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Solidification is one of the oldest processes for producing complex shapes for applications ranging from art to industry, and remains as one of the most important commercial processes for many materials. Since the 1980s, numerous fundamental developments in the understanding of solidification processes and microstructure formation have come from both analytical theories and the application of computational techniques using commonly available powerful computers. This book integrates these new developments in a comprehensive volume that also presents and places them in the context of more classical theories.

The three-part text is aimed at graduate and professional engineers. The first part, Fundamentals and Macroscale Phenomena, presents the thermodynamics of solutions and then builds on that subject to motivate and describe equilibrium phase diagrams. Transport phenomena are discussed next, focusing on the issues of most importance to liquid-solid phase transformations, then moving on to describing in detail both analytical and numerical approaches to solving such problems. The second part, Microstructure, employs these fundamental concepts for the treatment of nucleation, dendritic growth, microsegregation, eutectic and peritectic solidification, and microstructure competition. This part concludes with a chapter describing the coupling of macro- and microscopic phenomena in microstructure development. The third and final part describes various types of Defects that may occur, with emphasis on porosity, hot tearing and macrosegregation, presented using the modeling tools and microstructure descriptions developed earlier.

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#### **PREFACE**

The modern science of solidification began in the 1940's, when engineers began to use analytical methods and models to describe solidification processes. In 1940, Chvorinov applied the analysis of heat flow to predict solidification patterns and defect in sand castings. In the 1950's Chalmers and co-workers analyzed the heat and solute balance at the moving solid-liquid interface to understand why planar interfaces become unstable during unidirectional growth. This body of work culminated in a seminal text, *Principles of Solidification*, written by Chalmers in 1964.

In the 1960's, Mullins and Sekerka put Chalmers' analysis on a firmer mathematical footing by performing a formal stability analysis. Later in the 1960's and in the 1970's, Flemings and co-workers developed models for segregation and other microstructural features by applying heat and solute balances at the scale of the microstructural features themselves. Flemings followed Chalmers' text with *Solidification Processing* in 1974, presenting this next generation of achievements.

The next decade saw a great deal of activity in the study of microstructure as a pattern selection problem through the competition between the transport of heat and solute and inherent length scales in the material owing to surface energy. This body of work was summarized in 1984 in Fundamentals of Solidification, by Kurz and Fisher.

Kurz and Fisher's book appeared just at the beginning of a revolution in modeling of solidification, when low-cost powerful computers became available. Computational approaches allowed more accurate and detailed models to be constructed, shedding light on many important phenomena. Today, industrial users regularly model the solidification of geometrically complex parts ranging from directionally solidified turbine blades to automotive engines. At the microscopic scale, computational models have been used to great effect to understand the pattern selection process in ways that were only hinted at using the analytical techniques available earlier. In the 1990's, methods were developed to combine these microscopic and macroscopic views of solidification processes.

Although there have been a few specialty texts written in the intervening time between Kurz and Fisher's book and the present, none of them provides a comprehensive presentation of the fundamentals, analytical models, and computational approaches. Also in the 1990's and 2000's, a short course on solidification was developed in collaboration with

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Ecole des Mines de Nancy, EPFL and Calcom, that incorporated both the fundamental aspects described earlier and the developing computational techniques. Through teaching this course, and at our respective universities, we felt that there was a need for a new text, which led us to write the book you now hold in your hands. The subject is presented in three parts: Fundamentals, which provides the basics of thermodynamics, phase diagrams, and modeling techniques. Microstructure then uses these techniques to describe the evolution of the solid at the microscopic scale, from nucleation to dendrites, eutectics and peritectics to microsegregation. This section concludes with a chapter on coupling macro- and micro-models of solidification. The final part, Defects, uses the same principles to describe porosity, hot tearing and macrosegregation. We have striven to present this wide range of topics in a comprehensive way, and in particular to use consistent notation throughout.

