# Heat transfer model of the SUBSA furnace

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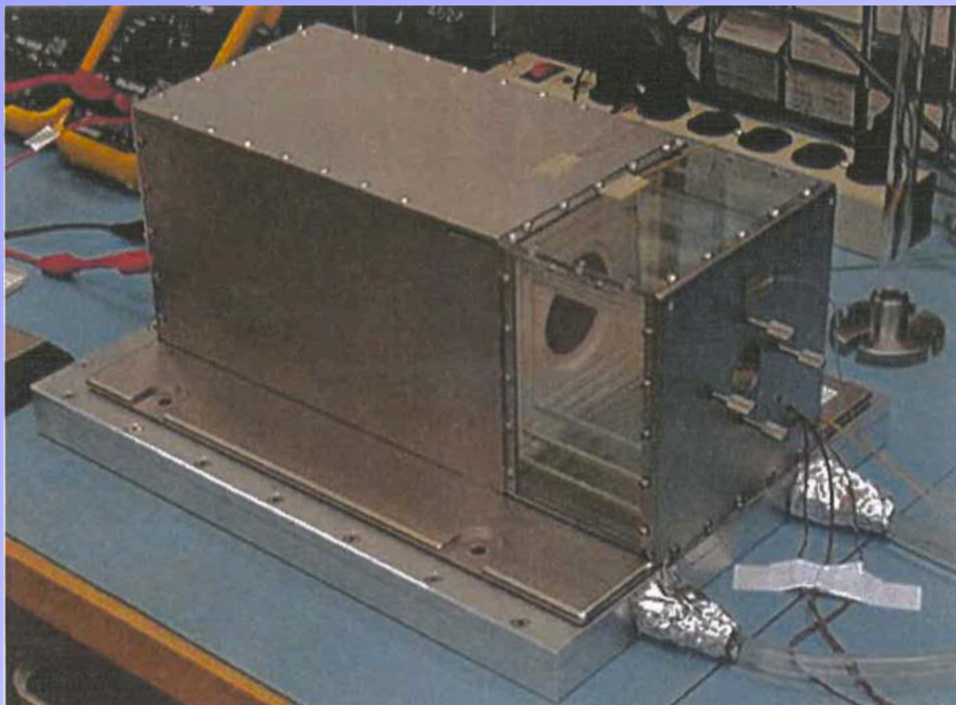
**1996 - 2002**

