Coupled Simulation of Transport Phenomena in Directionally Solidifying γ(TiAl) Alloy under Electromagnetic Fields

The Transport Phenomena here are described in term of Temperature, Melt Flow Velocity, Pressure, Solid-Volume Fraction and Concentration Fields *etc*

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INTRODUCTION

- Heat energy and species mass transfer, as well as melt flow are basic transport phenomena in solidification processes of various alloy ingots and castings (called " *Solidification Transport Phenomena* (STP)").
- These phenomena, in turn, play a critical role in controlling the solidification behaviors, structures and various defects formations, such as macrosegregation and porosity *etc*.

- In order to improve the qualities of the solidified alloy ingots/materials or to develop new materials processing methods, various electromagnetic (EM) techniques have been applied to materials solidification processes.
- Such as: Using alternating EM inductors or EM stirrers/brakes in continuous casting of Al alloy/steel ingots for melt flow/meniscus shape controls, or using an EM-inducted cold-crucible technique to obtain directionally solidified γ(TiAl)-base alloy ingots/materials (currently studied in the authors' research group).

• In such *EM materials processing* applications, the EM-induced solidification heat/mass transfer, and especially the melt flow behaviors can be *highly enhanced* (or *suppressed* in the case of a static magnetic field applied), through the *Lorentz forces* and *Joule heats*, and might be in a much more complex pattern.



The Aim of This Presentation

To present: An efficient multifield-coupled modeling method for the STP in alloy ingots/materials under an arbitrary EM-field, jointly using two different Computer Codes (One is FEM-Based/Commercial, another is FDM-based/Authors').

The Main Tasks:

- 1) To further extend a previous continuum solidificationmodel and the corresponding numerical solution algorithms(including an extended Direct-SIMPLE scheme for directly solving the EM-/gravity-/solidification-shrinkage-driven and strongly pressurelinked flow problems) to a more general EM-STP-case;
- 2) To propose an efficient technique for FEM→FDM dataconversion;
- 3) Try to apply the modeling to EM-directional solidification of Ti alloy castings/ingots.

Physical Model for EM-Directional Solidification





Electromagnetic solidification model

- A Continuum Model (based on Mixture Average Theory) with the following assumptions:
- 1) the external forces involved in a solidifying system are gravity and Lorentz force;
- 2) no pores will occur, i.e. the geometric continuity, $f_L+f_S=1$, holds for any region in the casting/ingot domain;
- **3**) the solid phase is macroscopically static during solidification;
- 4) local thermodynamic equilibrium holds at the microscopic solid-liquid interfaces
- 5) Newtonian and laminar liquid flow present;
- **6)** the model alloy is a binary system.

Solidification heat energy transfer

∂[(ρc_p)_mT]/∂t + ∇(f_Lρ_Lc_{PL}V T) = ∇[λ_m∇T] + ρ_Sh(∂f_S/∂t) + q_J
where, the electromagnetically inducted Joule heat is given by

q_J = J_GE = J_G²/σ

Solidification solute mass transfer

 $\partial(\rho C)_{\rm m}/\partial t + \nabla(f_{\rm L}\rho_{\rm L}VC_{\rm L}) = \nabla[D_{\rm L}\nabla(f_{\rm L}\rho_{\rm L}C_{\rm L}) + D_{\rm S}\nabla(f_{\rm S}\rho_{\rm S}C_{\rm S})]$

where:

 $\partial(\rho C)_{m}/\partial t = (\rho_{S}C_{S})^{*}\partial f_{S}/\partial t + \Phi f_{S}\partial(\rho_{S}C_{S})^{*}/\partial t + (\rho_{L}C_{L})\partial f_{L}/\partial t + f_{L}\partial(\rho_{L}C_{L})/\partial t \quad (4)$ $\Phi = \theta \phi/(1 + \theta \phi), \quad \phi = (D_{S}(T)/R_{f})\zeta \cdot \mathbf{A}_{2N} \quad \text{and} \quad \theta = k(1 + \beta)f_{S}/f_{L}^{2}$

