ON THE CONTROL OF THE EFFECTS OF GRAVITY ON SOLIDIFICATION MICROSTRUCURES USING OPTIMALLY DESIGNED BOUNDARY HEAT FLUXES AND ELECTROMAGNETIC FIELDS[1]

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The main objective of this work is to design and test computational techniques that can be used to control the microstructures that are developed during directional solidification processes.

Gravity plays an important role in the obtained microstructures mainly by influencing the melt flow mechanisms as well as the solute diffusion processes. Since these effects remain present even under a reduced gravity environment, we address inverse design solidification problems that result in desired microstructures at various gravity levels.

Our main design variables are the thermal mold/furnace conditions as well as the strength and orientation of an externally applied electromagnetic field. We select these continuous variables such that a desired growth velocity V and temperature gradient G are achieved near the freezing interface that correspond to desired microstructures. In our preliminary work, we are interested to design processes with spatially uniform growth velocity under stable growth conditions.

These design problems are inverse problems with overspecified thermal conditions (temperature and flux) on one part of the boundary and no-thermal conditions on another part of the boundary. They are posed as functional optimization problems. The exact gradient of the cost functional is obtained via the solution of an adjoint continuum problem. A sensitivity problem is also defined and is used in the implementation of the conjugate gradient method.

Since electromagnetic fields have a direct effect on the strength of the melt flow, the consideration of designing appropriate strengths and direction of electromagnetic fields simultaneously with continuous boundary heating/cooling conditions for various strengths of gravity enhances the success of the solidification design process.

These design techniques are useful for the development of the next generation of furnaces for controlled crystal growth. In particular, the availability of mathematical models for solidification control via optimally designed thermal boundary fluxes and electromagnetic fields is essential for the development of multiple-zone automated furnaces. Further development of such inverse techniques will enhance our ability to develop new advanced directional solidification process designs for cast microstructure control.

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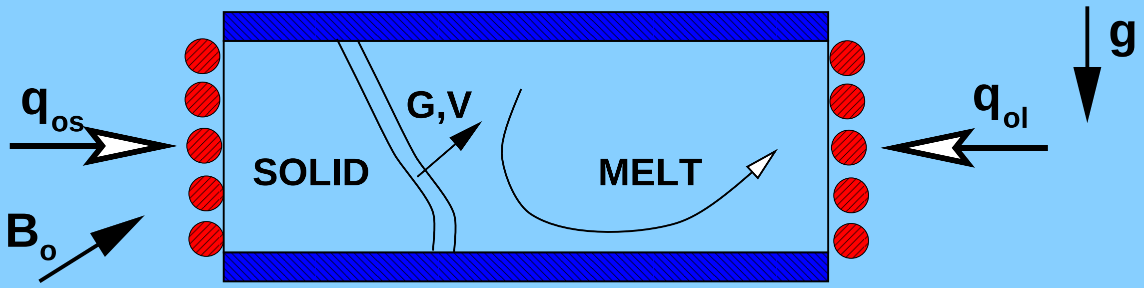
[1] NASA Materials Science Microgravity Conference, Huntsville, AL, June 6–8, 2000.

