



METRO
MEtallurgical TRaining On-line



Mass transport at the solid/liquid interface of growing composite *in situ*

Waldemar Wołczyński
IMMS PAS



Education and Culture



Microstructure of the growing composite *in situ*

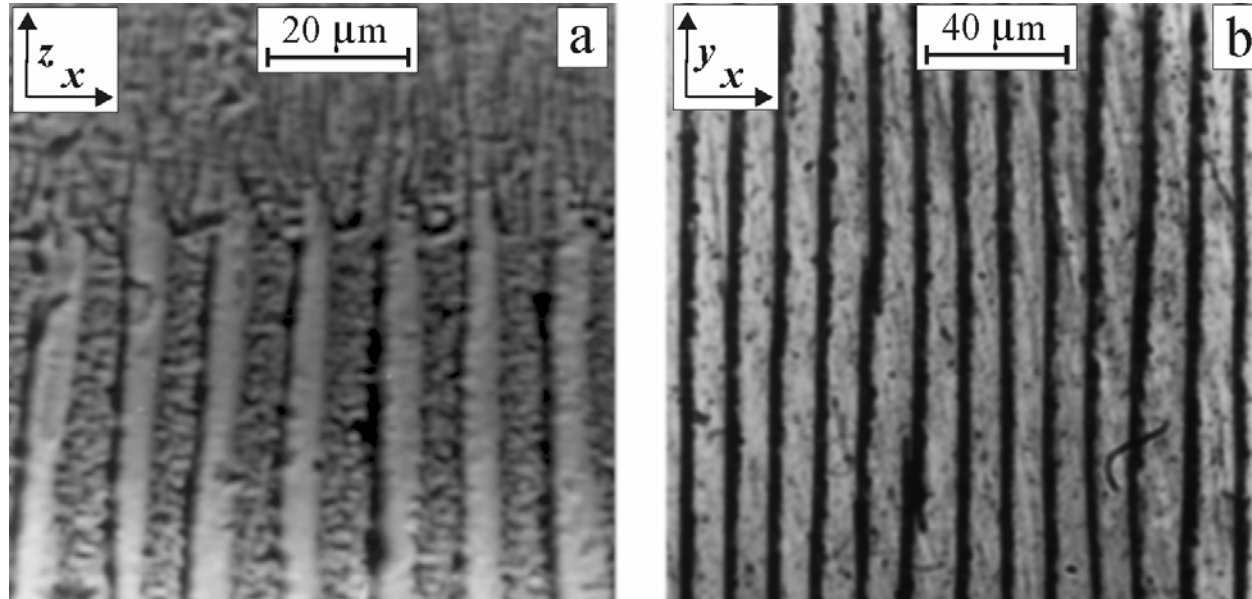


FIG. 1

Oriented growth of the (Pb) – (Cd) composite *in situ*
a/ frozen solid/liquid interface (s / l interface)
b/ typical structure of growing α / β composite *in situ*



Conditions applied to the diffusion equation by **Jackson-Hunt** theory



$$\nabla^2 C + \frac{v}{D} \frac{\partial C}{\partial z} = 0$$

$$\frac{\partial C}{\partial x} = 0$$

at

$$x = 0$$

and

$$x = S_\alpha + S_\beta$$

$$\frac{\partial C}{\partial z} = -\frac{vC_0^\alpha}{D}$$

for

$$0 \leq x < S_\alpha$$

$$\frac{\partial C}{\partial z} = +\frac{vC_0^\beta}{D}$$

for

$$S_\alpha < x \leq S_\alpha + S_\beta$$

C – solute concentration in the liquid at the solid/liquid interface
D – coefficient of diffusion in the liquid

K.A. Jackson, J.D. Hunt, Trans. AIME, **236**, 1129-1142, (1966)

