Crystal Growth Laboratory
Fraunhofer Institute of Integrated Circuits and Device Technology (IISB)
Erlangen, Germany

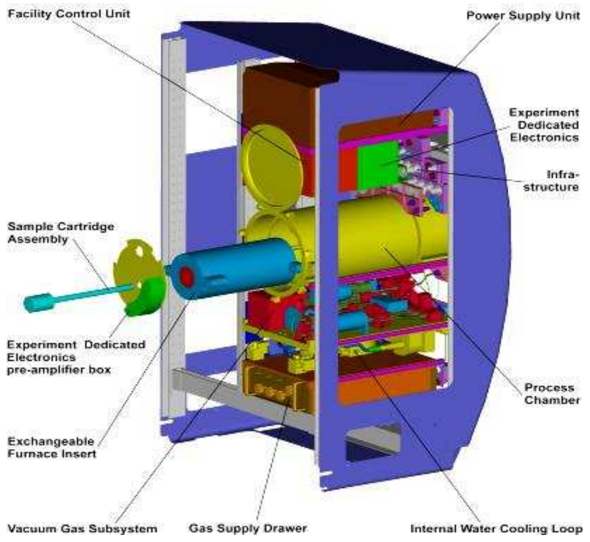
Simulation of Furnace Inserts and Sample-Cartridge Assemblies using the Thermal Modeling Tool CrysVUn

M. Hainke, J. Dagner, J. Friedrich, G. Müller

ESTEC contract No. 16462/02/NL/JS

Contents

The Material Science Laboratory and Modeling Tasks



Furnace inserts (FIs)
- Low Gradient Furnace (LGF)
- Solidification and Quenching Furnace (SQF)

Several types of different sample-cartridge assemblies (SCAs), dependent on FI and specific experimental requirements.

MSL User Support Program

Support users and hardware developer with a thermal modeling tool (TMT) in
- Construction of the SCA
- Definition of the process parameters
- Evaluation of experiments

Contents

Modeling of solidification processes with the TMT CrysVUn

Physical phenomena:

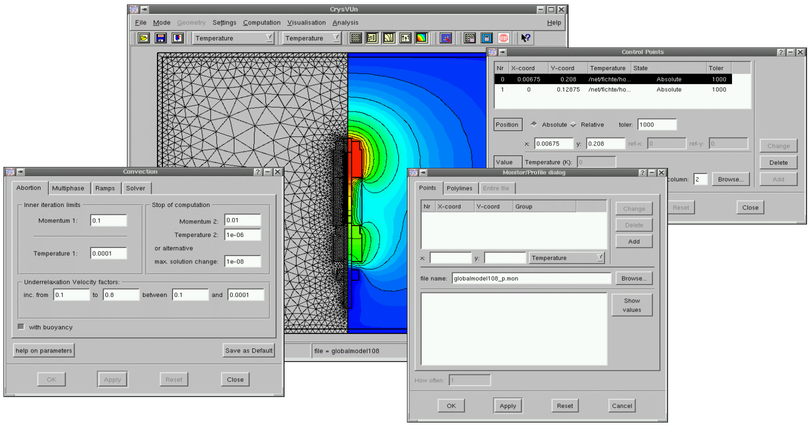
- (Laminar) convection
- Radiative heat transfer (semitransparent media)
- Heat transfer by conduction (anisotropic)
- Resistance and inductive heating
- Thermal stress
- Time-dep. magnetic fields
  (rotating, travelling, alternating)
- Alloy solidification
  Flow in porous media
  Macrosegregation
  Microsegregation modelling

Working with CrysVUn:

- *Inverse simulation*
- Unstructured grids
- Easy transfer of CAD-files
- Automatic grid generation
- *User-friendly graphical interface*

Technical details:

- Finite-volume technique
- Axisymmetric/2D-geometry
- Direct/indirect solvers
- Unix/Windows systems
- Parallelisation of view-factor
  computation

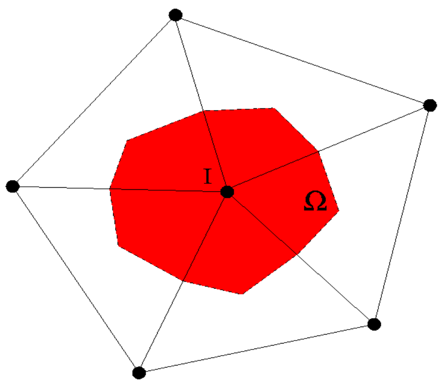


Finite Volume Technique on Unstructured Grids

Integral form of a general conservation equation:

