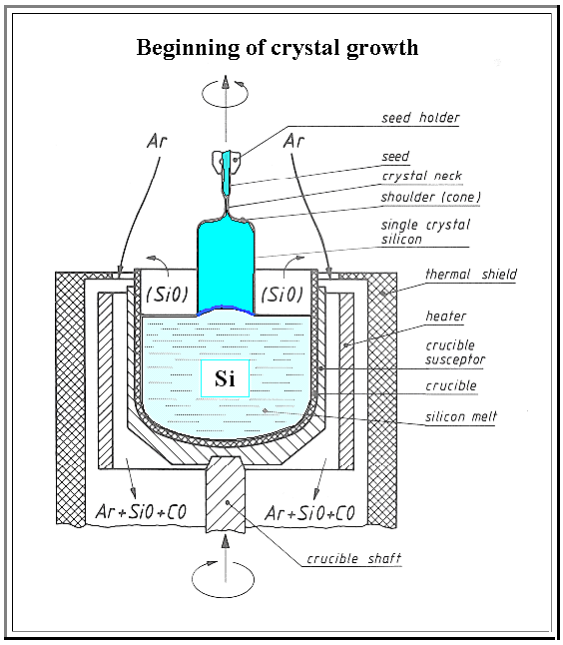
The Science and Art of Si Crystal Growth

Advanced

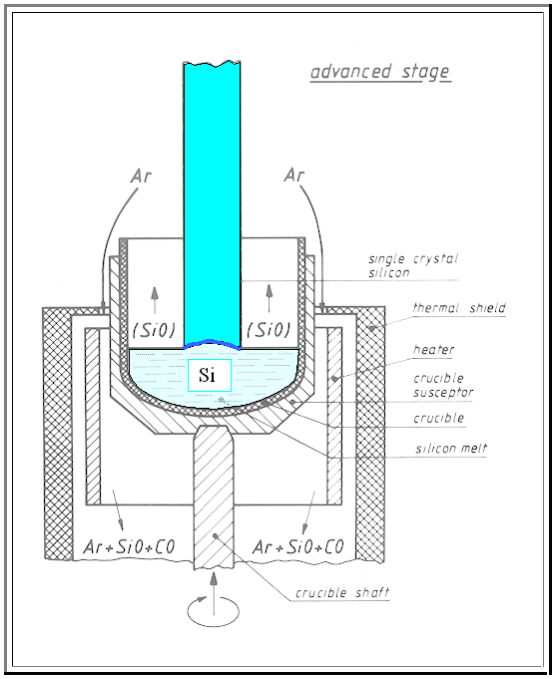
There are a few major points in Crochalski (or **CZ**) crystal growth that shall be outlined briefly. In particular, we will discuss

- The "**Dash**" **process** (or "necking") for the production of dislocation free crystals.
- **Bulk microdefects**, or the question of what happens to the point defects present in thermal equilibrium upon cooling down?
- **Convection** in the melt and the incorporation of oxygen.



