A Required Model For InSb Czochralski Growth

The Czochralski Growth Process

The most important and widely used technique of crystal pulling is known as the Czochralski technique. It is used to produce a large fraction of the crystals used by the electronics industry. The elements of the technique are shown schematically in Fig. 1. The charge material to be crystallized is contained in a crucible which is heated to above the melting point of the charge. A pull rod with a chuck containing a seed crystal at its lower end is positioned axially above the crucible. The seed crystal is dipped into the melt and the melt temperature adjusted until a meniscus is supported. The pull rod is slowly rotated and then lifted and, by careful adjustment of the power supplied to the melt, the crystal of the desired diameter is grown. (Rotation rates are commonly in the range 1−10 r.p.m. and lift rates 0.1−100 mm/hr.)

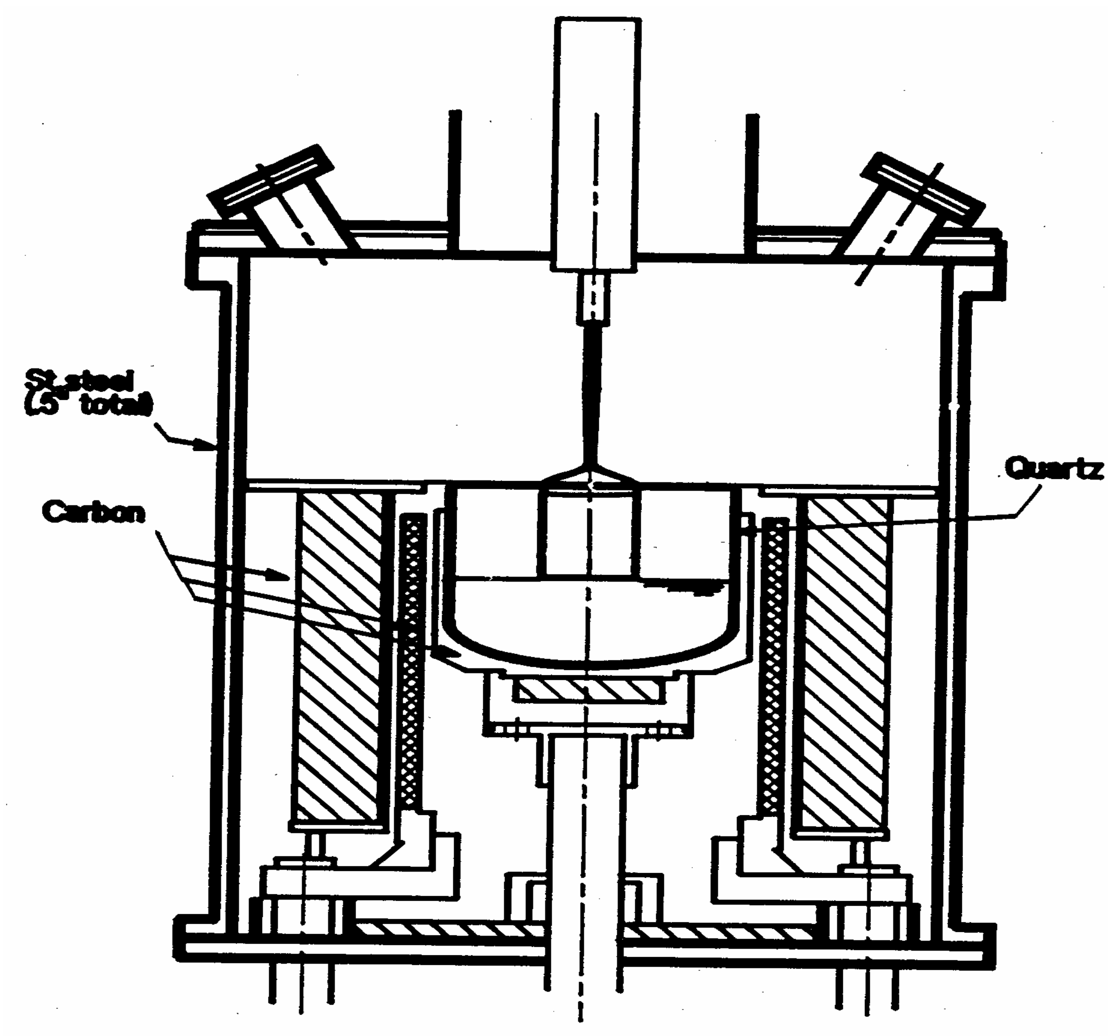

Figure 1: Typical Czochralski Grower

The whole assembly is maintained in an envelope that permits control of the ambient gas and enables the crystal to be observed visually. In the case of InSb, the ambient gas is hydrogen to ensure reduction of any InOx compounds. This hydrogen adds two complications to growth; namely high heat losses because of its fluidity and the necessity of avoiding any oxygen introduction to avoid explosions!

Major advantages of the technique include:

(a) The crystal is unconstrained as it cools and a high structural perfection can be obtained. For example, large single crystals containing very few dislocations within their volume are routinely produced for device fabrication.

(b) Crystal rotation produces a uniform distribution of deliberately added solute since the rotating crystal has a uniformly accessible boundary layer. Crystals are seldom required in an undoped state. For example donor or acceptor impurities are added to semiconductors to provide n or p−type. Automatic servo−control systems have been developed to control the diameter of the growing crystal.