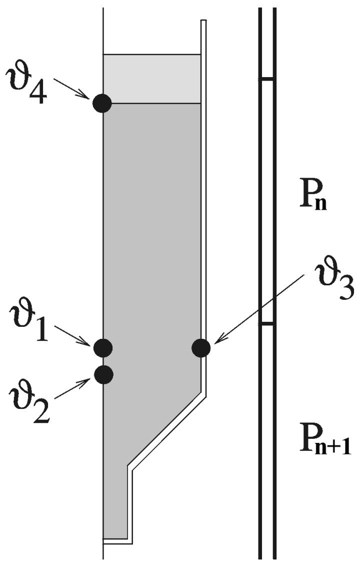
$$\int_{\Omega} \Lambda_t \frac{\partial \phi}{\partial t} dV + \oint_{\partial\Omega} \Lambda_c \phi \mathbf{v} \cdot \mathbf{n} dS = \oint_{\partial\Omega} \Lambda_d \nabla \phi \cdot \mathbf{n} dS + \int_{\Omega} s_\phi dV$$

unsteady term convection term conduction term source term



Unstructured grid and construction of a control volume, surrounding a vertex I.

Idea of Inverse Modeling



- forward simulation: $\{P_n\} \Rightarrow T(x)$
heater powers are given, like in experiments, problem is mathematically well posed
- inverse simulation :

selection of N points $\{x_1, \ldots x_n\}$
where N temperature $\{\vartheta_1, \ldots \vartheta_N\}$ are given

mathematical problem:
find the heating powers P_m so that $T(x_n)=\vartheta_n$ for all n ($1 \le n \le N$),
this problem is mathematically ill-posed

strategy of solution within CrysVUn

$$\tfrac{1}{2}\sum_n w_n \left(T(x_n) - \vartheta_n\right)^2 + \tfrac{\mu}{2}\sum_m \left(P_m\right)^2 = \min$$

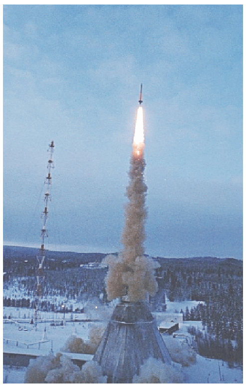
weak formulation *regularization*

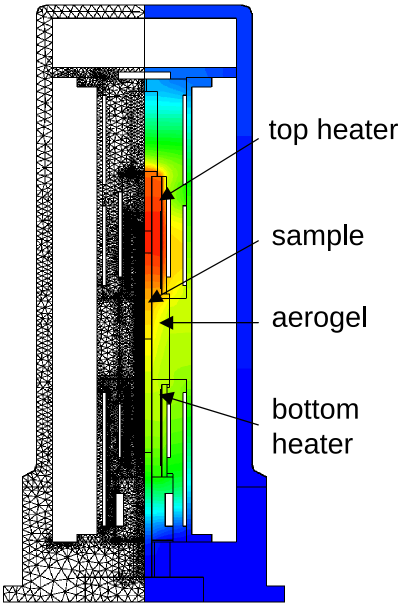
Contents

Application of CrysVUn in Microgravity Research I

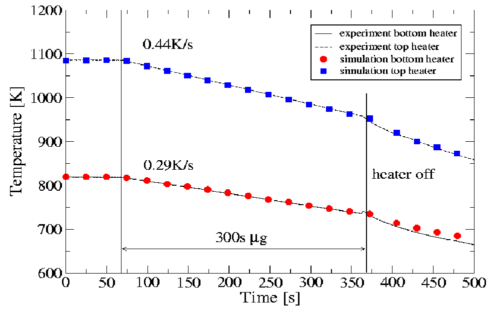
MICAST
MAP project No. AO-99-031

Thermal modeling of the ARTEX facility (IRS,DLR).