### Acknowledgment

This work represents the culmination of our education, training and practice over the last 25 years. We have had many mentors, colleagues and friends who have helped us along the way, too numerous to name them all. We would particularly like to express our gratitude to our mentors. Wilfried Kurz, Stephen Davis and Robert Pond, Sr. In addition to the authors mentioned above, we would like to acknowledge the very fruitful discussions we have had over the years with many esteemed colleagues: William Boettinger, Martin Glicksman, John Hunt, Alain Karma and Rohit Trivedi, to name just a few. Much of the structure of this text derived from the short course described above, and we would like to thank our colleagues and fellow teachers in that course, past and present, in particular Philippe Thévoz and Marco Gremaud who organize the course. Special thanks are due to Christoph Beckermann, Hervé Combeau, Arne Dahle and Mathis Plapp for their helpful comments and contributions to the manuscript, and to Sébastien Rappaz for the design of the cover. We also owe a special debt of gratitude to our students, postdocs and coworkers, whose contributions made this book possible. We would also like to thank our many colleagues and friends who graciously allowed us to use figures and movie sequences that appear throughout the book.

Most importantly, we would like to thank our families for their love and support.

Jonathan A. Dantzig Michel Rappaz Lausanne, 2009

# NOMENCLATURE AND DIMENSIONLESS GROUPS

#### Principal Nomenclature

A book that covers as many topics as this one does is bound to encounter some problems with nomenclature. We have tried to use standard notation wherever possible, and to be consistent in usage throughout. In order to help distinguish between dimensional quantities and their dimensionless counterparts after scaling, we use Roman alphabet symbols for dimensional variables and corresponding Greek letters for the dimensionless ones. For example, the dimensional coordinates  $(x,y,z) \to (\xi,\eta,\zeta)$ . For some variables, such as velocity  $v,v_i$ , this scheme is not possible because there is no Greek counterpart. Further, we need symbols for both the vector and its components. We handle this by using italic symbols for dimensional quantities and Roman symbols for the dimensionless ones, e.g.,  $(v,v_i) \to (v,v_i)$ .

Subscripts and superscripts can be complicated as well. We use upper case Roman letters to designate components, lower case Greek to represent phases, s or  $\ell$  to designate solid and liquid, respectively, and a superscript '\*' to designate quantities evaluated at the solid-liquid interface. Whereas the '\*' will always appear as a superscript, the other indices may appear as subscripts or superscripts, depending on what form provides the clearest description in the current context. As an example, the most complicated symbol used in the text is  $C_{J\ell}^{*\alpha}$ , which means the mass fraction of component J in the liquid, evaluated at the solid-liquid interface ahead of phase  $\alpha$ . This symbol appears in the discussion of the solidification of eutectic and peritectic alloys. The most important symbols are given below.

#### Roman alphabet

| $A, B, \dots$       | species (component) A                                 |
|---------------------|---|
| $A, A_{s\ell}$      | area, solid-liquid interfacial area                   |
| $A_{f\ell}, A_{fs}$ | surface area between foreign substrate and liquid, or |
|                     | foreign substrate and solid                           |
| $A_C, A_R$          | growth constants for eutectics                        |
| $A(\boldsymbol{n})$ | surface energy anisotropy function                    |