Since the crystal is heated from the side and from below with heat being extracted through the crystal at the top, there is a strong buoyancy−driven convective motion in the melt (Rayleigh numbers greatly in excess of 10’ are commonly encountered). Such motion tends to be turbulent and thus strongly time−dependent especially for the molten semiconductors where the Prandtl number is much less than unity. The resultant temperature fluctuations modulate the microscopic rate of growth of the crystal. (The mean value of the growth rate is of course equal to the crystal pulling speed plus the rate of fall of melt level in the crucible.) Since the rate of incorporation of solute into the crystal is dependent on the growth rate, growth rate fluctuations introduce fluctuations in the concentration of solute in the grown crystal. This lack of chemical homogeneity can be serious in some applications. A study of the hydrodynamic behaviour of the melt is vital to an understanding of the rate *of* uptake and of the spatial distribution of impurity concentration in the melt.

The pulling technique is applicable to a wide range of materials and is used commercially for the production of the elemental semiconductors silicon and germanium and *of* a wide range of materials. Some III−V semiconductors present a problem in that they tend to dissociate when heated. Thus for example, if one endeavours to melt a charge of gallium arsenide in the crucible the arsenic will distil off leaving a pool of molten gallium. To overcome this a low melting point glass (boric oxide commonly), is added to the crucible so that, on heating, this melts and flows over the charge encapsulating it and preventing dissociation provided that the external pressure is always maintained greater than the dissociation pressure. Pulling is performed by lowering the seed through the boric oxide layer, growth occurring at the interface between the two liquids. This technique, known as the Liquid Encapsulation (LEC) technique is <u>not</u> required for the growth of InSb which has a low Sb dissociation pressure thus quite modest Sb losses.

Heat and Fluid Flows

Figure 2 shows the principal heat flows in a Czochralski (CZ) system.