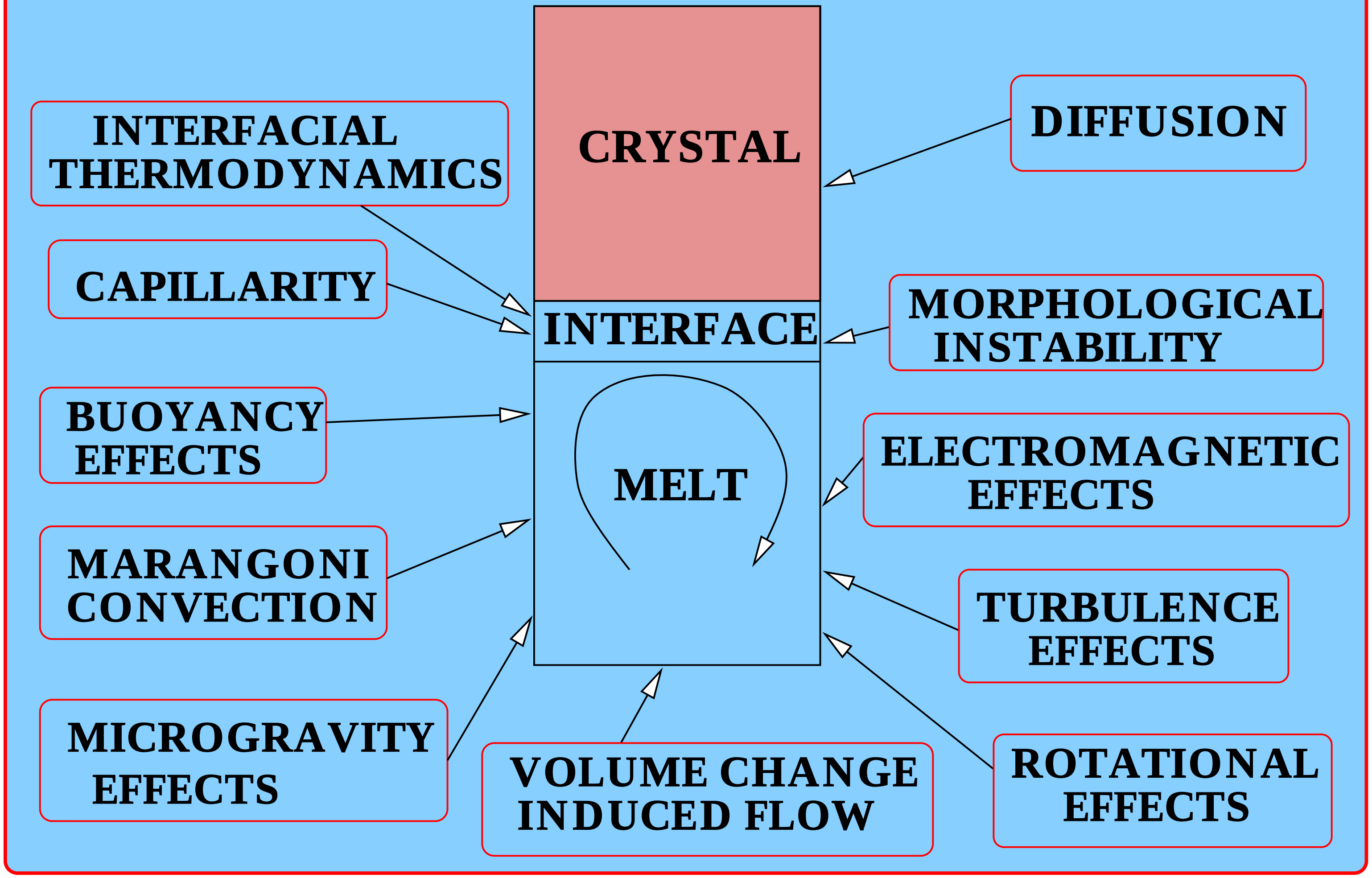
PROJECT OBJECTIVES



DEVELOP AND IMPLEMENT FEM BASED INVERSE METHODS FOR:

- Controlling growth velocity V and freezing interface heat flux G to obtain desired microstructures
- Delaying or eliminating morphological instability
- Eliminating or reducing the effects of convection on the solidification morphology
- Improving macroscopic and microscopic homogeneity of the final crystal