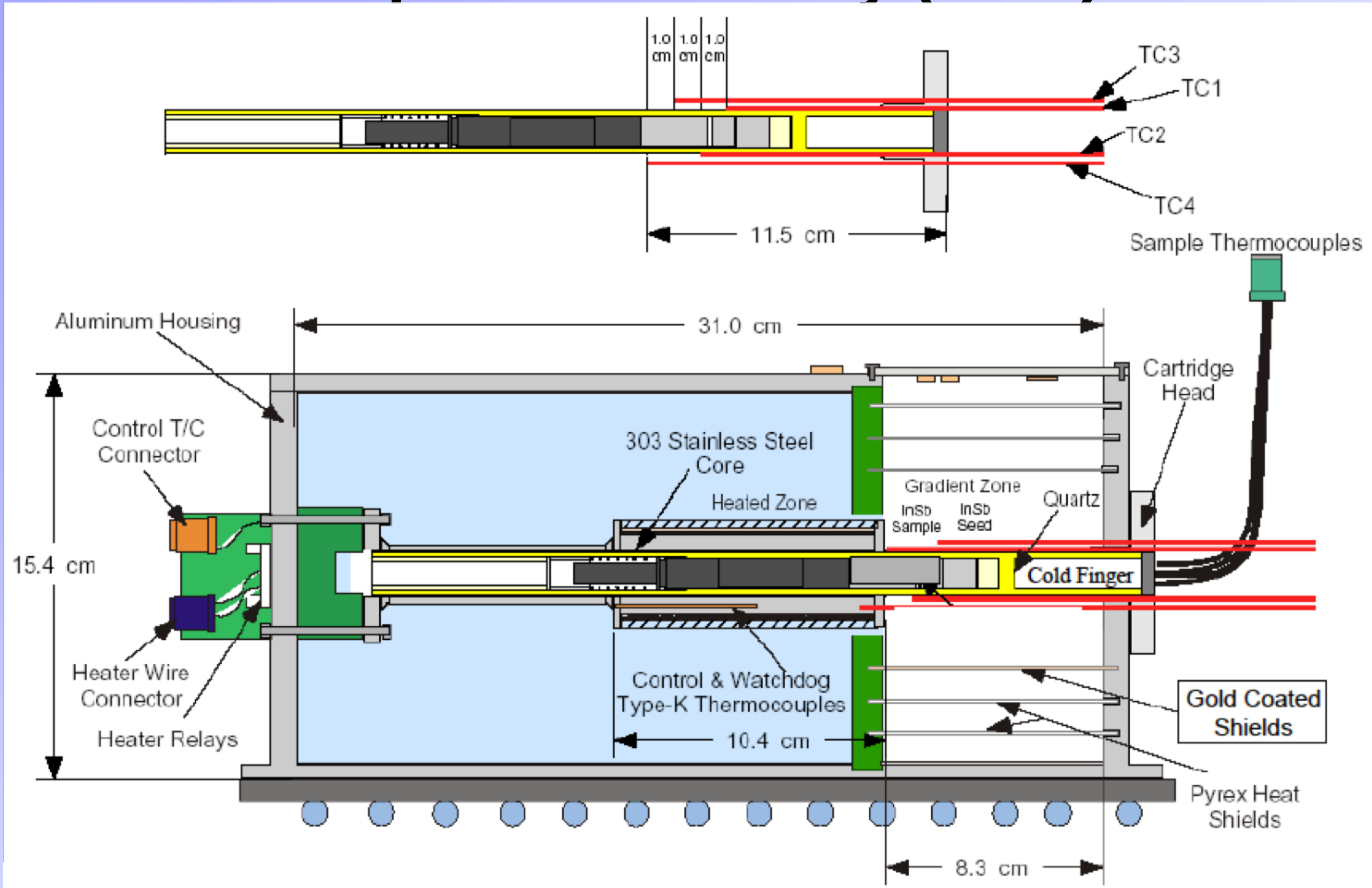

**2016 - present**

- The SUBSA (Solidification Using a Baffle in Sealed Ampoules) furnace was designed in 2002 for growth of indium antimonide in the Microgravity Science Glovebox at the International Space Station.
- The furnace features a transparent section, which allows a side view of the melt and growing crystal.
- At present, the SUBSA furnace is being used to grow the radiation detector materials InI and $Cs_2LiYCl_6$:Ce (CLYC)
- Heat transfer models of the SUBSA furnace have been developed using the modelling programs CrysMAS to help optimize the design of the experiments for these new materials.

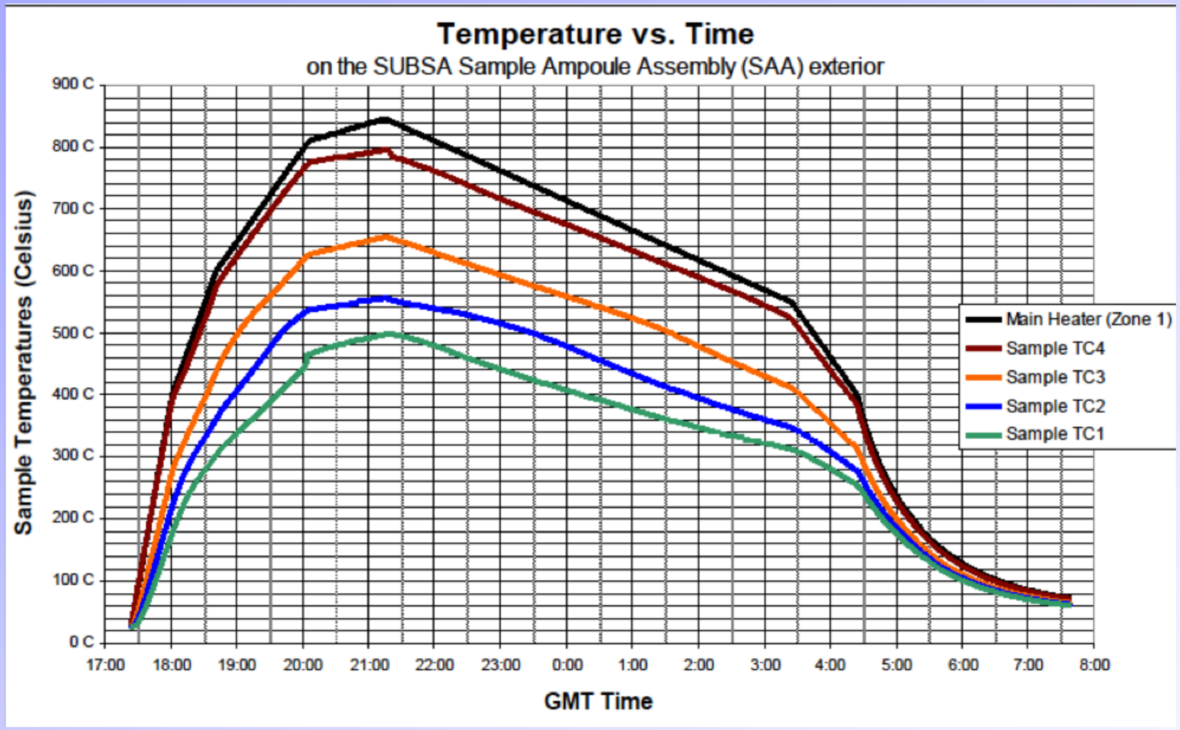
# SUBSA Furnace (left) and Microgravity Science Glovebox (MSG) Unit (right)