(1)

(2)

(3)

(5)

L-S phase-change characteristic function for a specific alloy
 T_{Liq} = T_{Liq}(C_L*)

Solidification mass conservation: $\partial \rho_{\rm m} / \partial t = -\nabla (\mathbf{f}_{\rm L} \rho_{\rm L} \mathbf{V})$ (6)where, $\partial \rho_{\rm m} / \partial t \approx \rho_{\rm S}^* \partial f_{\rm S} / \partial t + \Phi f_{\rm S} \partial \rho_{\rm S}^* / \partial t + \rho_{\rm L} \partial f_{\rm L} / \partial t + f_{\rm L} \partial \rho_{\rm L} / \partial t$ (7)Momentum transfer for bulk/interdendritic liquid flow: $\partial (\mathbf{f}_{\mathrm{L}} \boldsymbol{\rho}_{\mathrm{L}} \mathbf{V}) / \partial \mathbf{t} + \nabla [(\mathbf{f}_{\mathrm{L}} \boldsymbol{\rho}_{\mathrm{L}} \mathbf{V}) \cdot \mathbf{V}] = \nabla [\mu \nabla (\mathbf{f}_{\mathrm{L}} \mathbf{V})] - \nabla (\mathbf{f}_{\mathrm{L}} \mathbf{P}) - (\mu \mathbf{f}_{\mathrm{L}}^{2} / \mathbf{K}) \mathbf{V} + \mathbf{F}_{\mathrm{R}}$ (8)For the present modeling, the body force term induced by external fields includes the gravity and Lorentz force: (9) $\mathbf{F}_{\rm B} = f_{\rm L} \rho_{\rm L} \mathbf{g} + \mathbf{F}_{\rm L}$ the Lorentz force acting on the moving liquid phase during solidification: (10) $\mathbf{F}_{\mathrm{L}} = \sigma f_{\mathrm{L}} (\mathbf{E} + \mathbf{V} \times \mathbf{B}) \times \mathbf{B} = f_{\mathrm{L}} \{ \mathbf{J}_{\mathrm{G}} \times \mathbf{B} + \sigma [(\mathbf{V} \cdot \mathbf{B})\mathbf{B} - \mathbf{B}^{2}\mathbf{V}] \}$

- Maxwell's equations $\nabla \times \mathbf{H} = \mathbf{J} + \partial \mathbf{D} / \partial \mathbf{t} \quad (Law of Maxwell-Ampere) \quad (11)$ $\nabla \times \mathbf{E} = -\partial \mathbf{B} / \partial \mathbf{t} \quad (EM-Induction \ Law of \ Faraday) \quad (12)$ $\nabla \cdot \mathbf{D} = \rho_{e} \quad (Law of \ Gauss) \quad (13)$ $\nabla \cdot \mathbf{B} = \mathbf{0} \quad (Continuity \ of \ Magnetic \ Flux) \quad (14)$
- Constitutive equations for the involved EM-medium materials
 D = εE (Constitutive Relationship of Electric Properties) (15)
 B = μH (Constitutive Relationship of Magnetic Properties) (16)
 J = σ(E+f_LV×B) (Ohm Law for the Moving Metallic Melt) (17)



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Numerical Solution Methods to the Equations for Alloy Solidification Transport Processes



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Numerical Solution Methods to the Equations for Alloy Solidification Transport Processes

• Iterative Computations for the Nonlinear and Strong T–f_s–C_LCoupling



Figure 1 Solidification behaviors of a binary alloy of nominal composition $C_0 < C_{SM}$ and with different solid-back diffusion (SBD) extents (Thermodynamic equilibrium holds at the micro-scale S/L interface). (a) A portion of binary alloy phase diagram with the solidification paths of C_L , C_S^* and \overline{C}_S for different SBD; (b) The corresponding curves of solid fraction versus liquidus.

