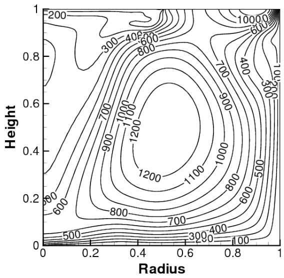
(d) Isothermal crucible surface, AR=0.5.

Figure 13: Streamline and isotherm contours for buoyancy driven flow coupled with Marangoni convection as well as crystal and crucible rotation.

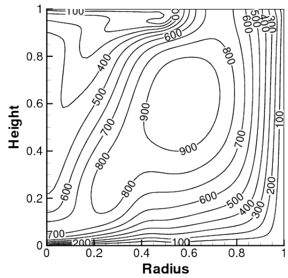
0.5.

Oxygen concentration at the melt crystal interface in presence of CUPS magnetic field shows a better radial uniformity as compared to case without magnetic field presence, as seen in Fig. 16. For melt aspect ratio of 1, presence of magnetic field results in lower oxygen concentration at melt crystal interface when experimental temperature is imposed at the crucible surface, as compared to isothermal scenario. This trend is just the opposite to all flow cases in absences of magnetic field. Values of oxygen concentration at the melt crystal interface are found to increase which can be attributed to the clockwise rotating cell below the crystal that transfers oxygen rich fluid from crucible bottom to the solidification zone below the crystal surface.

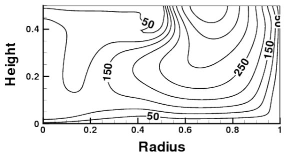
Value of maximum turbulent viscosity for different flow governing mechanisms considered is listed in Table 4. Value of maximum turbulent viscosity for melt aspect ratio of 0.5 is lower when compared to that of melt aspect ratio of 1, for similar flow mechanism and thermal boundary condition. This is expected as lower aspect ratio relates to drop in melt height and hence lower values



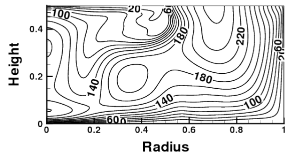
(a) Experimental temperature at crucible surface,AR =1



(b) Isothermal crucible surface, AR = 1



(c) Experimental temperature at crucible surface, AR = 0.5



(d) Isothermal crucible surface, AR = 0.5

Figure 14: Turbulent viscosity contours for buoyancy driven flow coupled with Marangoni convection as well as crystal and crucible rotation.

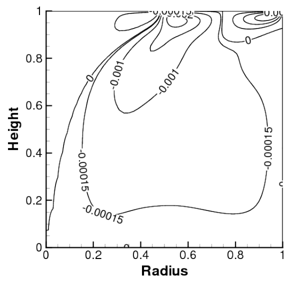
of related non dimensional number values. For melt aspect ratio of 1, value of turbulent viscosity when experimental temperature values are used as boundary information at crucible surface is higher as compared to turbulent viscosity for isothermal crucible surface case, except for case involving CUSP magnetic field. Melt aspect ratio of 0.5 however shows higher maximum turbulent viscosity for isothermal crucible surface boundary condition for flow governed by natural convection and Marangoni convection. It is worthwhile to note that in presence of CUSP magnetic field, the difference in turbulent viscosity for the two types of boundary information is insignificant for melt aspect ratio of 1.0.

Table 4: Maximum turbulent viscosity values - Experimental and Isothermal crucible surface boundary condition

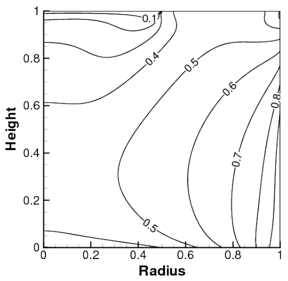
	Aspect Ratio 1		**Aspect Ratio 0.5**	
	Experimental temperature profile	**Isothermal crucible surface**	**Experimental temperature profile**	**Isothermal crucible surface**
NC	663.54	641.87	177.83	256.64
NC+MC	785.45	602.04	203.04	255.28
NC+MC+rotation of crystal and crucible	1314.99	993.41	435.68	269.20
NC+MC+rotation of crystal and crucible in presence of CUSP magnetic field	987.42	988.01	329.10	299.30

Simulation has been done to investigate effect of imposing an experimentally measured temperature profile along the crucible surface for a melt aspect ratio of 1, on to a crucible having an aspect ratio of 0.5. Melt motion inside the crucible is governed by natural convection, Marangoni convection as well as crystal and crucible rotation in presence of a CUSP magnetic field.

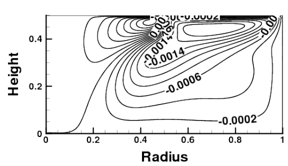
Variation of oxygen concentration at the melt crystal interface in such a scenario is shown in Fig. 17. As seen in the figure, oxygen concentration distribution along the melt crystal interface is of



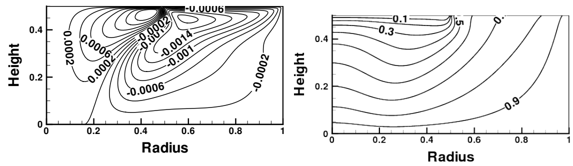
(a) Experimental temperature at crucible surface, AR=1



(b) Isothermal crucible surface, AR=1



(c) Experimental temperature at crucible, AR=0.5



(d) Isothermal crucible surface, AR=0.5.