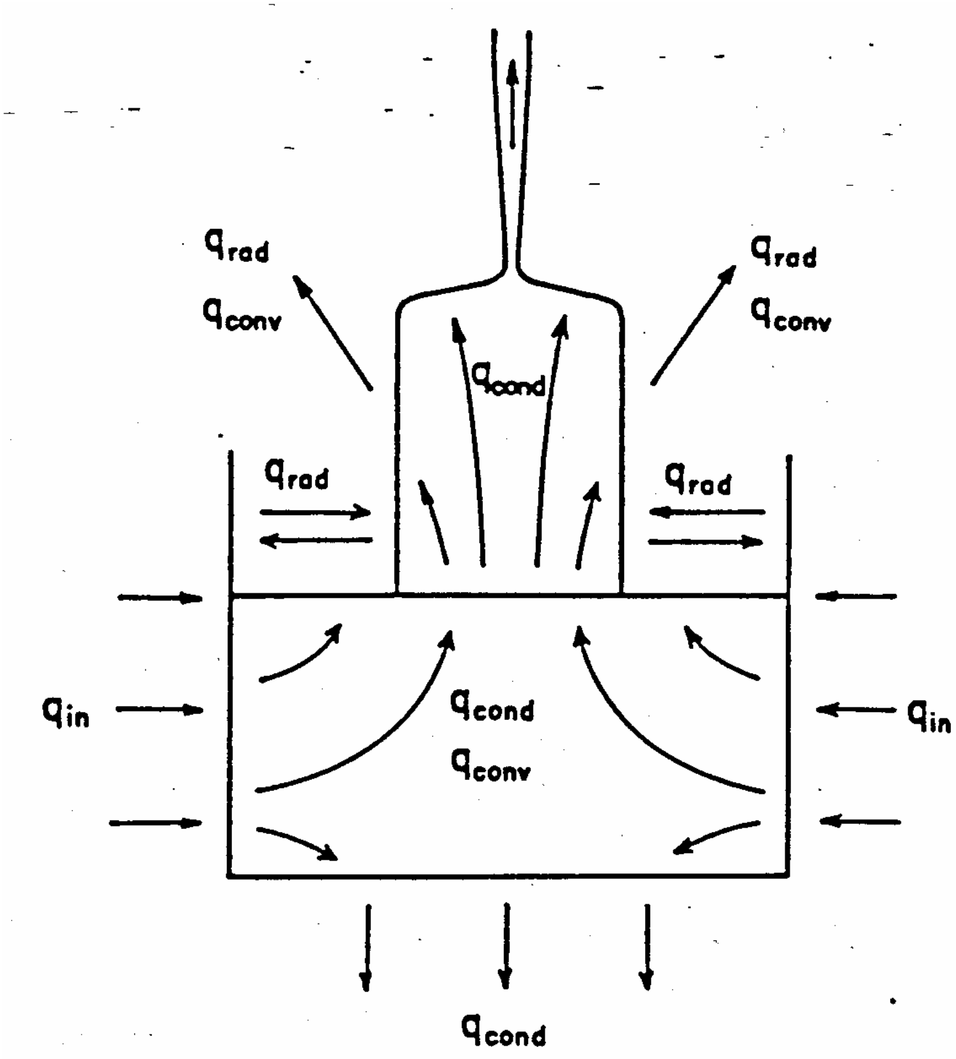

Figure 2: Czochralski Grower Heat Flows

Heat flows through the graphite susceptor and quartz crucible wall into the melt pool. The surface of the melt is cooled by radiation and contact with convective gas flows but gains the heat of freezing deposited at the melt−crystal interface. The crystal is hottest (presumably) at the melt interface. Heat is carried up the crystal conductively and is then dissipated by radiative and convective processes. The great majority of this is lost to the containment environment with only a minor amount exiting via the seed.

In the specific case of InSb, the radiative process no longer dwarfs convective losses (the case for higher melting materials such as Si, Ge and GaAs) so any modelling done in this system must adjust for this.

In addition to the thermal flows in the system, it is also useful to understand the liquid flows in the melt which transport heat . Figure 3 shows these flows.