Available for ANY Solid Back-Diffusion

Available for **BOTH** Single-Phase and Eutectic Solidification Portions



Fig. 4 Revised temperature by the latent heat release T^{i+1} (solid line) and the estimated temperature by Eq. (8) $T^{i+1'}$ (dashed line) for a control volume at the different nonequilibrium solidification stages for a binary eutectic system: (a) $f_{\rm S}^i = 0$, $T^{i+1'} \leq T_{\rm liq}(C_0)$; (b) $f_{\rm SE} > f_{\rm S}^i > 0$, $T_{\rm liq}(C_0) > T^{i+1'} \geq T_{\rm E}$; (c) $0 < f_{\rm S}^i < f_{\rm SE}$ ($T^i > T_{\rm E}$), $T^{i+1'} < T_{\rm E}$; (d) $1 > f_{\rm S}^i \geq f_{\rm SE}$ ($T^i = T_{\rm E}$), $T^{i+1'} < T_{\rm E}$, $f_{\rm S}^{i+1} < 1$; and (e) $1 > f_{\rm S}^i > f_{\rm SE}$, $T^{i+1'} < T_{\rm E}$, $f_{\rm S}^{i+1} = 1$.

(From: Daming Xu and Qingchun Li, "Numerical Method for Solution of Strongly Coupled Binary Aalloy Solidification Problems", *Numerical Heat Transfer, Part A*, 1991, Vol.20, 181-201.)

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Numerical Solution Methods to the Equations for Alloy Solidification Transport Processes

- Calculations of the Nonlinear and Strong Pressure– Velocity (P–V) Coupling in a Solidification Transport Process of Alloy Casting/Ingot Takes Most Portion (>90%) of the Entire Computational Efforts for the STP Numerical Simulation;
- Therefore, it is of Great Importance to Adopt a Algorithm of High Computational Efficiency for a Practical STP-Based Computer Simulation for the Solidification Processes of Alloy Castings/Ingots.

Numerical Solution Methods to the Equations for Alloy Solidification Transport Processes Numerical Computations of the Nonlinear and Strong P–V Coupling **SIMPLE** Scheme widely used for Fluid **Direct-SIMPLE** Scheme by present Authors (No Iteration Needed \rightarrow C. Efficiency $\uparrow \uparrow$ Available both for P-V**Transport Systems** by Subas V. Patankar Coupling in Pure Fluid Systems and Alloy Solidification Systems) Let $P = P^* + P'$, take an initial estimation: $P^0 = P^*$ Let: t^{i+1} time's pressure= t^i time's pressure + pressure change in the time interval Δt^{i+1} , i.e. $P^{i+1} = P^i + \Delta P^{i+1}$ (1)Let: tⁱ⁺¹ time's accurate V-field=an approximate V-field + the V-Calculate the approximate velosity: $V_x^* \& V_y^*$ based on corrections induced by the pressure change in time Δt^{i+1} : ΔP^{i+1} , the up-to-date pressure Pⁿ and Momentum Equations i.e. $V_X^{i+1} = V_X^* + V_X'$ and $V_Y^{i+1} = V_Y^* + V_Y'$ (2)/(3)Using V_x & V_v , V-correction eqs. and mass-conserv. eq. Using tⁱ time's pressure field: Pⁱ and tⁱ time's V-field: V_{v}^{i} and V_{v}^{i} , to calculate the approximate pressure: P' and $P^{n+1} = P^n + P'$ calculate the approxi. V-field: V_x^* and V_y^* from momentum eqs. Using the obtained t^{i+1} time's T, f_s and C_t fields, and the approxi. Using V_x^* , V_y^* , P'&V-corr. eqs. to calculate approxi. V: $V_x^{n+1} \& V_y^{n+1}$; calculate other fields that influence P&V V-field: V_x^*/V_x^* , solve the algebraical eq. set for ΔP^{i+1} which is derived from the mass conservation eq. and the V-correction eqs. If P^{n+1} Using V_x^* , $V_v^* \& \Delta P^{i+1}$ and the V-corr. eqs., calculate the accurate $V_{\mathbf{v}}^{n+1}$ and $V_{\mathbf{v}}^{n+1}$ converge? tⁱ⁺¹ time's pressure and velosity fieds: $P^{i+1} \& V^{i+1}$ from eqs.(1)-(3). No Yes End of **P-V** coupling calculation End of **P**-**V** coupling calculation (From: Daming Xu and Qingchun Li, " Gravity- and Solidification-Shrinkage-Induced (From: Subas V. Patankar, Numerical Heat Transfer and Fluid Flow, McGraw-Hill, Liquid Flow in a Horizontally Solidified Alloy Ingot", Numerical Heat Transfer, Part A, 1980) 1991, Vol.20, 203-221.)