PHYSICAL MECHANISMS TO BE CONTROLLED DURING SOLIDIFICATION



CRYSTAL

INTERFACE

MELT

INTERFACIAL THERMODYNAMICS

CAPILLARITY

BUOYANCY EFFECTS

MARANGONI CONVECTION

MICROGRAVITY EFFECTS

VOLUME CHANGE INDUCED FLOW

DIFFUSION

MORPHOLOGICAL INSTABILITY

ELECTROMAGNETIC EFFECTS

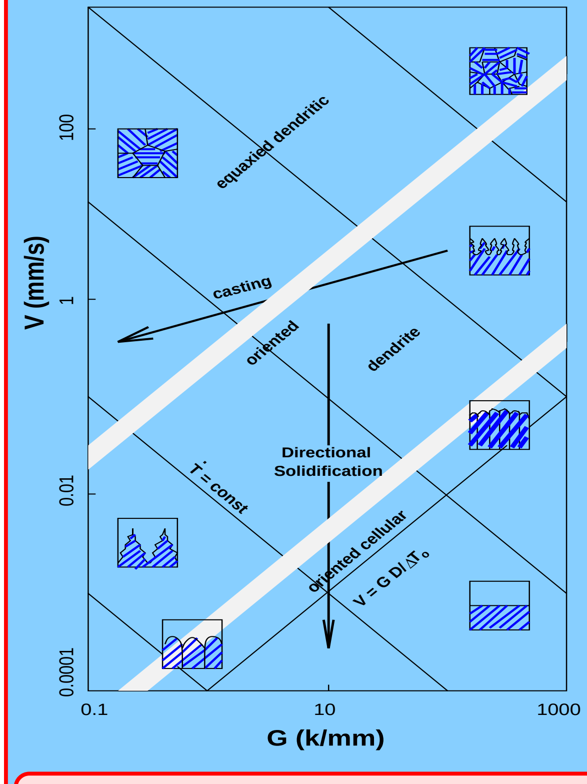
TURBULENCE EFFECTS

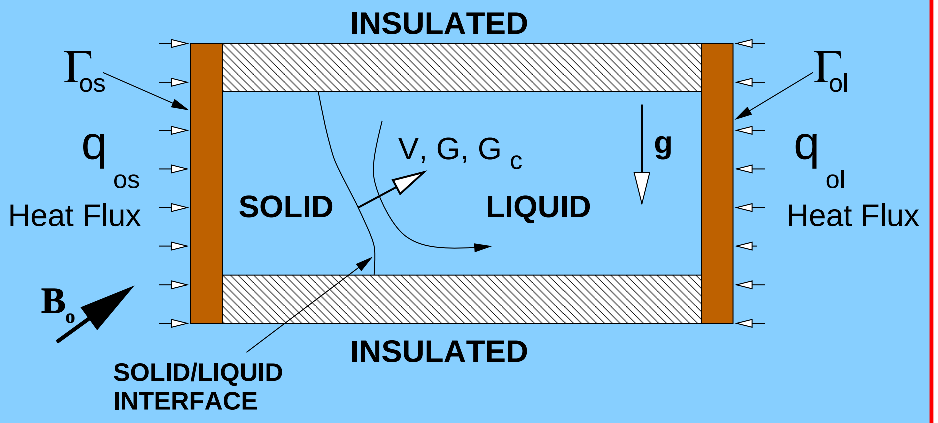
ROTATIONAL EFFECTS

MEANS FOR THE DESIGN OF DIRECTIONAL SOLIDIFICATION PROCESSES

- Proper adjustment of the cooling/heating furnace conditions
- Controlled variation of the solid-liquid interface growth velocity
- Use of electromagnetic fields for conducting melts in order to suppress or control the melt flow
- Proper rotation of the furnace/crucible to control the melt flow and solute distribution
- Solidification in reduced or gravity free environment to reduce the effects of buoyancy driven melt flow

DESIGN OF SOLIDIFICATION PROCESSES WITH DESIRED G/V STATE



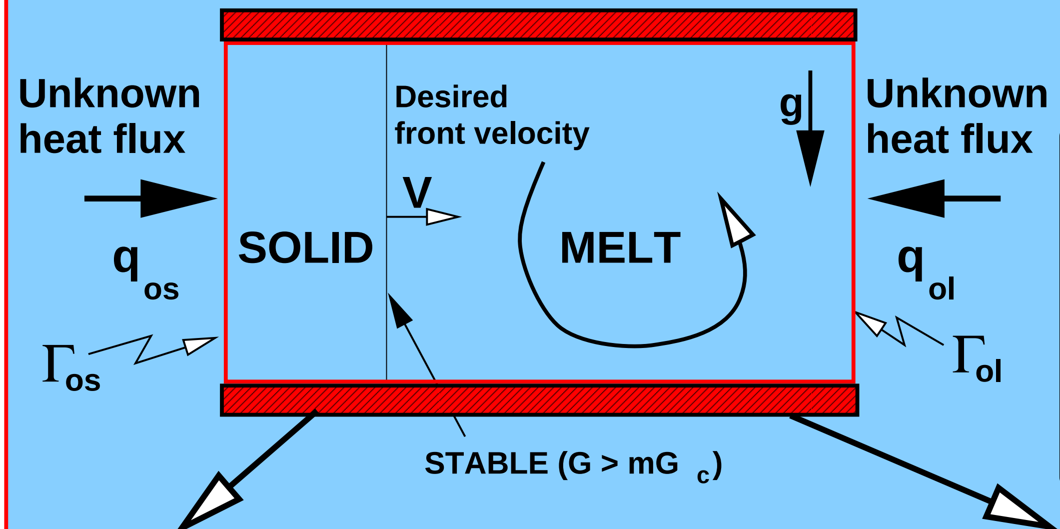


Thermal gradient (G) and growth velocity (V) are the main variables which determine the form and scale of microstructures