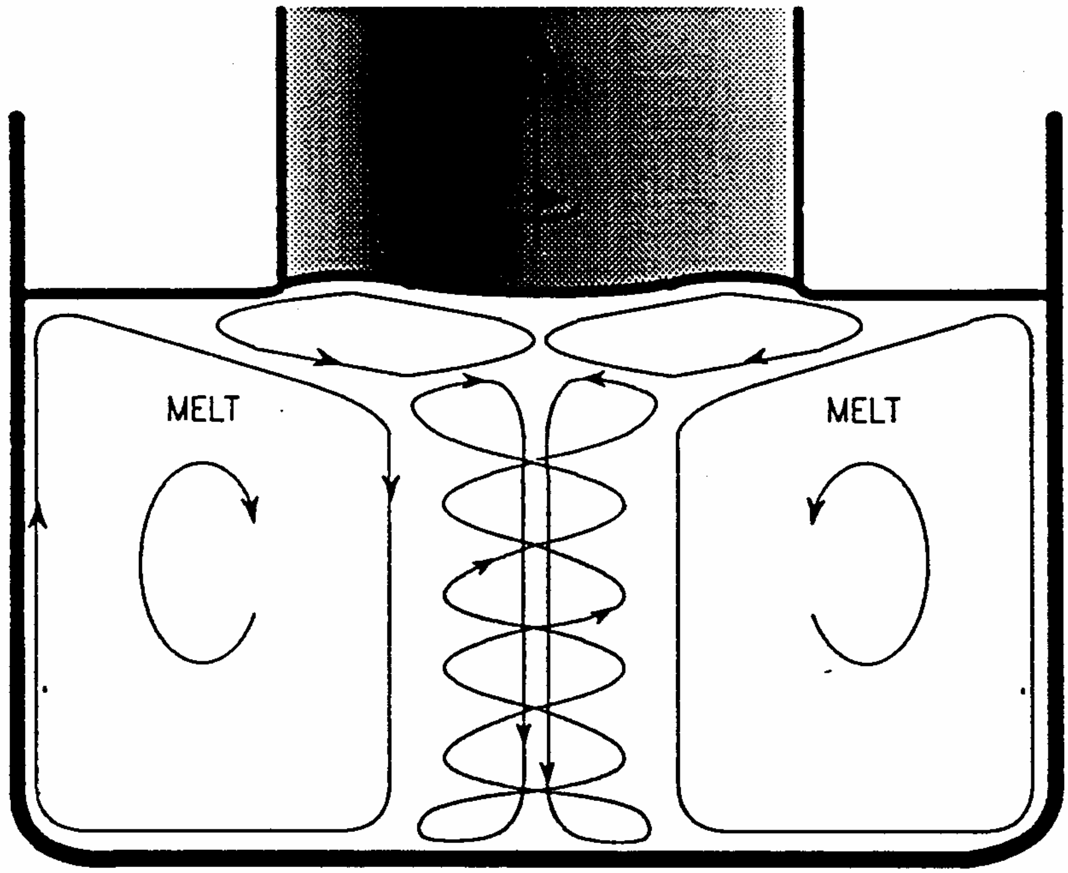

Figure 3: Melt Fluid Flows

To maintain quasi−uniformity in temperature, the crucible and seed are both slowly rotated (at 3−20 RPM) , usually in opposite senses. The seed rotation generates centripetal forces on the melt under the growth interface which causes an outward melt flow. The heat flows in the melt create a strong convective flow rising along the (hot) crucible walls and falling under the (relatively cool) crystal. Combined, these result in an upper centripetal cell, a lower convective one and (sometimes) a complex third region axially. In aggregate, the melt is well mixed but the model may have to account for the mechanics of the heat transfers in it.

Modeling

Most modeling approaches begin by postulating a formalism for the materials' thermal parameters and heat flows and then calculate the isotherms in the system. From these the interface shape can be derived.

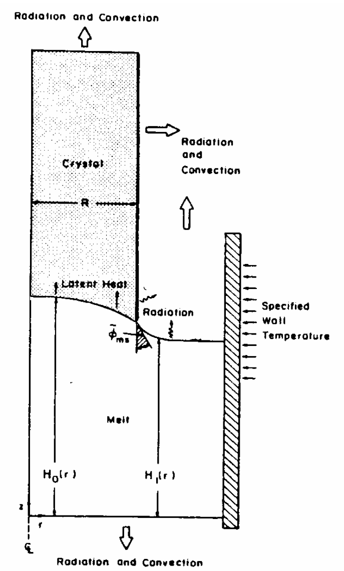

Fig. 1. Schematic of prototype LEC system.