Figure 15: Streamline and isotherm contours for buoyancy driven flow coupled with Marangoni convection as well as crystal and crucible rotation.

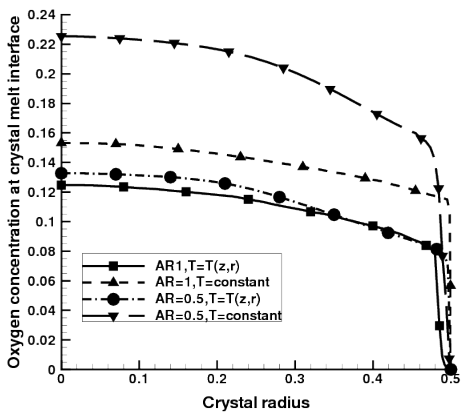


Figure 16: Oxygen variation at the crystal melt interface for natural convection combined with Marangoni convection and crystal as well as crucible rotation in presence of CUSP magnetic field.

similar trend, however, the values predicted by temperature profile of aspect ratio of 1 is lower as compared to that for aspect ratio of 0.5.

Streamline and isotherm contours for the two temperature profiles are shown in Fig. 18. Experimental temperature profile from melt aspect ratio of 1 shows reduction in depth of clockwise cell below the crystal, towards the axis. This in turn prevents direct transfer of oxygen rich melt to crystal melt interface, resulting in lower oxygen concentration.

Contours of turbulent viscosity shown in Fig. 19. show similar trend in distribution as well as the value of turbulent viscosity predicted by the two temperature profile.

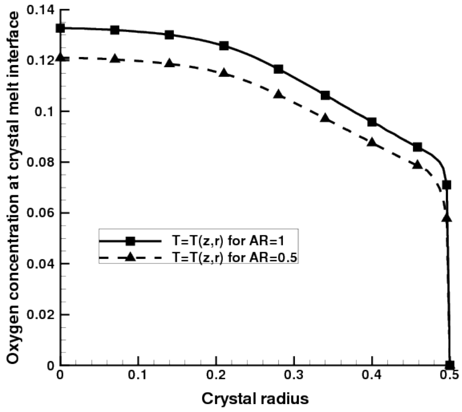
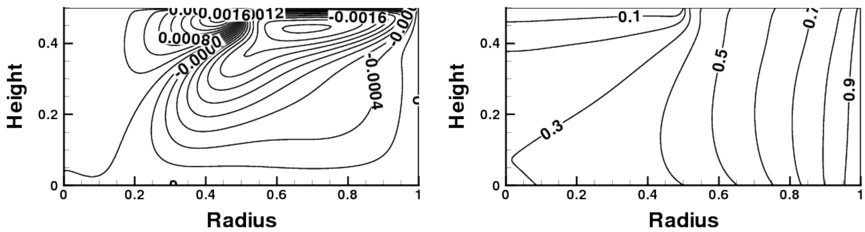
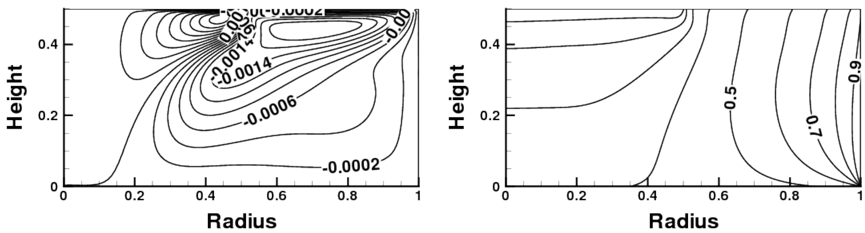


Figure 17: Oxygen concentration along melt crystal interface on imposing experimetal temperature profile for AR=1 on melt having AR=0.5



(a) Temperature profile measured on aspect ratio 1 imposed on melt aspect ratio of 0.5.

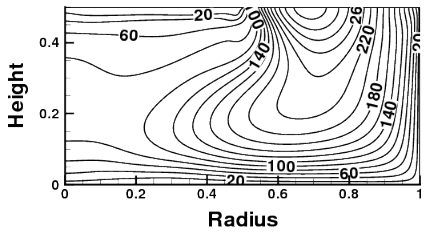


(b) Temperature profile measured on crucible having aspect ratio of 0.5 on melt aspect ratio of 0.5.

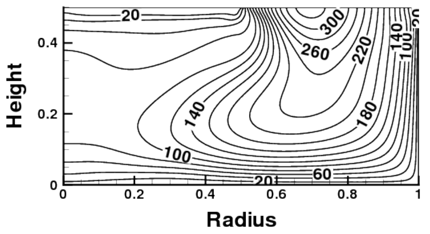
Figure 18: Streamline and isotherm for melt AR=0.5, with experimental temperature profile for AR = 1 and AR = 0.5 at the crucible surface.