DESIGN OBJECTIVE

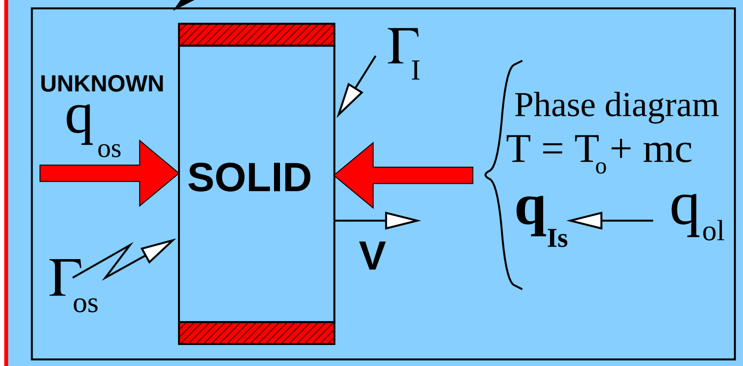
FIND THE OPTIMAL SOLID SIDE FLUX q_{os} AND THE LIQUID SIDE FLUX q_{ol} AS WELL AS THE DIRECTION AND INTENSITY OF THE APPLIED MAGNETIC FIELD AND GRAVITY SUCH THAT A DESIRED G-V STATE IS ACHIEVED

DESIGN OF BINARY ALLOY SOLIDIFICATION PROCESS



INVERSE PROBLEM STATEMENT

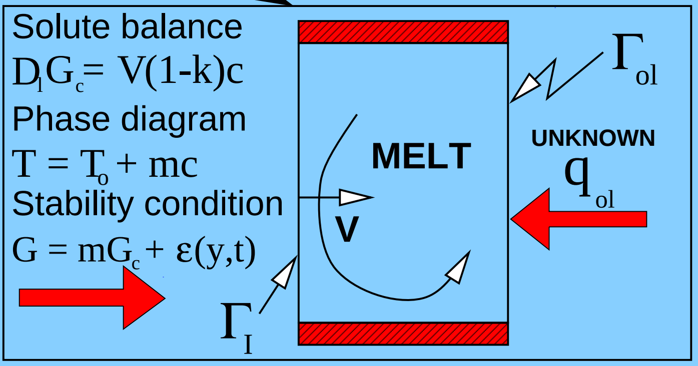
FIND THE COOLING CONDITIONS ON Γ_{os} AND THE HEATING CONDITIONS ON Γ_{ol} SUCH THAT A DESIRED STABLE GROWTH IS ACHIEVED



