Chapter 6

Conclusion

Semiconductor devices play a vital role in every aspect of our life ranging from communication to the modern day automobile. Bulk of the silicon crystal required for these devices are grown using the Czochralski method. Size and quality of crystal are key crystal characteristics with present day trend to grow silicon crystal of 450 mm diameter. Control of oxygen species concentration and its distribution along the radial direction along the length of the silicon crystal is of vital importance for growing good quality crystal. An external magnetic field is an industry norm to control dynamics of melt motion and there by the crystal quality in an industrial scale Czochralski setup.

Owing to challenges related to experimental investigation like restrictive environment, high melt temperature, flow field measurement issues etc, numerical investigation is still the preferred tool for investigation of Czochralski growth process.

Flow inside a CZ crucible for growth of silicon crystal of 450 mm diameter has been investigated numerically using finite volume approach by solving conservation equation of mass, momentum, energy and oxygen species. Effect of an external CUSP magnetic field and location of Zero Gauss Plane (ZGP), on the melt motion and oxygen species at the crystal melt interface has been studied. Three locations of ZGP, namely, at the crystal melt interface, 10% below and 10% above the crystal melt interface have been considered. Reduction in the melt height inside the crucible with growth of solid crystal is accounted by reduction of melt aspect ratio. Melt aspect ratio of 1, 0.5 and 0.25 corresponding to high, moderate and low melt level inside the crucible have been considered. Effect of melt motion owing to buoyancy, forced convection owing to crystal as well as crucible rotation and surface tension driven flow at free melt surface have been considered.

For laminar buoyancy driven flow inside the melt, oxygen concentration at crystal melt interface reduces with reduction in melt aspect ratio, irrespective of location of ZGP. However, the effect of location of ZGP below or above the melt free surface on the oxygen concentration depends on the melt aspect ratio. For melt aspect ratio of 1, ZGP 10% below the melt crystal interface results in increase in oxygen concentration at the crystal melt interface. However, for melt characterized by aspect ratio of 0.25, ZGP 10% above the crystal
melt interface shows increase in oxygen concentration at the crystal melt interface. 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 of higher melt aspect ratio of 1 and the variation is almost insignificant for low melt aspect ratio of 0.25. Forced convection owing to rotation of crystal coupled with buoyancy driven flow leads to uniform distribution of oxygen at the crystal melt interface for all three aspect ratio in consideration. The concentration of oxygen species is however higher as compared to that of natural convection flow case. For flow governed by buoyancy as well as forced convection owing to crystal and crucible rotation, change in ZGP location show characteristics similar to that for pure buoyancy driven flow.

Flow inside the crucible used for growth of 450 mm diameter silicon crystal by CZ method is invariably turbulent in nature. Reynolds Average Navier Stokes (RANS) equations have been solved coupled with low Reynolds number formulation to resolve near wall flow to simulate turbulent flow in Czochralski melt. Imposing an external CUSP magnetic is an important mechanism to control the melt motion. Two magnetic filed of 0.04 T and 0.2 T corresponding to low and high values of magnetic filed actually employed in industrial growth scenario have been considered. 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 exists radial oxygen concentration variation for higher melt aspect ratio of 1.

Type of temperature profile imposed at the crucible surface as boundary information plays a vital role in dictating the temperature and flow field inside the melt. 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, 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 types 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.

Often, owing to lack of information, temperature profile measured on crucible surface having a particular aspect ratio is used as boundary information on a melt of different aspect ratio all together. Melt aspect ratio of 1 and 0.5 have been considered to investigate the effect of such an approach, as experimentally measured temperature data on crucible surface are available in literature for these two melt aspect ratios only. Imposing an experimental temperature profile measured on a crucible of aspect ratio 1, on a crucible characterized by actual aspect ratio of 0.5 results in lower oxygen concentration at the crystal melt interface. Similar trend is observed when experimental temperature profile measured on a crucible of aspect ratio of 0.5 is imposed on a crucible having an actual aspect ratio of 1. Distribution of turbulent viscosity and value of maximum turbulent viscosity is however the same for both the temperature profiles for a particular aspect ratio. Local Nusselt number at crucible wall is lower for temperature profile for aspect ratio of 1 imposed on crucible having aspect ratio of 0.5. For melt aspect ratio of 1, imposing temperature profile of melt aspect ratio of 0.5 results in higher value of local Nusselt number. For both the melt aspect ratio, difference in local Nusselt number value on crucible wall is observed in zone near the crucible bottom. Local Nusselt number values on crucible wall towards the free melt surface are similar, irrespective of the temperature profile imposed on the crucible surface.