| $a_1, a_2, a_3, \dots$                               | surface energy anisotropy coefficients  |
|--|---|
| $a_{Alpha}$  | chemical activity of species $A$ in phase $\alpha$  |
| B  | ratio of solutal and thermal expansion coefficients   |
| SKS 7W   | $(=eta_C/(m_\elleta_T))$  |
| $[oldsymbol{B}^e]$                                   | spatial derivatives of element shape functions  |
| $\boldsymbol{b}$                                     | vector of body force per unit mass; design vector   |
| $[oldsymbol{C}^e], [oldsymbol{C}]$                   | element and global capacitance matrices in FEM  |
|  | mass fraction of solute in a binary alloy   |
| $C_J$  | mass fraction of species $J$ in a mixture   |
| $C_s^*, C_\ell^*$                                    | mass fractions of solute in the solid and liquid phases of a                                      |
|  | binary alloy at the solid-liquid interface  |
| $c_0, c_1, \dots$                                    | constants of integration  |
| $c_p, c_V$   | specific heat at constant pressure; at constant volume  |
| D  | chemical diffusivity of solute; diameter  |
| d  | diameter of a sphere  |
| D  | $\textbf{rate-of-deformation tensor} \ (= (\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T)/2)$ |
| $d_0, d_0^C$   | thermal capillary length; chemical capillary length   |
| E  | Young's modulus   |
| $E, E^m, e$ $\dot{E}$                                | total, molar and specific internal energy   |
| $\dot{E}$  | cumulative average deformation rate   |
| $oldsymbol{\mathcal{E}},\mathcal{E}_{ijkl}$          | elasticity tensor, indecial form  |
| $oldsymbol{\mathcal{E}}, \mathcal{E}_{ijkl} \ e^I_J$ | second-order interaction coefficient between solute   |
|  | element I and gas element J   |
| $\mathfrak{F}, F$                                    | total and volumetric free energy in phase-field model   |
| $oldsymbol{F}$                                       | deformation gradient tensor, $F_{ij} = \partial x_i / \partial X_j$                               |
| $f_A,f_V$  | geometric factors for nucleation in a conical pit   |
| $f_{J\ell}, f^0_{J\ell}$                             | activity coefficient for species J in an alloy and in a pure                                      |
|  | material  |
| $f_{lpha}$   | mass fraction of phase $\alpha$   |
| G  | temperature gradient  |
| $G,G^m,g$  | total, molar and specific Gibbs free energy   |
| $G_C$  | composition gradient  |
| g  | acceleration due to gravity, $9.82~\mathrm{m~s^{-2}}$   |
| $g_{lpha}$   | volume fraction of phase $\alpha$   |
| $g_d, g_e, g_g$                                      | volume fraction of interdendritic liquid, extradendritic  |
|  | liquid and grain  |
| $g_s$  | volume fraction of solid  |
| $g_{se}$   | extended volume fraction of the solid phase   |
| $g_{si}$   | internal volume fraction of the solid phase in a grain  |
| $H, H^m, h$  | total, molar and specific enthalpy  |
| $h_T$  | heat transfer coefficient   |
| I  | unit tensor (identity tensor); the $ij$ component is $\delta_{ij}$                                |
| $I^{homo}, I^{heter}$                                | homogeneous or heterogeneous nucleation rate  |
| $I_0^{homo}, I_0^{heter}$                            | prefactors for homogeneous or heterogeneous nucleation  |
|  | rate  |
| $Iv_{2D}$ , $Iv_{3D}$                                | Ivantsov function in 2-D or 3-D   |
| i  | $\sqrt{-1}$   |
| $\boldsymbol{j}_A$                                   | mass fraction flux for species A  |
| J  | $\operatorname{Jacobian}\left(\det F ight)$   |
| [J]  | element Jacobian for isoparametric FEM  |
|  |   |

permeability tensor; value of isotropic permeability K, Kelement and global conductance matrices in FEM  $[K^e], [K]$ thermal conductivity tensor; value of isotropic conductivity k, kthermal conductivity ratio (=  $k_s/k_\ell$ )  $k_T$ partition coefficient (mass); partition coefficient (molar)  $k_0, k_0^m$ Boltzmann's constant,  $1.38 \times 10^{-23} \text{ J K}^{-1}$  $k_B$ characteristic length  $L, L_c$  $L_f$ latent heat of fusion per unit mass  $L_v$ latent heat of vaporization per unit mass mass of a system; morphological number M $M_{I}$ molecular weight of species J slopes of the liquidus and solidus curve (mass fractions)  $m_\ell, m_s$  $[N^e]$ element shape functions in FEM Avagadro's number,  $6.02 \times 10^{23}$  atoms mol<sup>-1</sup>  $N_0$ number of components  $N_C$  $N_F$ number of degrees of freedom for phase equilibria total number of atoms of species I in a mixture  $N_I$  $N_b$ bond coordination number number of grid points in a computational domain  $N_a$ No number of phases number of moles  $\boldsymbol{n}, (n_x, n_y, n_z)$ unit vector normal to a surface and its Cartesian components density of grains  $n, n_a$ maximum density of particles available  $n_{max}$ density of potent nucleant particles; density of pores  $n_p$  $O(\cdot)$ order of magnitude Ppower input to a system; penalty parameter  $P(r; R_{tip})$ surface of a paraboloid of revolution (dimensional)  $\mathcal{P}(\varrho)$ surface of a paraboloid of revolution (dimensionless) pressure, atmospheric pressure  $p, p_a$ probability of capture  $p_c$ orientation distribution function  $p(\phi)$  $\tilde{p}, p'$ intermediate pressure and pressure correction in SIMPLE algorithm  $\hat{p}$ modified pressure (=  $p + \rho_0 qh$ ) Qheat input to a system boundary heat flux  $q_b$ heat flux vector  $\boldsymbol{q}$ radius R $R_q; R_{q0}$ radius of grain; final grain radius  $R_1, R_2$ principal radii of curvature gas constant, 8.31 J mol<sup>-1</sup> K<sup>-1</sup> R R dimensionless radius for a spherical solid particle  $\dot{R}_a$ specific heat generation rate  $R_c$ radius of a critical nucleus  $R_p$ pore radius tip radius of a paraboloid  $R_{tip}$ 