Phase diagram
$T = T_o + mc$

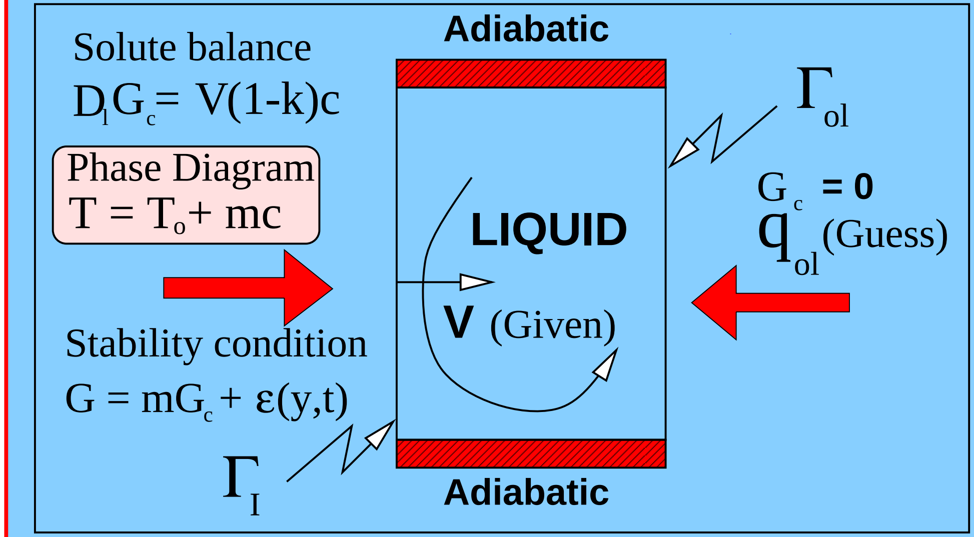
INVERSE HEAT CONDUCTION PROBLEM

Solute balance
$D_l G_c = V(1-k)c$
Phase diagram
$T = T_o + mc$
Stability condition
$G = mG_c + \varepsilon(y,t)$



INVERSE DESIGN WITH COUPLED HEAT, MASS AND MOMENTUM TRANSPORT

INVERSE THERMAL-SOLUTAL CONVECTION PROBLEM



Solute balance

$D_l G_c = V(1-k)c$

Phase Diagram

$T = T_o + mc$

Stability condition

$G = mG_c + \varepsilon(y,t)$

$G_c = 0$

q_{ol} (Guess)

With a guessed heat flux q_{ol} and without using the equilibrium equation solve the following direct problem

Define the cost functional as a measure of the deviation from thermodynamic equilibrium

$$J(q_{ol}) = \frac{1}{2}\left\| T(x,t;q_{ol}) - [T_m + mc(x,t;q_{ol})] \right\|^2_{\Gamma_I \times [0,t_{max}]}$$

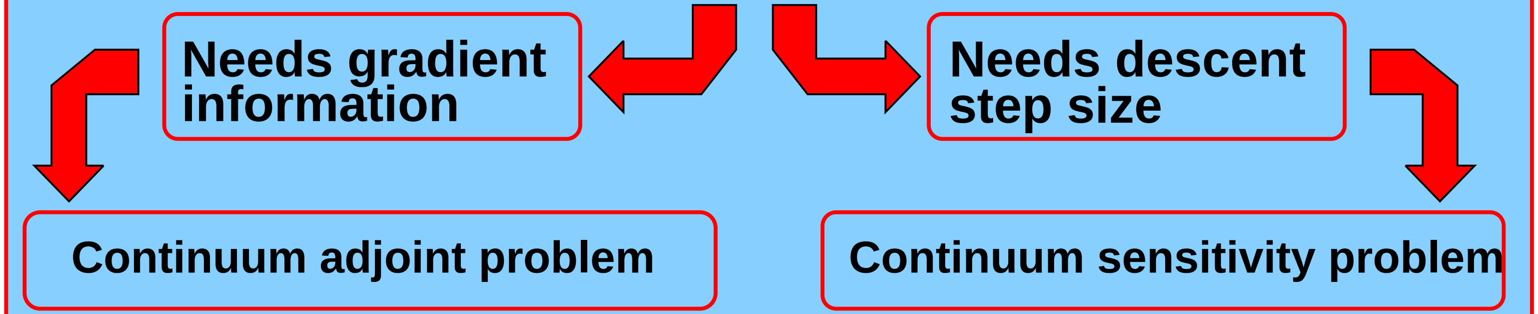
INVERSE THERMAL-SOLUTAL CONVECTION PROBLEM

- Define the inverse problem in the liquid domain in an optimization sense

Find a quasi solution $\overline{q}_{ol} \in L_2(\Gamma_{ol} \times [0, t_{max}])$ such that

$$J(\overline{q}_{ol}) \leq J(q_{ol}) \quad \forall \quad \overline{q}_{ol} \in L_2(\Gamma_{ol} \times [0, t_{max}])$$

- Solve the above minimization problem using the nonlinear Conjugate Gradient Method (CGM)