# Original Experiments WITH InSb: A schematic of the furnace and a sample ampoule assembly (SAA)



# Temperatures measured by the sample thermocouples during growth of InSb



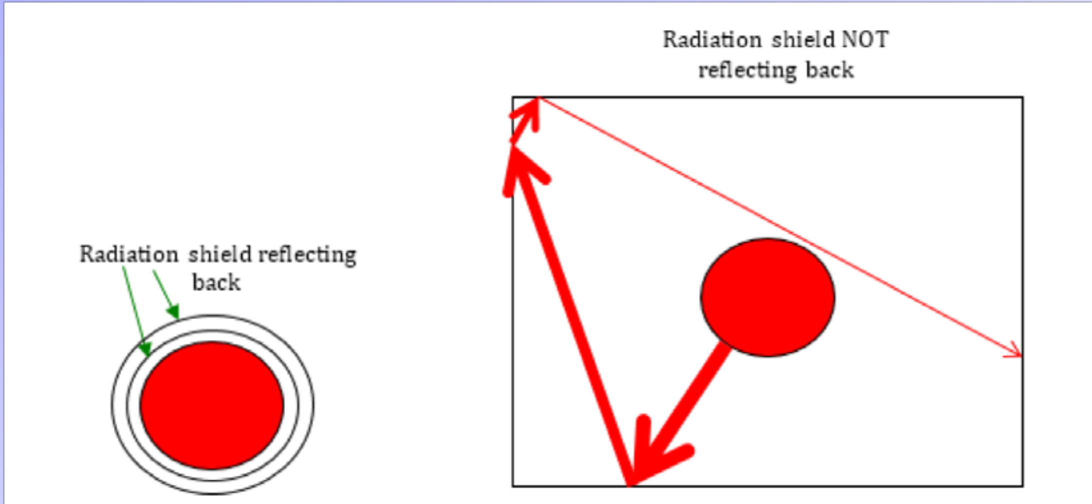

- Transparent section was feasible, because of the low melting point (512 C) and high thermal conductivity of InSb (10 $W/m-K$ for liquid and 18 $W/m-K$ for solid InSb)

- During "seeding" i.e. peak temperature, $T_{TC4}\,\_\,TT_{C3}\,{}_{=}\,{}_{120}K$. $T_{TC3}\,\_\,TT_{C2}\,{}_{=}\,{}_{100}K$. Thus, $\boldsymbol{dT/dx > 100\ K/cm}$

# Heat transfer in the transparent zone
# Radiation shields

The radiation shields are effective if they:

- reflect radiation back towards the ampoule (are cylindrical and coaxial)
- have high reflectivity and low emissivity
- Are small and close to the heat source to be relatively "hot" (to reduce $\Delta T^4$).
- Are not transparent, $\tau=0$ (except in the visible range).




a) Effective coaxial radiation shields. b) Radiation shield in the SUBSA furnace.