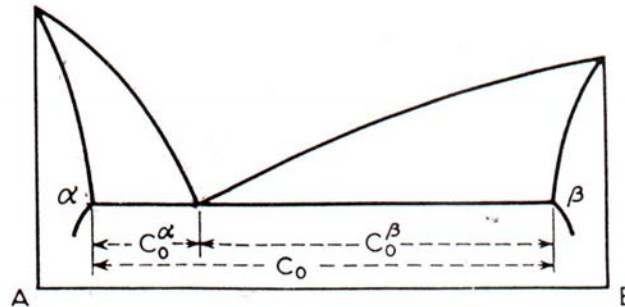
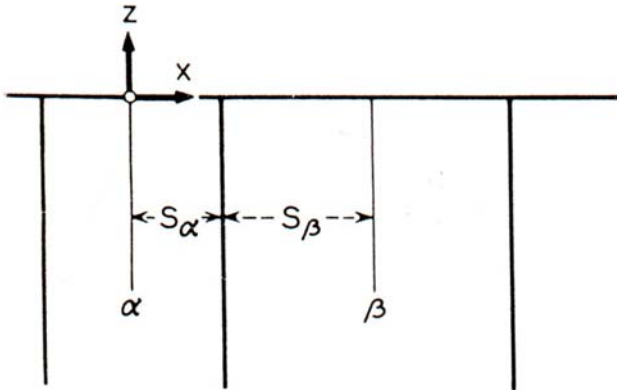


Solution to the diffusion equation by Jackson - Hunt theory



FIG. 2

$$C = C_E + C_\infty + \sum_{n=1}^{\infty} B_n \cos\left(\frac{\pi n x}{S_\alpha + S_\beta}\right) \exp\left(-\frac{\pi n z}{S_\alpha + S_\beta}\right)$$



with

$$B_0 = \frac{C_0^\alpha S_\alpha - C_0^\beta S_\beta}{S_\alpha + S_\beta}$$

Composite *in situ* growth:
 a/ J-H planar s/l interface
 b/ adequate J-H phase diagram

K.A. Jackson, J.D. Hunt,
 Trans. AIME, **236**, 1129-1142, (1966)



A solid / liquid interface behaviour according to Jackson-Hunt theory

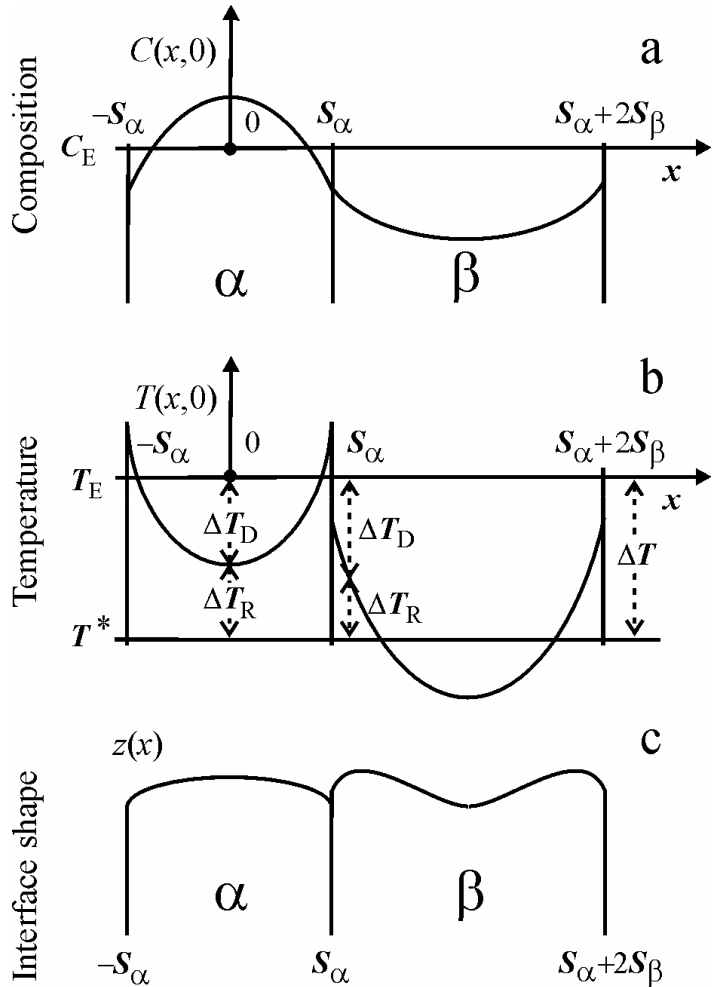


FIG.3

Imperfections of the J-H theory

- a/ no mass balance:
 $C(x,0) - C_E$ for α phase lamella is not equal to $C_E - C(x,0)$ for β phase lamella
- b/ mass balance is satisfied for $S_\alpha = S_\beta$ and $C_0^\alpha = C_0^\beta$, only, in J-H theory
- c/ undercooling greater than $\Delta T = T^* - T_E$ assumed in concept of *ideally coupled growth*
- d/ discontinuity of temperature at the α / β inter-phase boundary
- e/ non-realistic curvature of the solid / liquid interface shape