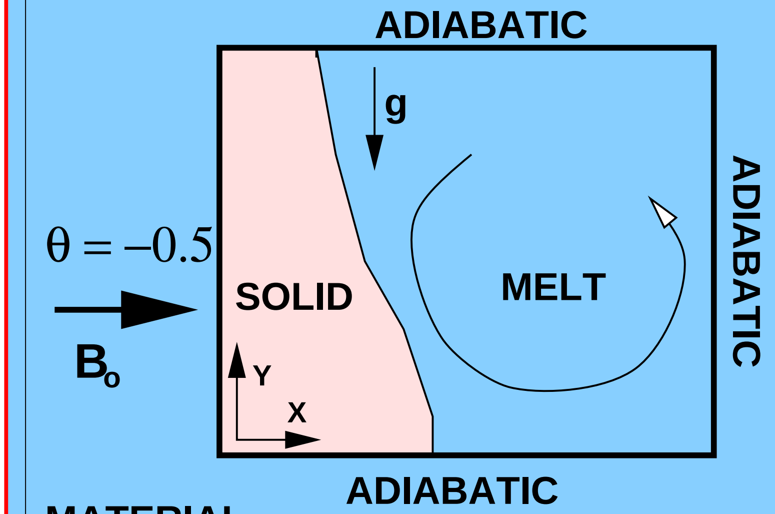
Needs gradient information

Needs descent step size

Continuum adjoint problem

Continuum sensitivity problem

REFERENCE BINARY ALLOY SOLIDIFICATION PROBLEM UNDER THE INFLUENCE OF AN EXTERNAL MAGNETIC FIELD



MATERIAL

Germanium + dopants

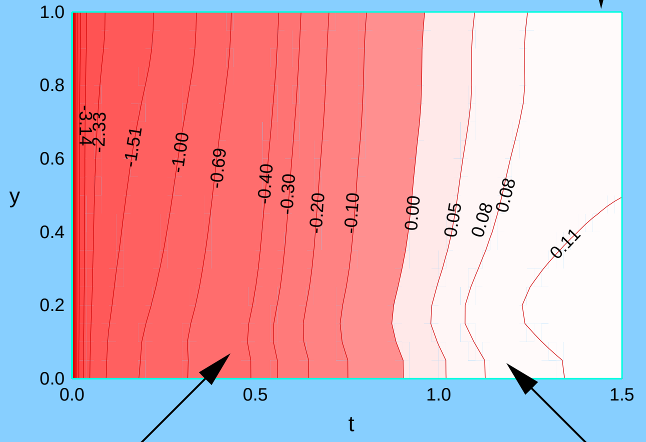
- **Properties from Brown et al., 1988**

FE MESH

800 bi-linear quadrilateral elements in the solid and liquid domains

FE SIMULATION

POST PROCESS

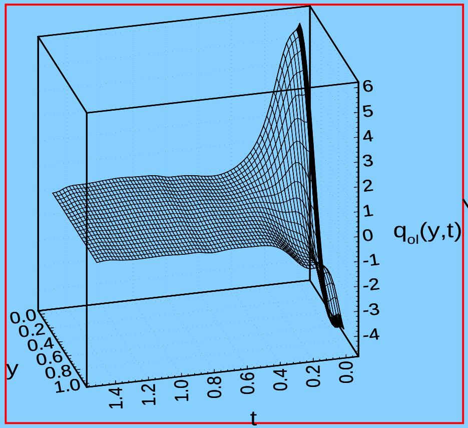


STABLE GROWTH

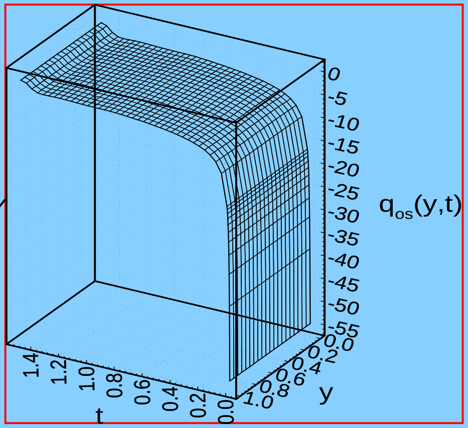
MORPHOLOGICAL INSTABILITY

THE WELL POSED MATHEMATICAL PROBLEM VIOLATES THE A-PRIORI ASSUMPTION OF STABILITY!