7. Achievements with respect to objectives

- Laminar flow inside a CZ crucible in presence of a CUSP magnetic field has been simulated. Effect of ZGP location on the oxygen concentration at the crystal melt interface has been investigated.
- Turbulent flow inside a CZ crucible used to grow 450 mm diameter silicon crystal, in presence of CUSP magnetic field and effect of ZGP location in relation to the crystal melt interface, on oxygen species at melt crystal interface has been investigated.
- Effect of two types of boundary conditions, namely, experimental temperature profile at the crucible and isothermal crucible, on melt flow and oxygen species transfer, for melt aspect ratio of 1 and 0.5 has been investigated.



(a) Temperature profile measured for aspect ratio 1 imposed on melt aspect ratio of 0.5



(b) Temperature profile measured for crucible having aspect ratio of 0.5 on melt aspect ratio of 0.5.

Figure 19: Contours of turbulent viscosity for melt AR=0.5, with experimental temperature profile for AR = 1 and AR = 0.5 at the crucible surface.

8. Conclusion

Flow inside a CZ crucible for growth of silicon single crystal has been investigated numerically. Effect of an external CUSP magnetic field and location of ZGP, on the melt motion and oxygen species at the crystal melt interface has been studied. Change in melt height with growth of solid crystal is accounted by change of melt aspect ratio.

For laminar flow inside the melt, oxygen concentration at crystal melt interface reduces with reduction in melt aspect ratio, irrespective of location of ZGP. Effect of location of ZGP, below or above the melt free surface on the oxygen concentration depends on the melt aspect ratio. Change of location of ZGP above or below the melt free surface effects oxygen concentration at melt interface significantly during initial stage of crystal growth, characterized by higher melt aspect ratio. Oxygen concentration at the crystal melt interface dose not vary significantly with change in ZGP location for lower melt aspect ratio. There exists significant radial variation of oxygen species distribution in growing crystal for higher melt aspect ratio and the variation is almost insignificant for low melt aspect ratio.

Flow inside the crucible used for growth of 450 mm diameter silicon crystal by CZ method is invariably turbulent in nature. Here too the location of ZGP for a given magnetic field strength strongly effects the oxygen concentration for high aspect ratio melt. For melt aspect ratio of 0.5, magnetic field on 0.2 T shows increase in oxygen concentration at melt crystal interface where as for melt aspect ratio of 0.25, 0.04 T magnetic field shows higher oxygen species concentration. Distribution of oxygen species along the radius is uniform irrespective of ZGP location and magnetic field strength for melt aspect ratio of 0.5 and 0.25. There exist radial oxygen concentration variation for higher melt aspect ratio of 1.

Effect of two types of thermal boundary conditions, namely isothermal crucible surface and experimentally measured temperature at the crucible surface, on melt flow and oxygen concentration at the melt crystal surface has been investigated. For melt aspect ratio of 1.0, in absence of an external magnetic field, experimental temperature at the crucible surface predicts higher oxygen concentration at the melt crystal interface as compared to case of isothermal crucible scenario. For melt aspect ratio of 0.5 the trend is reverse with isothermal crucible surface showing higher oxygen concentration at the melt free surface, in absence of magnetic field. Presence of a CUSP magnetic field results in relatively higher oxygen concentration as compared to case without a magnetic field. However, the distribution of oxygen species is uniform along the crystal for both types of boundary conditions.

Value of maximum turbulent viscosity predicted by isothermal crucible surface is lower as compared to experimental temperature at the crucible surface, for melt aspect ratio of 1. Contours of turbulent viscosity are remarkably similar for both type of thermal boundary condition at the crucible surface, for melt aspect ratio of 0.5 as well as 1.0. Maximum turbulent viscosity value is almost identical for melt aspect ratio of 1.0 in presence of an external magnetic field.

Imposing an experimental temperature profile for melt aspect ratio of 1, on a melt of aspect ratio of 0.5 results in prediction of lower oxygen concentration at the melt crystal interface. Distribution of turbulent viscosity and value of maximum turbulent viscosity is however the same for both the temperature profiles.

List of Publication

1. Mitesh Vegad and N M Bhatt. Review of some aspects of single crystal growth using Czochralski crystal growth technique. *Procedia Technology* 14 (2014) 438-446.
2. Mitesh Vegad and N M Bhatt. Effect of location of zero gauss plane on oxygen concentration at crystal melt interface during growth of magnetic silicon single crystal using Czochralski technique crystal growth technique.*Procedia Technology* 14 (2014) 438-446.
3. Mitesh Vegad and N M Bhatt. On Effect of Location of Zero Gauss Plane on Oxygen Concentration During Growth of Silicon Crystal using Czochralski Technique. *International Conference on Fluid Mechanics and Fluid Power*, December 15-17 2016 at MNIT, Allahabad.

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