residual vector

cylindrical coordinates

 $\{R\}$ 

 $r, \theta, z$ 

 $\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}$ 

 $r, \theta, \phi$   $r_J^I$ spherical coordinates second-order interaction coefficient between solute element I and gas element J bounding surface  $S, S^m, s$ total, molar and specific entropy molar entropy of mixing Sv. Sv solid-liquid interfacial area per unit volume  $S_{V}^{de}$ interfacial area per unit volume for inter-extradendritic liquid  $S_V^{sd}$ interfacial area per unit volume for solid-interdendritic liquid Ttemperature  $\dot{T}$ cooling rate boundary temperature; temperature where  $G_s^m = G_\ell^m$  $T_0$  $T^*$ solid-liquid interface temperature  $T_b$ boundary temperature  $T_{col}$ temperature of a columnar front  $T_{eut}$ eutectic temperature  $T_f$ equilibrium melting temperature of pure material  $T_{lia}$ liquidus temperature  $T_{per}$ peritectic temperature  $T_{ref}, T_0$ reference temperature solidus temperature  $T_{sol}$  $T_v$ vaporization temperature at atmospheric pressure  $\{T^e\}, \{T\}$ local and global vector of nodal temperatures  $t, t_c$ time, characteristic time  $t_f$ local solidification time  $t_n$ time of nucleation surface traction vector displacement vector  $V, V^m, v$ total, molar and specific volume  $V_R$ volume of representative volume element  $V_s, V_\ell$ volume of solid and liquid phases in representative volume element scalar velocity vvelocity normal to the surface of a grain  $v_g$  $\boldsymbol{v}, v_i$ (dimensional) velocity vector and its  $i^{th}$  component (dimensionless) velocity vector and its  $i^{th}$  component  $\mathbf{v}, \mathbf{v}_i$  $\mathbf{v}_K$ velocity vector for species K $v_n$ normal component of velocity of the solid-liquid interface speed of sound  $v_{sound}$ isotherm velocity  $v_T$ Wwidth; total work done by external forces  $W_0$ phase-field interface width  $X_I$ molar composition of species I  $\boldsymbol{X}$ material coordinate vector  $\{X\}, \{Y\}, \{Z\}$ element vectors of nodal coordinates in FEM xposition vector  $x^*$ interface position in 1-D problems Cartesian coordinates; also  $x_1, x_2, x_3$ x, y, z