DESIGN TO ACHIEVE A DIFFUSION-BASED STABLE GROWTH IN THE PRESENCE OF MELT CONVECTION



OPTIMAL LIQUID SIDE HEAT FLUX



OPTIMAL SOLID SIDE HEAT FLUX

INPUT

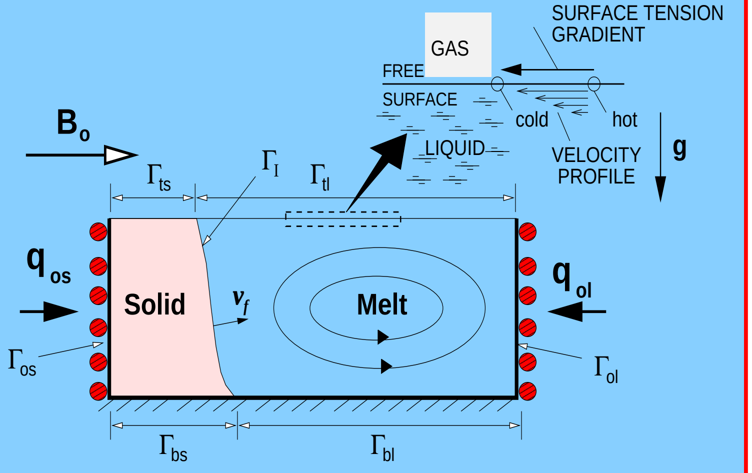
INPUT

DIRECT ALLOY SOLIDIFICATION SOLVER INCLUDING THE COUPLED EFFECTS OF BUOYANCY AND ELECTROMAGNETIC CONVECTION

FLAT-INTERFACE STABLE GROWTH CORRESPONDING TO A DIFFUSION BASED SOLIDIFICATION PROBLEM

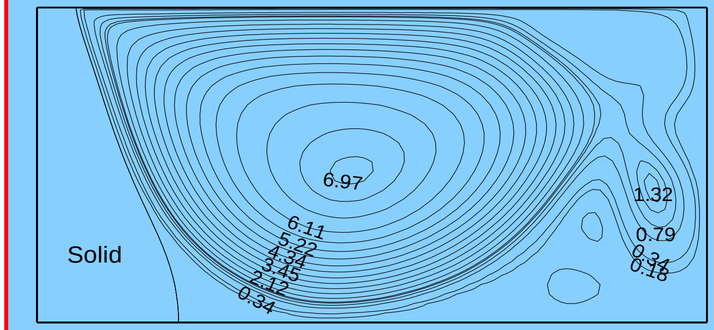
CONTROL OF CONVECTIVE EFFECTS IN THE MELT THROUGH ELECTRO-MAGNETIC AND MICROGRAVITY DESIGN

- In low-gravity environment the action of Marangoni convection is significant
- A preliminary design study has shown that thermal flux design combined with appropriate magnetic field and microgravity strength and orientation can lead to a desired flat-interface growth

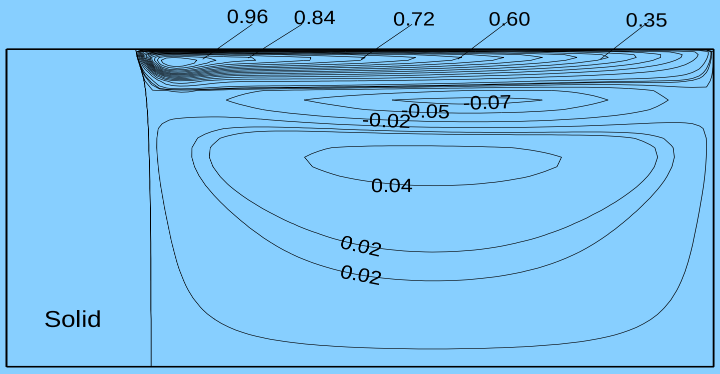


SOLIDIFICATION SIMULATION

MATERIAL: Germanium-Antimony



Normal gravity
No magnetic field



Reduced gravity
Horizontal magnetic field

IMMEDIATE RESEARCH OBJECTIVES

- Implement design methods for desired interface growth conditions for several metallurgical and semiconductor materials
- Address flow control problems to stratify or restrict the melt flow to achieve macroscopic homogeneity
- Develop computational methods for simultaneous design of magnetic fields and thermal fluxes
- Incorporate microstructure evolution models to achieve desired microstructures based on optimal macroscopic design solutions
- Develop inverse methods for computational design of eutectic solidification models

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