The radiation shield geometry used in the SUBSA furnace uses the radiation reflectors that are flat and far from the ampoule (Fig. 2 b),and the conditions i, and iii are not satisfied. Only a small fraction of radiation is reflected back to the ampoule. Instead, it is absorbed in the shields after multiple reflections. **As a result dT/dr and dT/dx are high.**

# Convection and Radiation heat transfer coefficient in the transparent zone on Earth in microgravity (ISS)

$q_{conv} = h_{conv}(T - T_{fluid});$ $q_{rad} = h_{rad} * (T - T_{sur})$

$h_{conv} - empirical\ model$ Type equation here.

| g | Gr_D | Gr_L | h_Hori | h_Vert | h_rad | h_Total |
|---|---|---|---|---|---|---|
| | | | W/m2-K | W/m2-K | W/m2-K | W/m2-K |
| **9.81E-06** | 0.01585 | 0.2477 | 1.306 | 1.221 | 18.16 | 19.46 |
| **9.81E-05** | **0.1585** | **2.477** | **1.57** | **1.493** | **18.16** | **19.73** |
| **9.81E-04** | 1.585 | 24.77 | 2.04 | 1.943 | 18.16 | 20.2 |
| **9.81E-03** | 15.85 | 247.7 | 2.876 | 2.709 | 18.16 | 21.03 |
| **9.81E-02** | 158.5 | 2477 | 4.363 | 4.065 | 18.16 | 22.52 |
| **9.81E-01** | 1585 | 24771 | 7.006 | 6.551 | 18.16 | 25.16 |
| **9.81E+00** | **15853** | **247710** | **11.71** | **11.27** | **18.16** | **29.86** |

Conclusions:

- On Earth, $h_{convection}$ =11 W/m-K and $h_{rad}$ ~ 18 W/m-K. $h_{Total}$ ~ 30 W/m-K.
- At $10^{-6}g_0$, $h_{convection} = 1.3\frac{W}{m} - K$, $h_{Total}$ ~ 20 W/m-K.
- Heat transfer is dominated by radiation

# Experiments with InI and CLYC in 2016-present

- At present, the SUBSA furnace is being used to grow the radiation detector material InI and scintillator $Cs_2LiYCl_6$:Ce (CLYC) both of which have low thermal conductivity, k~ 0.5 W/m-K (~10x lower than the thermal conductivity of InSb).

InI detector

CLYC crystal

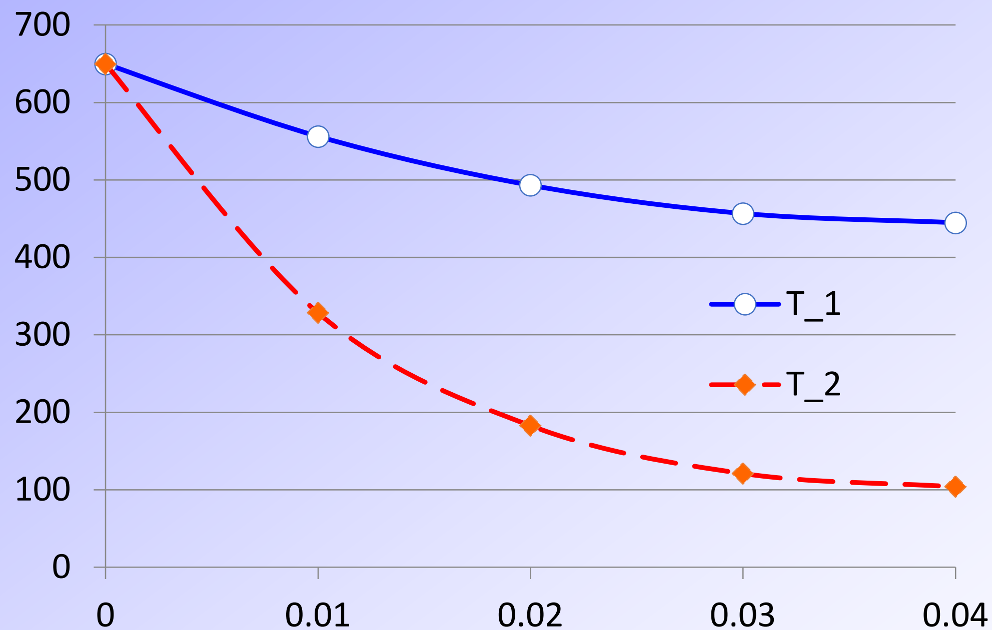
Image source: https://www.nasa.gov/sites/default/files/thumbnails/image/imclyc.jpg

- Both salts have low thermal conductivity, k~ 0.5 W/m-K (~10x lower than the thermal conductivity of InSb).
- At the ISS in 2002, one experiment failed, because 0.503 g of molten salt LiCl-KCl eutectic was present. LiCl-KCl has similar properties as InI or CLYC (k~ 1 W/m-K)