K.A. Jackson, J.D. Hunt, Trans. AIME, **236**, 1129-1142, (1966)



A solid / liquid interface behaviour according to Jackson-Hunt theory



according to the J-H scheme (FIG. 3a) some parts of α - phase should grow from the liquid of the solute concentration adequate to the formation of β - phase, rather it could lead to the changes in inter-lamellar spacing and instability of a solid/liquid interface

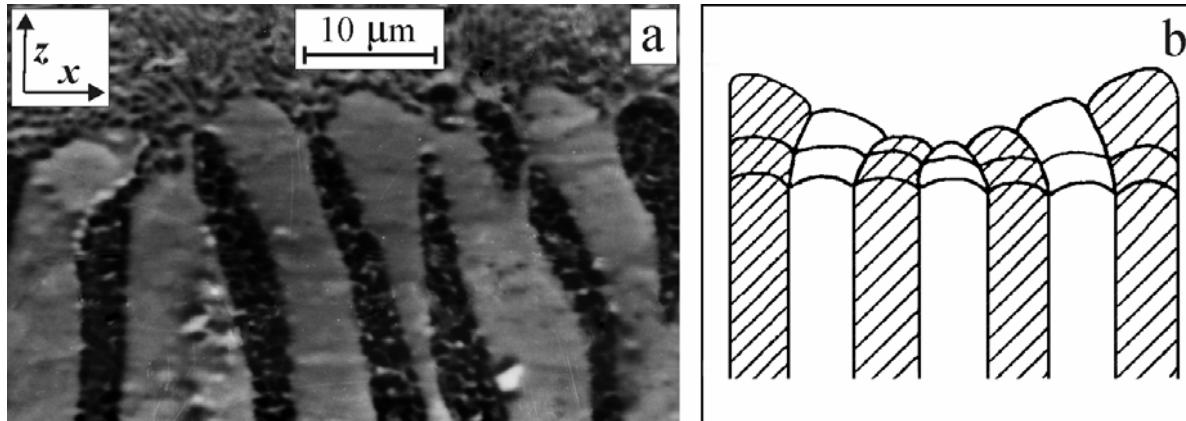


FIG. 4

instability at the solid / liquid interface

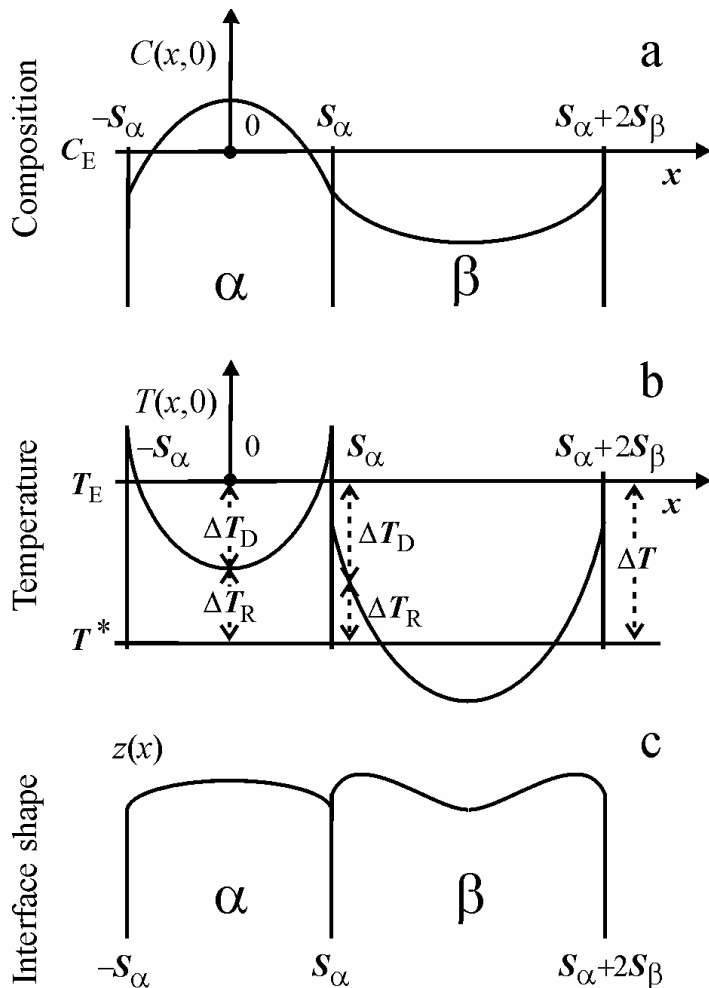
a/ observed during composite *in situ* growth