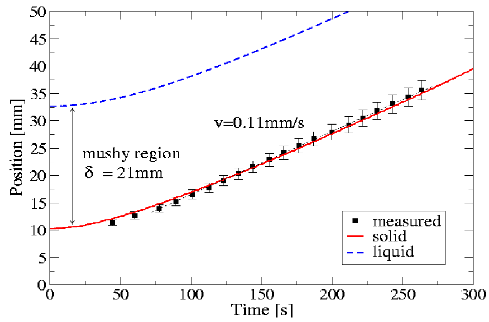




Heater temperature profiles as used on TEXUS39



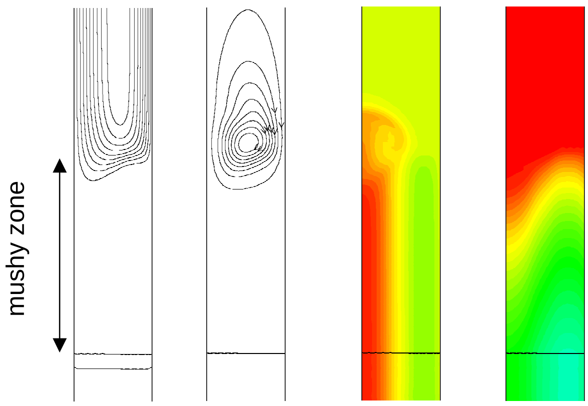
Resulting solidification process



Application of CrysVUn in Microgravity Research II

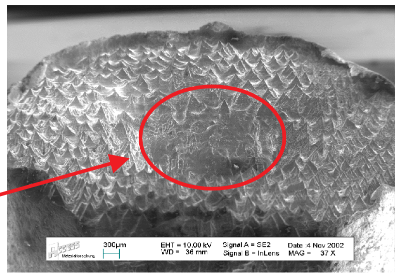
→ Modeling task: Definition of process conditions for the re-flight of ARTEX, scheduled for TEXUS41, but now equipped with an additional rotating magnetic field (RMF).

Example: Solidification of AlSi7 including a RMF



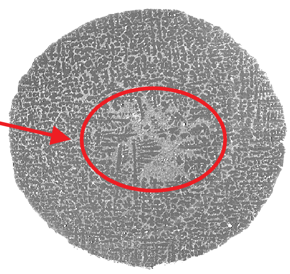
from left to right: azimuthal flow velocity, streamlines, segregation and liquid volume fraction

liquid channel formation



(source: ACCESS, e.V.)

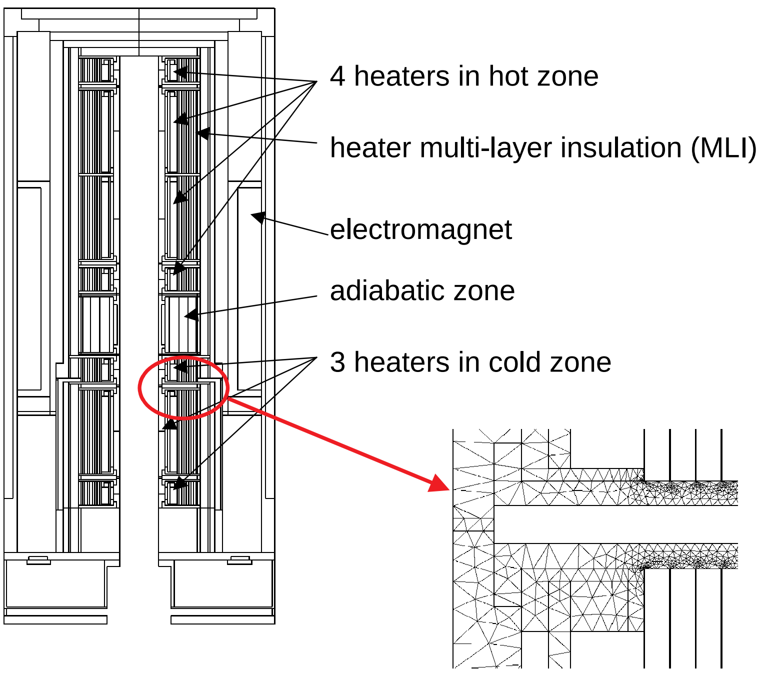
axial Si segregation



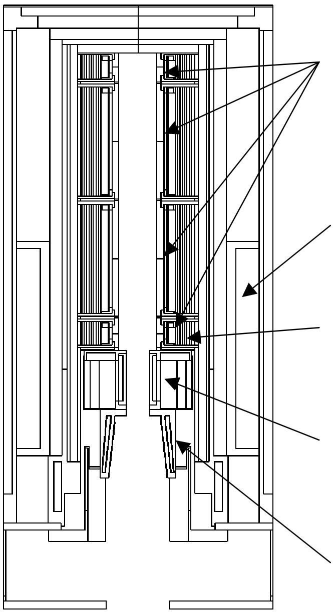
(source: IRS, DLR)

Contents

Thermal Model of LGF

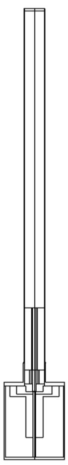


Thermal Model of SQF

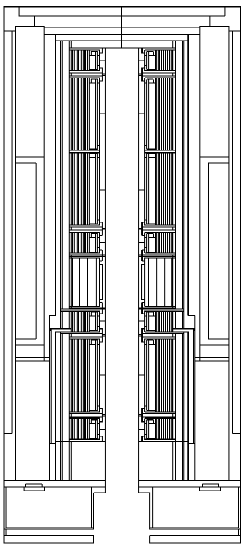


Pre-Processing SCA Models Independently from FI Models

2 select appropriate FI model from a list



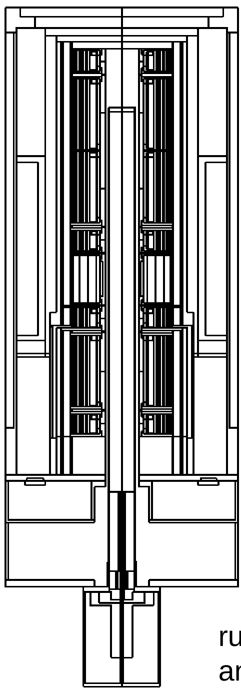
+



=

generate engineering model (EM)