# Axial temperature gradient dT/dx as a function of melt thermal conductivity

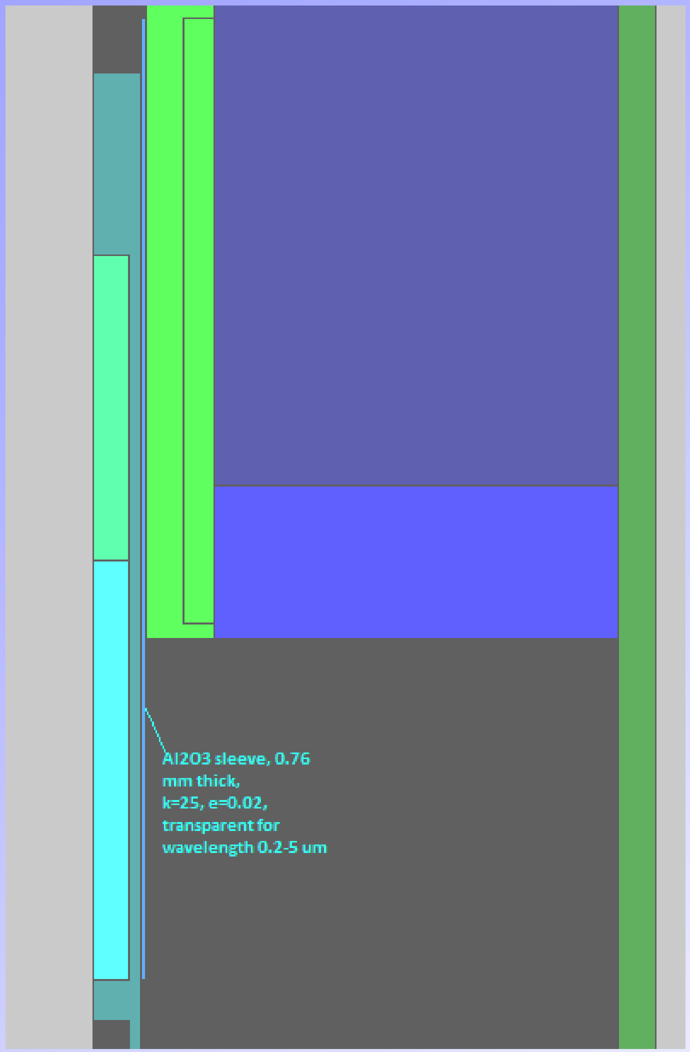
Using the “fin” model we show that the resulting the temperature profile T(x) and gradient dT/dx, depend on the the thermal conductivity of the charge in the ampoule.

- dT1/dx ~ 100 K/cm, is in excellent agreement with the data from InSb-SUBSA experiments
- dT2/dx ~ 300 K/cm. One must overheat the melt by 300 C, for 1 cm to be visible in the transparent zone




Axial profile in SUBSA SAA. T_1 for InSb, k1=10 W/m-K and T_2 for a salt, k2=1 W/m-K,