b/ concluded from the J-H theory (as above)

K.A. Jackson, J.D. Hunt, Trans. AIME, **236**, 1129-1142, (1966)



A solid / liquid interface behaviour according to Jackson-Hunt theory



according to J-H solution of diffusion equation
 concentration profile is **common** for both
 lamellae of the composite *in situ*

^assumption of non separation of concentration
 micro-field (in the J-H theory)
 together with concept of *ideally coupled growth*
 $\Delta T_\alpha^* = \Delta T_\beta^* = \Delta T$ results in discontinuity
 of undercooling at α / β inter-phase boundary
 ^moreover, some parts of the α as well as β phase
 lamellae should grow outside of the regime

FIG.5

undercooling
 ΔT_D results from changes
 of the solute concentration
 ΔT_R results from
 the s / l interface curvature



Application of Jackson-Hunt theory to the phase diagram

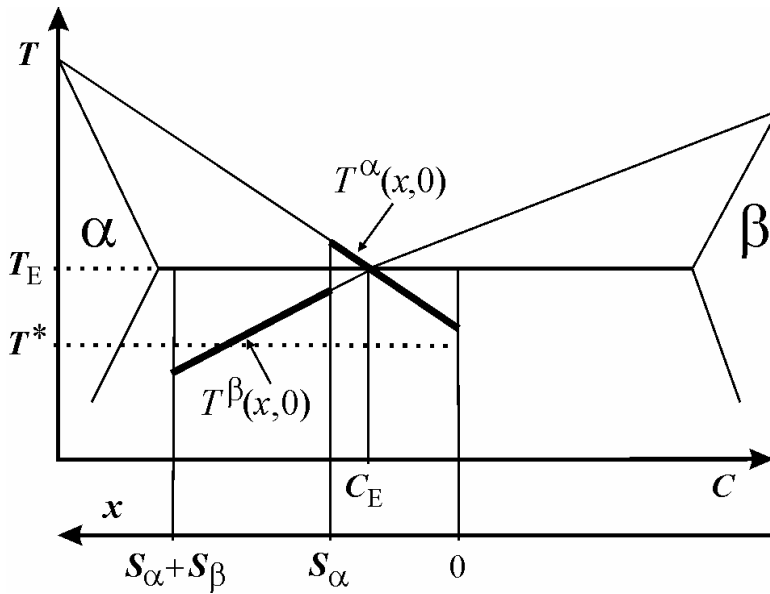


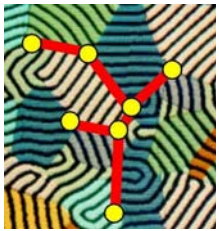
FIG.6

undercooling – phase diagram

total undercooling: $\Delta T = T^* - T_E$

- C** solute concentration
- C_E** solute concentration at eutectic point
- S_α** half the width of the α phase lamella
- S_β** half the width of the β phase lamella
- T** equilibrium temperature
- $T^\alpha(x,z)$** equilibrium temperature corresponding to changes in solute concentration at the α phase solid / liquid interface ($z = 0$)
- $T^\beta(x,z)$** equilibrium temperature corresponding to changes in solute concentration at the β phase solid / liquid interface ($z = 0$)
- T^*** real temperature of the solid/liquid interface
- T_E** temperature of eutectic transformation