3



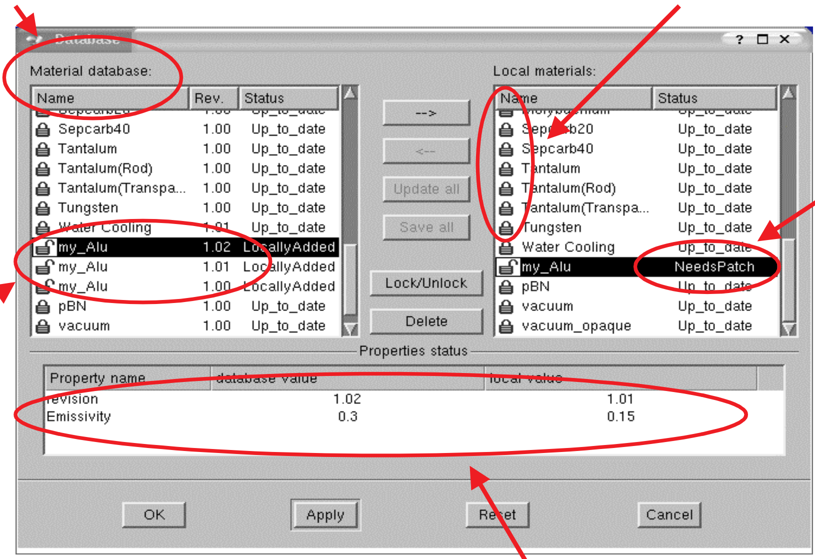
1 modify pre-processed SCA model or design SCA model from the scratch

4 run thermal analysis

Extended Material Database in CrysVUn

Materials used in the FIs and test SCAs are taken from a central material database.

FI related materials are locked for the Users.



Old material properties used in a thermal model are identified.

Revision control in the case of changed material properties.

Changed material properties are displayed in the GUI.

Contents

Conclusion and Outlook

The TMT CrysVUn was further developed according to ESA's software standard PSS05-lite to fulfill the user requirements defined by ESA.

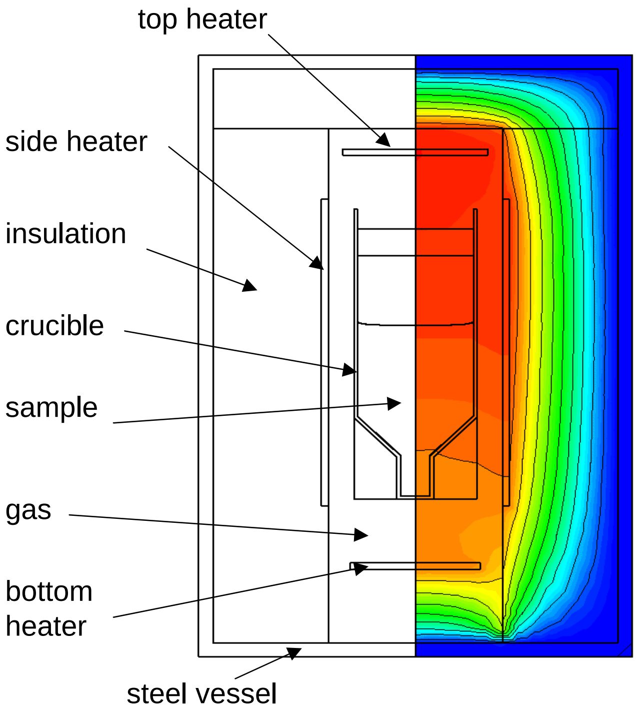
Thermal models for the FI Low Gradient Furnace (LGF) and Solidification and Quenching Furnace (SQF) were developed according to ESA's software standard PSS05-lite.

The detailed validation of the thermal models is underway.

Currently, CrysVUn is applied on behalf of EADS to support the development of the Sample-Cartridge Assemblies which shall be used by the different European MSL users.

Contents

Online Demonstration of CrysVUn using a VGF toymodel



Quick-start in CrysVUn:
- making a forward simulation
- making a inverse simulation
- evaluation of results
- changing the geometry