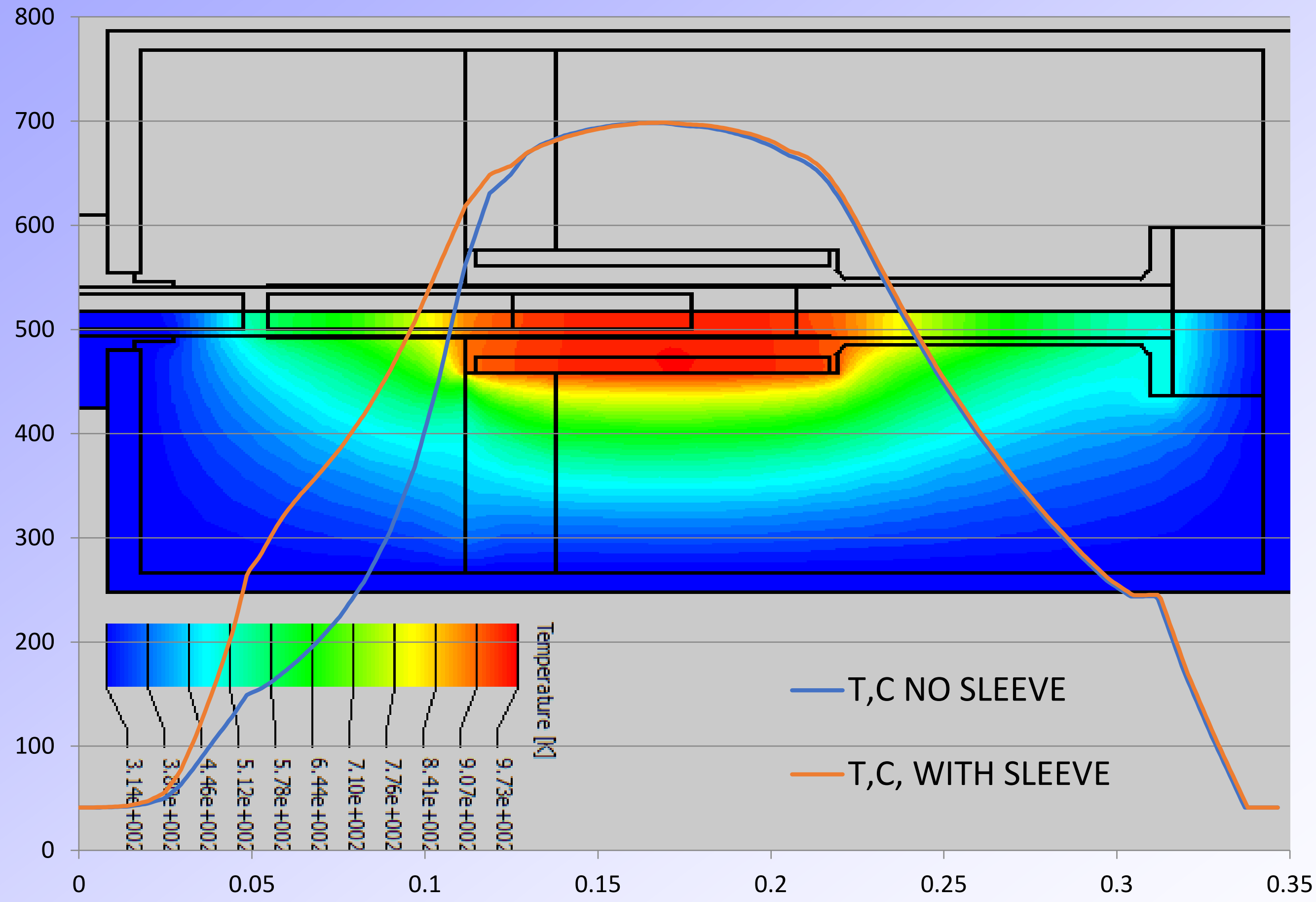
# Modeling for optimization



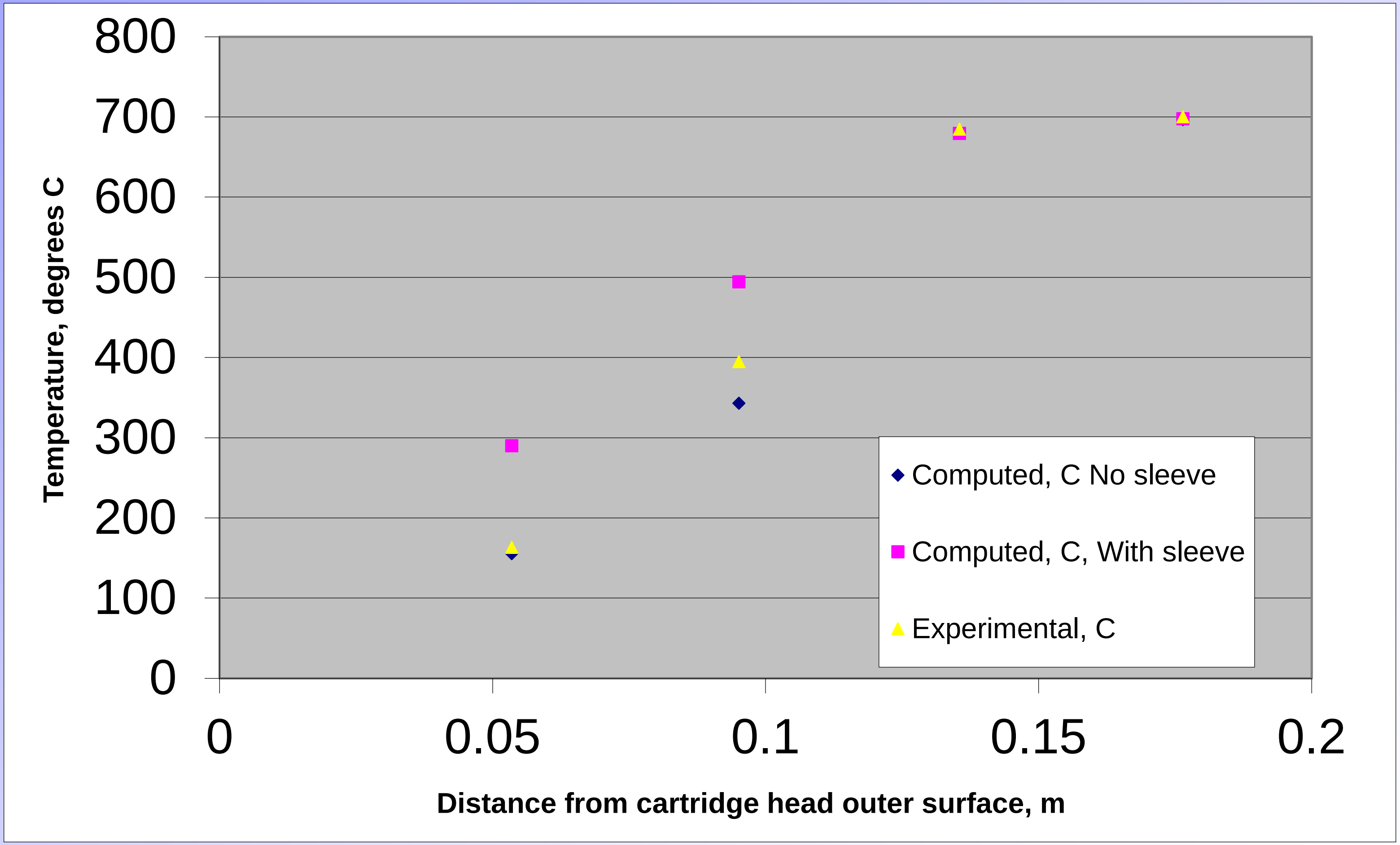

- Using CrysMas software package, Axi-Symmetric Heat conduction and radiation model was developed to explore the application of highly conductive sleeve on SAA to help supply heat from the heater core into the transparent zone and to **reduce dT/dx**

# Axial temperature profile and field in the model

- CrysMass calculations show significant reduction of dT(x)/dx when 15 cm long, OD=17.6 mm, ID=16 mm sapphire pipe is used



# Comparison of temperatures measured by sample TC's in experimental run Inl-G1 with values obtained by simulation



# Conclusion

- ***The step