K.A. Jackson, J.D. Hunt, Trans. AIME, **236**, 1129-1142, (1966)



An initial correction of Jackson-Hunt theory

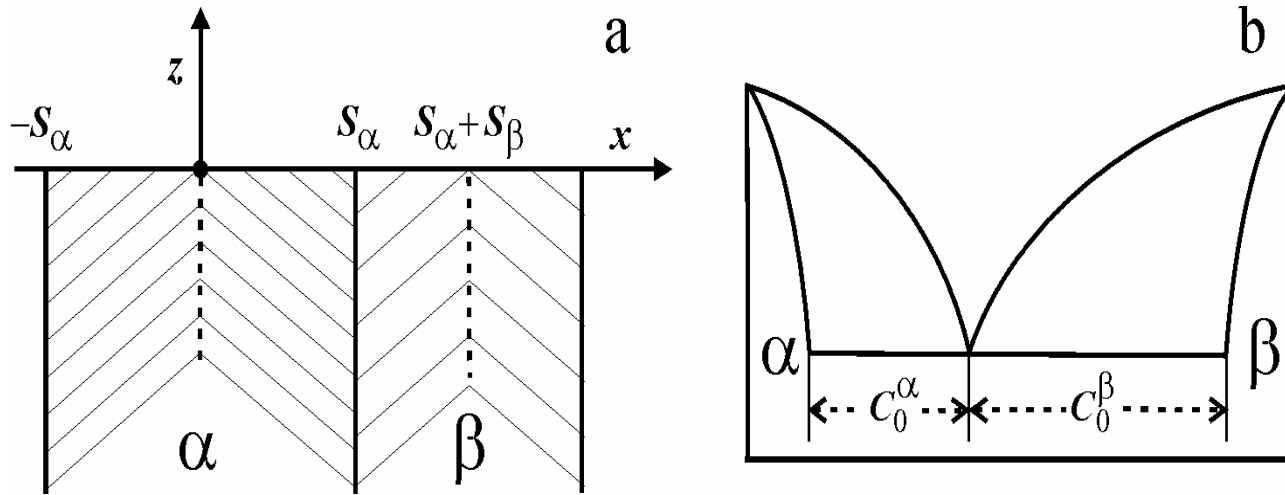


FIG. 7

now

$$C_0^\alpha S_\alpha = C_0^\beta S_\beta$$

thus

$$B_0 = \frac{C_0^\alpha S_\alpha - C_0^\beta S_\beta}{S_\alpha + S_\beta} = 0$$

a/corrected planar solid / liquid interface
b/corresponding arbitrary phase diagram

$$C = C_E + C_\infty + \sum_{n=1}^{\infty} B_n \cos\left(\frac{\pi n x}{S_\alpha + S_\beta}\right) \exp\left(-\frac{\pi n z}{S_\alpha + S_\beta}\right)$$