unit vectors in Cartesian coordinates

#### Greek alphabet

| Greek alphabet  |  |
|---|--|
| $\alpha$  | thermal diffusivity (= $k/(\rho c_p)$ )                                  |
| $\alpha, \beta, \gamma$   | generic phases   |
| $\alpha_T$  | linear thermal expansion coefficient (= $\beta_T/3$ )                    |
| $\beta$   | Solidification shrinkage (= $\rho_s/\rho_\ell - 1$ )                     |
| $\beta_T$   | volumetric thermal expansion coefficient (= $3\alpha_T$ )                |
| $\beta_C$   | volumetric solutal expansion coefficient                                 |
|   | coefficient of compressibility   |
| $eta_p$   | Gibbs-Thomson coefficient (= $\gamma_{s\ell}T_f/(\rho_sL_f)$ )           |
| $\Gamma_{s\ell}$ $\Gamma_{s,\ell}^{m*}, \mathbf{\Gamma}_{s,\ell}^{\sigma*}, \Gamma_{s,\ell}^{h*}, \Gamma_{s,\ell}^{C*}$ |  |
| $1_{s,\ell}$ , $1_{s,\ell}$ , $1_{s,\ell}$ , $1_{s,\ell}$   | interfacial mass, momentum, energy or species term for                   |
|   | solid or liquid  |
| $\gamma_{f\ell}$  | surface energy between foreign substrate and liquid                      |
| $\gamma_{fs}$   | surface energy between foreign substrate and solid                       |
| $\gamma_{gb}$   | grain boundary energy  |
| $\gamma_{s\ell}, \gamma_{s\ell}^0$  | surface energy between solid and liquid; value of isotropic              |
|   | surface energy   |
| $\Delta$  | dimensionless undercooling $c_p \Delta T/L_f$ (Stefan number)            |
| $\Delta C_0$  | difference in compositions across eutectic plateau                       |
| $\Delta G_n^{homo}, \Delta G_n^{hetero}$  | free energy barrier for homogeneous or heterogeneous                     |
|   | nucleation   |
| $\Delta H_{mix}^m$  | molar enthalpy of mixing   |
| $egin{array}{l} \Delta S_f^m \ \Delta s_f^J \end{array}$  | molar entropy difference between solid and liquid                        |
| $\Delta s_f^J$  | specific entropy of fusion of species $J (= L_f^J/T_f^J)$                |
| $\Delta ec{T}$  | total undercooling   |
| $\Delta T_b$  | undercooling for bridging or coalescence                                 |
| $\Delta T_c$  | characteristic temperature difference                                    |
| $\Delta T_0$  | Equilibrium freezing range (= $T_{liq} - T_{sol}$ )                      |
| $\Delta T_k$  | kinetic undercooling   |
| $\Delta T_n$  | nucleation undercooling  |
| $\Delta T_R$  | curvature undercooling   |
| $\Delta T_C$  | solutal undercooling   |
| $\Delta T_T$  | thermal undercooling   |
| $\Delta x, \Delta y, \Delta z$  | grid spacing in various coordinate directions                            |
| δ   | dimensionless solidified layer thickness; boundary layer                 |
|   | thickness  |
| $arepsilon_{JK}$  | bond energy between atoms of $J$ and $K$                                 |
| ε   | strain tensor  |
| $arepsilon_{eq}$  | equivalent strain  |
| $\varepsilon_4, \varepsilon_n$  | 4-fold, n-fold coefficient for the planar anisotropy of $\gamma_{s\ell}$ |
| $\eta$  | dimensionless $y$ -coordinate; paraboloidal coordinate                   |
| ζ   | dimensionless $z$ —coordinate; fractional time step                      |
| $\dot{\theta}$  | dimensionless temperature; angular coordinate;                           |
|   | wetting angle  |
| $ar{\kappa},\!\kappa_G$   | mean and Gaussian curvature of a surface                                 |
| Λ   | ratio of eutectic spacing to extremum value (= $\lambda/\lambda_{ext}$ ) |
| λ   | wavelength of instability; eutectic spacing                              |
| $\lambda_1, \lambda_2$  | primary, secondary dendrite arm spacing                                  |
| $\mu_{\ell}$  | shear viscosity of a Newtonian fluid                                     |
| $\mu_{Jlpha}$   | chemical potential of species $J$ in phase $\alpha$                      |
| $\mu J \alpha$  | enemical potential of species 3 in phase a                               |

| $\mu_k$            | kinetic attachment coefficient                         |
|--------------------|--|
| $ u_{\ell}$        | kinematic viscosity (= $\mu_\ell/\rho_\ell$ )          |
| $ u_0$             | atomic vibration frequency                             |
| $ u_e$             | Poisson's ratio  |
| ξ                  | dimensionless $x$ -coordinate; parabolic coordinate    |
| ξ                  | Cahn-Hoffmann vector (= $\nabla(r\gamma_{s\ell}(n))$ ) |
| $\pi$              | 3.14159  |
| П                  | dimensionless scaled pressure                          |
| $\rho$             | density  |
| $ ho_0$            | density at reference temperature and pressure          |
| $\varrho$          | dimensionless radial coordinate                        |
| $\sigma$           | total stress tensor                                    |
| $\hat{m{\sigma}}$  | effective stress tensor (= $\sigma + pI$ )             |
| $\sigma_{eq}$      | equivalent stress                                      |
| $\sigma^*$         | dendrite tip selection constant                        |
| $\sigma_n$         | instability growth rate exponent for mode $n$          |
| $\sigma_y$         | yield stress   |
| au                 | extra stress tensor                                    |
| au                 | dimensionless time                                     |
| $	au_0$            | time scale factor in phase-field model                 |
| Υ                  | noise in phase-field equation                          |
| $\phi$             | constant used to describe interface position           |
| $\phi_s,\phi_\ell$ | existence function for solid, liquid phase             |
| $\chi_{\alpha}$    | mole fraction of phase $\alpha$                        |
| $\psi$             | phase-field order parameter                            |
| $\Psi$             | surface stiffness                                      |
| $\Omega^m$         | regular solution parameter                             |
| $\Omega$           | supersaturation  |
| $\omega$           | vorticity vector (= $\nabla \times v$ )                |
|                    | 5  |