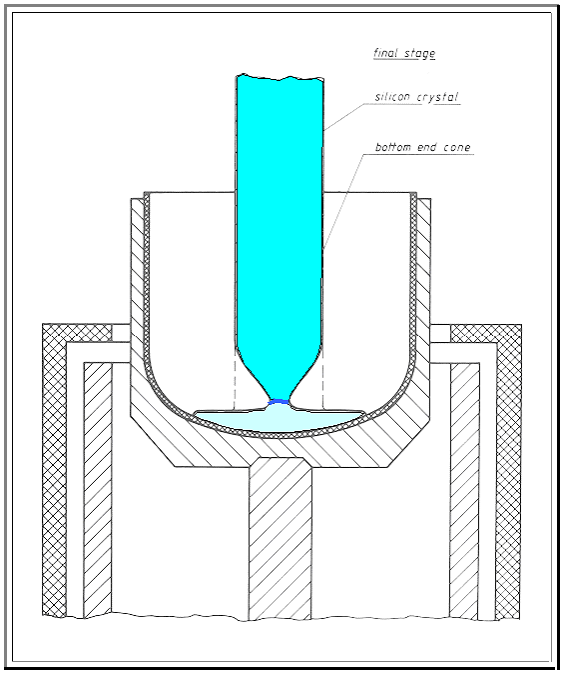
Dash Technique

- How do you obtain perfectly dislocation free crystals? Always considering that your seed crystal may not be dislocation free, and even if it is, the unavoidable thermal shock upon dipping the seed crystal in the melt will almost certainly produce some dislocations (this is real easy at temperatures close to the melting point).
- You just do two things:
  1. Reduce the strain as driving force for dislocation movement and multiplication, and
  2. Make sure that existing dislocations are never lined up in growth direction, so that they will sooner or later terminate at the surface.
- Both points are satisfied if you just make the first part of the growing crystal very thin, i.e. you form a "neck" as shown on the left.
- This technique was pioneered by W.C. **Dash** in **1959**. It was one of the many "little" inventions necessary to allow Si technology.



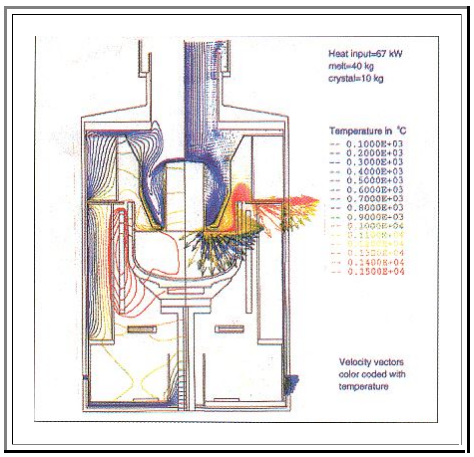
Bulk Micro Defects

- Just after crystallization, the crystal is at a temperature close to the melting point, and thus contains the maximum equilibrium concentration of point defects (vacancies and interstitials). As it cools down, the equilibrium concentration goes down to practically zero at room temperature.
- But how? In normal crystals the point defects disappear at grain boundaries or dislocations - whatever internal sinks there are. In dislocation free single crystalline Si there is only the surface available as sink - and for most point defects, the surface is far away and will never be reached by diffusion.
- What will happen is that some, if not most, of the point defects form small clusters or agglomerates, the so-called bulk micro defects, (***BMD***), ***COPs*** (crystal originated particles or pits), or, as they were called in the eighties, swirl defects.
- They are unavoidable, and they are bad for **ICs**. All you can do is to try and make them very small. Manipulating these defects is one oft the recurrent themes in **Si** crystal growth, made difficult by the fact that - quite ironically - we know far less about point defects in Si than in metals.



Convection Effects

- Even if crystal and crucible would not be rotated, there would be convection in the melt, driven by density gradients coupled to temperature gradients. The only way to totally avoid this would by to switch off gravity. This is the reasoning behind all those " *Very Important*" experiments with crystal growth in space.
- Don't fall for it. First, you also can suppress convection with a strong magnetic field (its actually done for large diameter crystals) at an incredibly tiny fraction of the prize for space-grown crystals, and secondly, why should you suppress convection?
- Well, uncontrolled convection is bad for many reasons. Lets just look at one: The melt streaming by the crucible walls dissolves some **SiO_2** and later deposits it into the crystal. The **O** - concentration then is not only higher compared to convection-free melts, but its radial distribution mirrors the flow pattern - and nothing is worse than inhomogeneities in **Si** crystals.
- Does this mean that you do not want convection? No - all it means that want to have convection that is precisely right for your crystal at every stage of its growth. If you have that, you can control **O** - concentration and keep the doping concentration about constant through the length of the crystal despite the effects of segregation.



Science and Art

- So, in growing a large **Si** crystal, you have a number of buttons to fiddle with. which you must turn in the right directions as your crystal grows. Consider the major parameters:
  1. Growth speed,
  2. Rotation of the crystal,
  3. Rotation of the crucible - same or opposite direction,
  4. Magnetic field (strength and direction)

  5. Power fed to crucible.
- Changing anyone of this parameters a little bit will influence everything in a way not easily cast into formulas - diameter of the crystal, **BMD** size and distribution, **O**-concentration and distribution, dopant concentration and distribution, and much more.
- Growing good crystals certainly was (and to some extent still is) an therfore an art.
- Only in the nineties of the **20.** century, theory and simulation progressed enough to be of help. Now it is indispensable.
- The picture on the left shows one result: the complete temperature distribution in the whole machine (including, of course, melt and crystal) and the flow field in the melt (little arrows). Now you can change some parameters and see what will happen without actually growing (and later destroying for analysis) an expensive crystal.