Initially corrected Jackson - Hunt theory

Solute concentration and undercooling

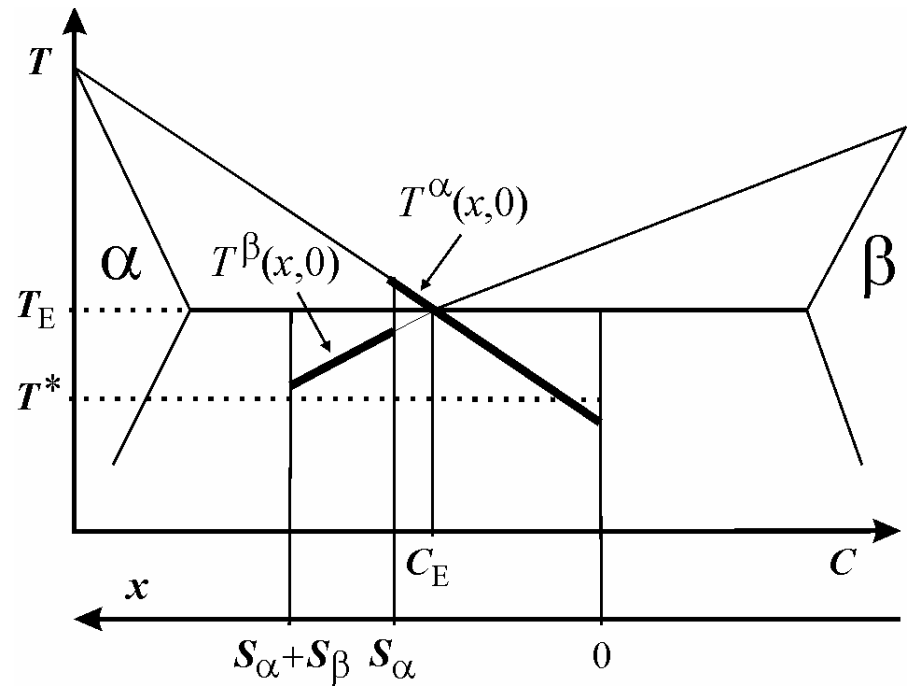
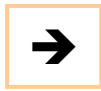
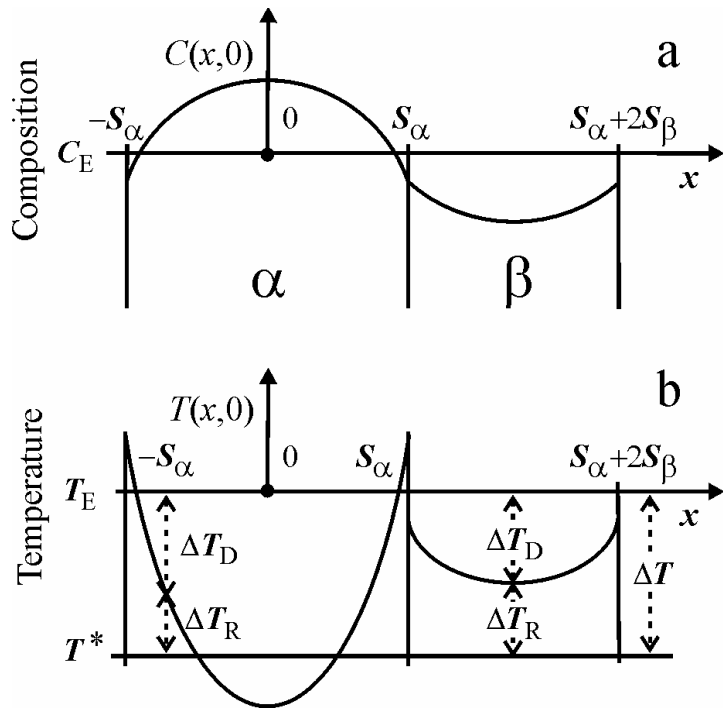