### Subscripts, superscripts and indices

 $A^*$ 

|             | evaluated on the sond figure finterface         |
|-------------|---|
| $A_C$       | composition                                     |
| $A_c$       | characteristic value                            |
| $A_{col}$   | columnar zone                                   |
| $A^{el}$    | elastic deformation                             |
| $A_{eut}$   | eutectic  |
| $A_\ell$    | liquid phase                                    |
| $A_g$       | gas phase                                       |
| $A_k$       | attachment kinetics                             |
| $A_I,A_J$   | species I, species J                            |
| $A_{liq}$   | liquidus  |
| $A^m$       | amount per mole                                 |
| $A_n$       | component of vector $A$ normal to the interface |
| $A_p$       | pores   |
| $A^R$       | surface with radius of curvature $R$            |
| $A_s$       | solid phase                                     |
| $A_{sol}$   | solidus   |
| $A_{s\ell}$ | solid-liquid interface                          |
|             |   |

evaluated on the solid-liquid interface

| $A^{th}$                       | thermal deformation                    |
|--------------------------------|--|
| $A^{tr}$                       | transformational deformation           |
| $A^{vp}$                       | viscoplastic deformation               |
| $A_{\alpha}, A_{\beta}, \dots$ | quantity in phase $\alpha$ , $\beta$ , |
| $A_x, A_y, A_z$                | x, y, z components of a vector         |
| $A_0$                          | nominal or reference value             |
| $A^{\infty}$                   | flat surface $(R \to \infty)$          |

#### **Mathematical functions**

| Symbol                              | Meaning                        | Representation  |
|-------------------------------------|--------------------------------|---|
| $\mathrm{E}_1(u)$                   | exponential integral           | $\int\limits_{u}^{\infty}\frac{e^{-s}}{s}ds$  |
| $\operatorname{erf}\left(u\right)$  | error function                 | $\frac{2}{\sqrt{\pi}} \int_{0}^{u} e^{-s^2} ds$   |
| $\operatorname{erfc}\left(u\right)$ | complementary error function   | $1 - \operatorname{erf}(u)$   |
| $f(\theta)$                         | nucleation geometric factor    | $\frac{(2+\cos\theta)(1-\cos\theta)^2}{4}$  |
| $\mathcal{L}_n(x)$                  | Laguerre polynomial            | $\frac{e^x}{n!} \frac{d^n}{dx^n} \left( e^{-x} x^n \right)$   |
| $P_{nm}(x)$                         | associated Legendre polynomial | $\frac{(-1)^m}{2^n n!} (1 - x^2)^{m/2} \frac{d^{n+m}}{dx^{n+m}} (x^2 - 1)^n$  |
| $Q_4$                               | first cubic harmonic function  | $n_x^4 + n_y^4 + n_z^4$   |
| $S_4$                               | second cubic harmonic function | $n_x^2 n_y^2 n_z^2$   |
| $Y_{nm}(\theta,\phi)$               | spherical harmonic function    | $\sqrt{\frac{(2n+1)(n-m)!}{4\pi(n+m)!}}e^{-im\phi}P_{nm}(\cos\theta)$   |
| $\delta(x)$                         | Dirac $\delta$ -function       | $\delta(x) = \begin{cases} +\infty & x = 0\\ 0 & x \neq 0 \end{cases}$  |
|                                     |                                | $\int_{-\infty}^{\infty} \delta(x)dx = 1$   |
| $\delta_{ij}$                       | unit tensor (Kronecker delta)  | $\delta_{ij} = \left\{ \begin{array}{ll} 1 & i = j \\ 0 & i \neq j \end{array} \right.$   |
| $arepsilon_{ijk}$                   | permutation tensor             | $ \begin{cases} 1 & i, j, k \text{ even permutations} \\ -1 & i, j, k \text{ odd permutations} \\ 0 & \text{otherwise}  \end{cases} $ |