change in temperature, between the heated and the unheated zone**, **causes large temperature gradients, dT/dx,*** which are

  (a) undesirable for single crystal growth
  (b) may cause convective interference with diffusion in microgravity experiments.

  (c) For InI, CLYC and there non-metallic melts, ~1 cm of melt is visible.

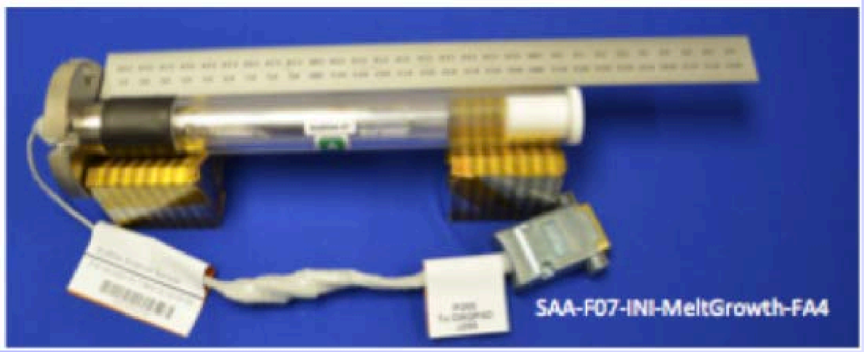
- temperature gradient in the SAA should be reduced to a value of 20 to 50 K/cm in order to:

  - reduce overheating the melt
  - reduce thermal stresses and stress induced dislocations.
  - reduce convection on Earth and in microgravity.
  - allow 3 to 4 cm of the melt to be visible (as this was the case with InSb).