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FEM-calculated results from **ANSYS 6.1** (TiAl casting, CaO mould, under a harmonic EM-field of 20kHz and with loads of 10kAt. The shaped casting has moved down for 40mm relative to the coils): **a**) meshed pattern for the whole EM-directional solidification system (right-half, with the EM-boundary definitions); **b**) the local meshed element grids around the casting; **c**) calculated distribution of the Az magnetic potential contours.

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outside the FEM-element.

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FEM-EM Results → **FDM Format Conversion**





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The comparison of the data between before and after conversion (Inducted current density)

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The physical properties used for the present computer modeling of solidification transport phenomena of γ (TiAl)-Al%at. pseudo-binary alloy

| • | Thermal conductivity: $\lambda_{s}(T) = \lambda_{L}(T) = 2.3 \times 10^{-2}$ | | [W/mm·°C] |
|---|---|--|---------------------------|
| • | Solid specific heat: | | |
| | $\left(\begin{array}{c} 0.67832 - 6.4328 \times 10^{-6} \cdot \mathrm{T} + 2.5417 \times 10^{-13} \cdot \mathrm{T}^3 \end{array} \right)$ | $(25^{\circ}\mathrm{C} < \mathrm{T} \leq 660^{\circ}\mathrm{C})$ | |
| | $c_{PS}(T) = \begin{cases} 0.68286 + 1.3644 \times 10^{-5} \cdot T \end{cases}$ | $(660^{\circ}C < T \le 882^{\circ}C)$ | [J/g·°C] |
| | $0.65193 + 1.0513 \times 10^{-5} \cdot T$, | $(882^{\circ}C < T \le 1490^{\circ}C)$ | |
| • | Liquid specific heat: $c_{PL}(T,C_L) = 0.86074$, (1490°C < T | ≤ 2727°C) | [J/g·°C] |
| • | Solid density of the alloy: $\rho_{\rm S}({\rm T},{\rm C}_{\rm L}) = 3.8 \times 10^{-3}$, | | [g/mm ³] |
| • | Liquid density of the alloy: | | |
| | $\rho_L(T,C_L) = 3.632 \times 10^{-3} - 2.0 \times 10^{-7} \cdot (T-T_{liq.}) - 9.32 \times 10^{-6} \cdot (C_L - C_O)^{-6} \cdot (C_L - C$ |) | [g/mm ³] |
| • | Latent heat of fusion: $h(C_s) = 435.4$ | | [J/g] |
| • | Liquidus of the γ(TiAl)-Al%at. alloys: | | |
| | $T_{liq}(C_{L/Al}) = 802.19745 + 23.01678 \cdot C_L - 0.20279 \cdot C_L^2 ,$ | $(C_L \in [54.86, 74.61at.\%Al])$ | [°C] |
| • | Partition coefficient: | | |
| | $k(C_{L/Al}) = 69.24438 - 4.03153 \cdot C_{L} + 8.894 \times 10^{-2} \cdot C_{L}^{-2} - 8.70031 \times 10^{-4} \cdot C_{L}^{-2} \cdot C_{L}^{-2} - 8.70031 \times 10^{-4} \cdot C_{L}^{-2} \cdot C_{L}^$ | $_{L}^{3}$ + 3.18595×10 ⁻⁶ ·C $_{L}^{4}$ | |
| | | $(C_{L} \in [54.86, 74.61at.\%A1])$ | [-] |
| • | Liquid diffusion coefficient: $D_{L/Al}(T^{\circ}C) = 5 \times 10^{-3}$ | | $[mm^2/s]$ |
| • | Solid diffusion coefficient: $D_{S/AI}(T^{\circ}C) = 0.11 \cdot exp[-14504/(T+2)]$ | 273.15)] | $[mm^2/s]$ |
| • | Dynamic viscosity coefficient: $\mu(T) = 3.5 \times 10^{-3}$ | $[Pa \cdot s] (= [N \cdot s/m^2)$ | $^{2}] = [g/mm \cdot s])$ |
| | $4.0 \times 10^{-4} f_L^{3.0}$, $(f_L \le 0.7088)$ | | |
| • | Permeability coefficient: $K = \begin{cases} 1.6318 f_L^{27.155}, (0.7088 < f_L \le 1.6318) \end{cases}$ | 0.99999) | [mm ²] |
| | (1.0×10^{18}) , (f _L >0.99999) | | |
| • | Primary dendrite spacing: $d_1 = 1.4 \times 10^{-1}$ | | [mm] |
| • | Secondary dendrite arm spacing: $d_2 = 3.0 \times 10^{-2}$ | | [mm] |
| | | | HIT-MSE |