### **Mathematical operators**

| Symbol           | Meaning                               | Representation |
|------------------|---------------------------------------|----------------|
| $m{A}\cdot m{B}$ | dot product of two vectors            | $a_ib_i$       |
| $oldsymbol{A}^T$ | transpose of a second rank tensor     | $a_{ji}$       |
| A:B              | scalar product of second rank tensors | $a_{ij}b_{ji}$ |

| $D\psi/Dt$  | material derivative of $\psi$            | $\frac{\partial \psi}{\partial t} + (\boldsymbol{v} \cdot  abla) \psi$  |
|---|--|---|
| ${ m tr} {m A}$   | trace of a second rank tensor            | $a_{ii}$  |
| $\nabla A$  | gradient of a scalar                     | $\frac{\partial A}{\partial x_i}$   |
| $ abla \cdot oldsymbol{A}$                                    | divergence of $A$                        | $rac{\partial a_i}{\partial x_i}$  |
| $ abla	imes oldsymbol{A}$                                     | curl of a vector                         | $\varepsilon_{ijk} \frac{\partial a_j}{\partial x_k}$   |
| $\nabla^2 A$  | Laplacian of $A$                         | $rac{\partial^2 A}{\partial x_i \partial x_i}$   |
| $\ oldsymbol{A}\ $  | $L_2$ norm of a vector                   | $\sqrt{a_i a_i}$  |
| $\langle A \rangle$   | volume average of ${\cal A}$             | $\frac{1}{V_R} \int A \ dV$   |
| $\langle A_{s,\ell} \rangle$                                  | phase average of $A_s$ or $A_\ell$       | $\frac{1}{V_R} \int\limits_V^{V_R} \phi_{s,\ell} A \ dV$  |
| $\langle A \rangle_{s,\ell}$                                  | intrinsic average of $A_s$ or $A_\ell$   | $\frac{1}{V_R} \int_{V_R} A  dV$ $\frac{1}{V_R} \int_{V_R} \phi_{s,\ell} A  dV$ $\frac{1}{V_{s,\ell}} \int_{V_R} \phi_{s,\ell} A  dV$ |
| $\left\langle A_{s,\ell}^{*}\boldsymbol{n}\right\rangle ^{*}$ | interfacial average of $A_s$ or $A_\ell$ | $rac{1}{A_{s\ell}}\int\limits_{A_{s,\ell}}^{V_R}A_{s,\ell}^*m{n}dA$  |
| $\langle C \rangle_M$   | mass average composition                 | $\int_{0}^{f_s} C_s df_s + \int_{0}^{f_\ell} C_\ell df_\ell$  |

### Classical dimensionless numbers

| Name             | Expression  | Physical Meaning   |
|------------------|---|--|
| Biot             | $Bi = \frac{h_T L_c}{k}$  | ratio of heat advection from a<br>surface to heat conduction inside        |
| Boussinesq       | $Bo = \frac{g\beta_T \Delta T_c L_c^3}{\alpha_0^2}$                 | ratio of heat advected by buoyancy to conducted heat                       |
| Fourier          | $Fo = \frac{\alpha t_c}{L_c^2}$                                     | ratio of characteristic time $t_c$ to the time for conduction $L_c^2/lpha$ |
| Grashof          | $Gr = \frac{g\beta_T \Delta T_c L_c^3}{(\mu_\ell/\rho_{\ell 0})^2}$ | ratio of buoyant advective flow to viscosity                               |
| Lewis            | $Le = \frac{\alpha}{D}$   | ratio of thermal diffusion to mass diffusion                               |
| Péclet           | $Pe = \frac{v_c L_c}{\alpha}$                                       | ratio of heat advection to heat conduction                                 |
| Péclet (solutal) | $Pe_C = \frac{v_c L_c}{D}$  | ratio of solute advection to solute dif-<br>fusion                         |
| Prandtl          | $\Pr = \frac{c_p \mu_\ell}{k} = \frac{\nu_\ell}{\alpha}$            | ratio of momentum and thermal diffusivities in a fluid                     |

| Rayleigh | $Ra = \frac{\rho_0 g \beta_T \Delta T_c L_c^3}{\mu_\ell \alpha_0}$           | ratio of buoyant advection to the product of viscosity and heat conduction |
|----------|--|--|
| Reynolds | $Re = \frac{\rho v_c L_c}{\mu_\ell} = \frac{v_c L_c}{\nu_\ell}$              | ratio of inertia to viscosity  |
| Schmidt  | $Sc = \frac{\mu_{\ell}}{\rho_{\ell} D_{\ell}} = \frac{\nu_{\ell}}{D_{\ell}}$ | ratio of momentum diffusivity to mass diffusivity                          |
| Stefan   | $Ste = \frac{c_p \Delta T}{L_f}$   | ratio of sensible heat to latent heat                                      |

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