Figure 4: Model Heat Flows

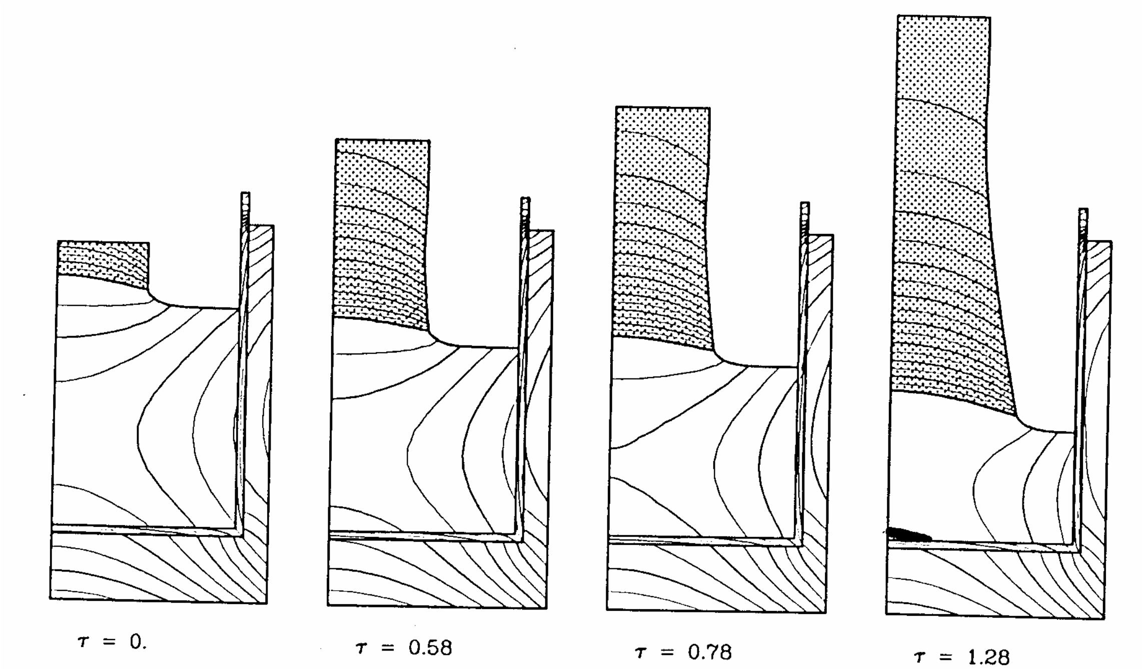

Figure 5: Modeled Isotherms as Growth Progresses

Note that the centre−bottom of the crucible can actually reach a temperature below the melting point of the charge. This warns of incipient disaster for the crystal grower!

Object of the Modeling Exercise

In the growing crystal the thermal conductivity of the crystalline material governs the isotherms as heat flows to identified sinks. The cooling of the crystal implicit in the isotherms can be used to derive stress fields from the elastic parameters of the solid. For example, if the surface is cooling more rapidly than the interior, the surface material is in tension while the core is in compression. The radial and axial variation of these stresses is the required end result of the model and calculation.

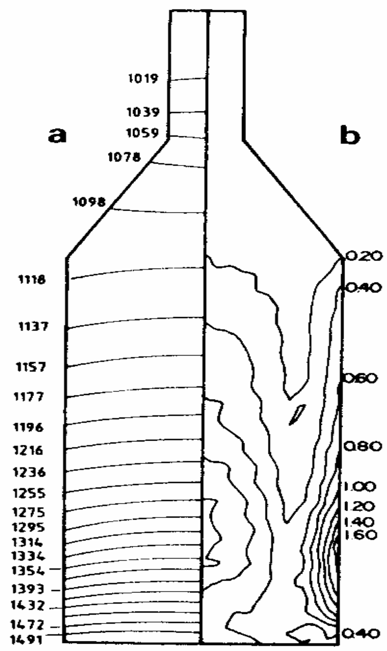

Fig. 7. (a) Temperature (K) and (b) stress (kg mm^{-2})

Figure 6: Isotherms & Calculated Thermal Stress (GaAs case)

The ultimate object of the entire process is the estimation of the thermal stress field in the growing crystal with parameterization amenable to “tweaking” to permit prediction of what changes would reduce these thermal stresses. The “tweaks” that the model predicts will lower stress are then tested experimentally, the model retuned iteratively until the problem (ideally) goes away!

In the case of InSb where the annual demand for material and great cost of each growth run dictates that typically 50 growths are made each year –each with a considerable pressure to yield saleable material. Given this constraint, there is a great benefit to modeling the process to speed the growth optimization process.