Animation: $V\&f_{S}$ Evolution in a Blade-like γ (TiAl)-55at.%Al

Casting directionally Solidifying under Zero & a Harmonic EM-Field



Only under Gravity

Under Gravity + Harnonic EM-Field (20kHz,500kAt)

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Solidification Transport Processes of a Blade-like Al-4.5%Cu Casting under Transverse Static Magnetic Fields of different Load Strengths (in At)



Comparisons of liquid flow and directional solidification behaviors of Al-4.5%Cu shaped casting under static magnetic fields inducted by different current-turns at t=21.0 sec: (a) Velocity vectors of liquid phases; (b) Contours of relative pressure in the liquid; (c) Contours of solid volume fraction; (d) Contours of temperature.

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Solidification Transport Processes of a Blade-like In718-4.85%Nb Casting under Transverse Static Magnetic Fields of different Load Strengths (in At)

Influences of transverse static magnetic strengths on the liquid flow behaviors and temperature /concentration distributions in directionally solidified In718 shaped castings at t=21.0 sec.: (a) Velocity vectors of liquid phases; (b) Contours of temperature; (c) Contours of liquid concentration, Nb%wt..

Solidification Transport Processes of a Blade-like In718-4.85%Nb Casting under Transverse Static Magnetic Fields of different Load Strengths (in At)

Influences of transverse static magnetic strengths on the liquid flow behaviors and temperature /concentration distributions in directionally solidified In718 shaped castings at t=21.0 sec.: (a) Velocity vectors of liquid phases; (b) Contours of temperature; (c) Contours of liquid concentration, Nb%wt..

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Influences of transverse static magnetic strengths on the liquid flow behaviors and temperature /concentration distributions in directionally solidified In718 shaped castings at t=21.0 sec.: (a) Velocity vectors of liquid phases; (b) Contours of temperature; (c) Contours of liquid concentration, Nb%wt..

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Application on the Way to: Directional Solidification of Cold Crucible Titanum Alloy Strip Ingot

Directional Solidification Apparatus of Cold Crucible Ti Alloy Strip Ingot Currently Used in the Authors' Group

Revised Continuum Model for EM-STP

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Solidification heat energy transfer

- $\mathcal{A}(\rho c_p)_m]/\mathcal{A} + \nabla (f_L \rho_L c_{pL} VT) + V_0 \mathcal{A}(f_L \rho_L c_{pL} T) + (f_S \rho_S c_{pS} T)]/\mathcal{A}$
- $= \nabla [k_m \nabla T] + \rho_s h(\partial f_s / \partial t) + q_J$

Solidification solute mass transfer

 $\frac{\partial}{\partial (\rho C)_m} \frac{1}{\partial t} + \frac{\nabla}{(f_L \rho_L C_L V)} + \frac{V_0 \partial}{\partial (f_L \rho_L C_L)} + \frac{(f_S \rho_S C_S)}{\partial t} \frac{1}{\partial t}$