- Using a sapphire (or other highly conductive material) tube will significantly reduce the step change in the boundary conditions

# Flight samples – Melt growth



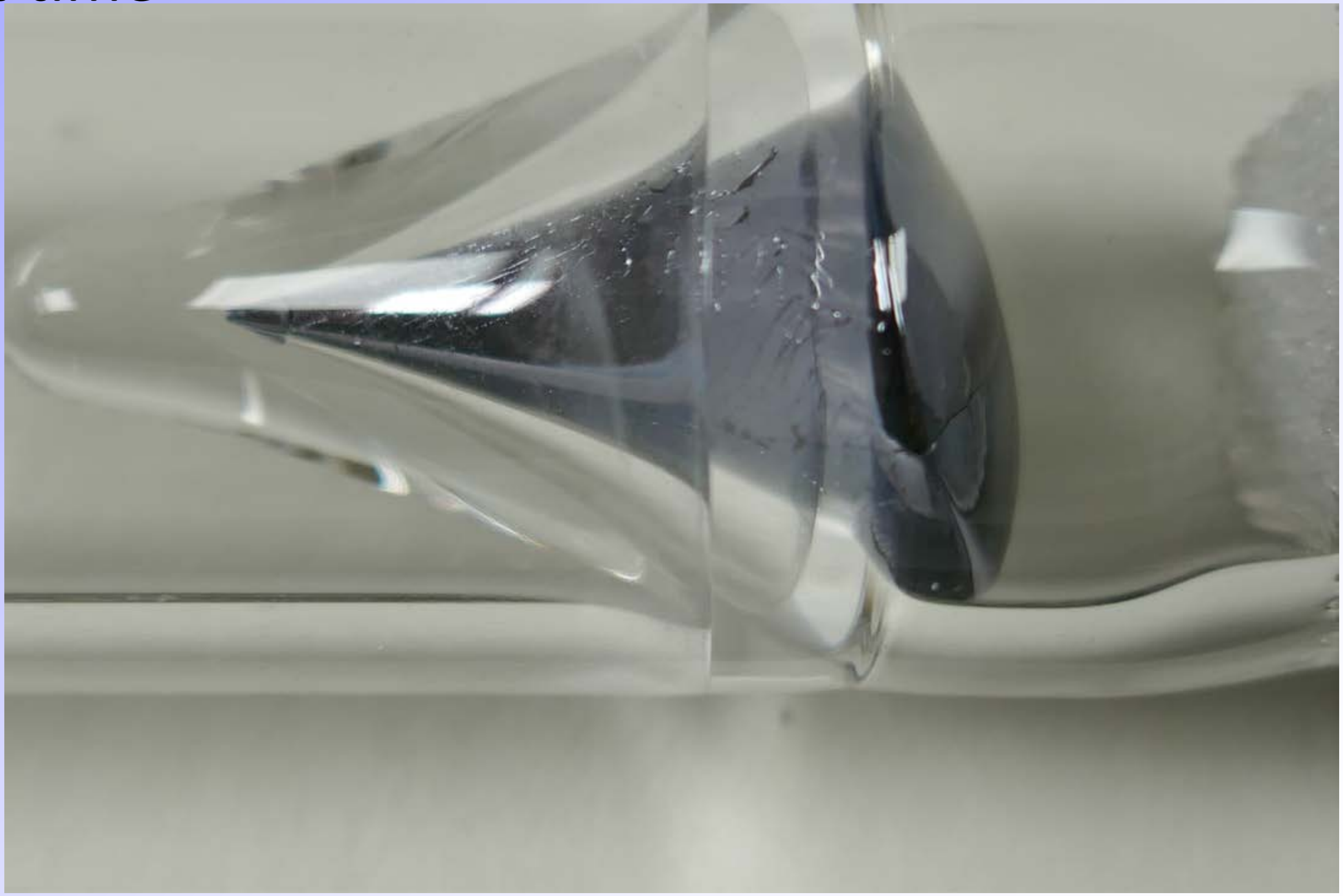




- The design of SAA featuring highly conductive silver and sapphire sleeves was implemented in the flight experiment samples
- Four melt growth samples of InI were delivered to the ISS in March 2017

# Vapor growth of InI

Over the course of this investigation a bulk crystals of InI were produced by physical vapor transport for the first time



# Flight samples – vapor growth

Two vapor growth samples of InI were delivered to the ISS in March 2017

# Acknowledgement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