 $= \nabla [\rho_L D_L \nabla (f_L C_L) + \rho_S D_S \nabla (f_S \rho_S C_S)]$

Solidification mass conservation

 $\partial \rho / \partial t + \nabla (f_L \rho_L V) + V_0 \partial \rho / \partial z = 0$

Momentum transfer for bulk/interdendritic liquid flow $\frac{\partial f_L \rho_L V}{\partial t} + \nabla [(f_L \rho_L V)V] + V_0 \nabla (f_L \rho_L V) + V_0 \partial (f_L \rho_L V)/\partial t = \nabla [\mu \nabla (f_L V) - \nabla (f_L P) + f_L \rho_L g - (\mu f_L^2/K)V + f_L \rho_L g + F_L t]$

Schematic FEM and FDM Meshing for the Top and Bottom Hump Regions

Magnetic Flux Density Vectors Output from Ansys 6.1 FEM-Analysis

EM-FEM q_I **Results** \rightarrow **FDM** Format Conversion

Schematic Radiation Heat Transfer between the Top and Bottom Humps

$$T = (\alpha \sum_{JI+1}^{JI2} T_{J,K+1/2} + T_M) / [\alpha (JI2 - 1 - JI) + 1]$$

 α is an approximate average of the sum of view factor $\cos\theta$ (0< α <1)

EM-Inducted Heating Processes in Top and Bottom Ingots (at x=12mm)

EM-Inducted Heating Processes in Top and Bottom Ingots (at x=12mm)

EM-Inducted Heating Processes in Top and Bottom Ingots (at x=12mm)

尔滨エルナ **Summary** The proposed modeling methods appear practical and efficient in numerical computation (The each above demonstrated sample usually takes 2-5 hours on a PC with a 1.6GHz-CPU) The computational results show that the solidification-shrinkage-driven interdendritic liquid flow in mushy zone, though usually smaller than the convection in bulk liquid region by order(s), can not be easily suppressed by a static magnetic field applied. (The inner force caused by solidification-shrinkage might be much stronger than Lorentz force)

Table I Initial and technological parameters for the presentexample simulations with 3 different kinds of Alloys

| Alloys | IN718 base-4.85wt.%Nb | γ(TiAl)-55at.%Al | Al-4.5wt.%Cu |
|---|-----------------------|------------------|--------------|
| Pouring temperature, T _P | 1450 °C | 1500 °C | 700 °C |
| Initial mold temperature, $T_{\rm M}$ | 1500 °C | 1550 °C | 700 °C |
| Heating zone temperature, T _h | 1600 °C | 1600 °C | 950 °C |
| Cooling zone temperature, $T_{\rm C}$ | 45 °C | 45 °C | 25 °C |
| Bottom cooler temperature, T_{BC} | 45 °C | 45 °C | 25 °C |
| Withdrawal velocity, V_0 | 0.15 mm/sec | 0.15 mm/sec | 0.15 mm/sec |

Configurations of Directionally Solidifying Blade-like Alloy Casting under a Harmonic EM-Field at Different Withdrawal Positions —At Each Position, an Ansys EM-FEM Analysis Made for EM-Field Interpolations for the Continuous EM-Solidification Process

Free Surface Tension:

Determining the free surface morphology of alloy melt corporately with gravity/ Lorentz force and the dynamic pressure resulted from the melt flow.

(in a continuously changing state)

The Force Balance on a Free Surface of Alloy Melt:

表面张力 + 熔体的静、动压力 + 电磁力(Lorentz力) = 0

Two types of Cold Crucible Processes

Fully numerical description for a 3-D free surface morphology of alloy melt in a dynamically changing state is a stiff task for the modelers in materials metallurgy and solidification fields.

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" Liquid Metal Flow with Heat Transfer in a Cold Crucible Confined by a Free Surface and a Solidification Front",

by T. TANAKA et al, ISIJ International, 1991, v.31, pp.1416-1423.

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