FIG. 8 solute concentration and undercooling

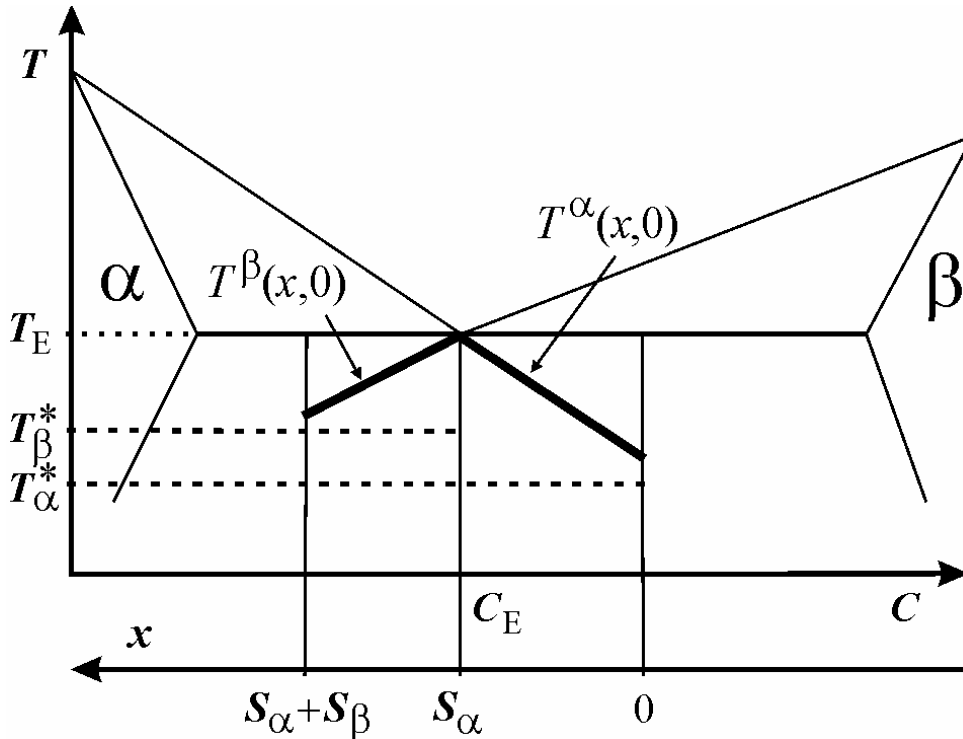
FIG. 9 undercooling – phase diagram

no significant improvement of the J-H theory ! - as it is seen in FIG. 9 (to be compared with the scheme in FIG. 6)



Fundamentals of the current analysis

Concept of the *coupled growth*



coupled growth is a new concept to improve J-H theory

$$\Delta T^*_\alpha = T^*_\alpha - T_E$$

$$\Delta T^*_\beta = T^*_\beta - T_E$$

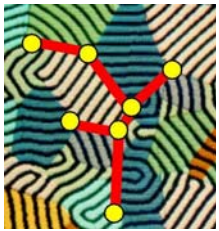
desired relation: undercooling – phase diagram

FIG. 10

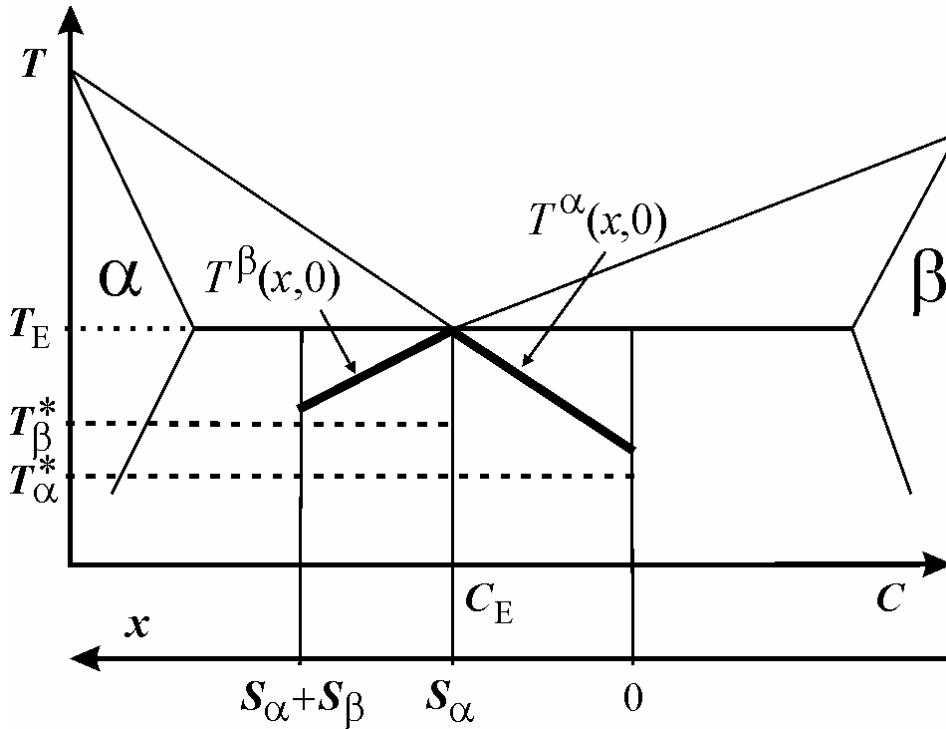
but generally



$$\Delta T^*_\alpha \neq \Delta T^*_\beta$$



Undercooling of the s/l interface due to the concept of *coupled growth*



curvature undercooling

$$\delta T_R^\alpha(x,0) = T_\alpha^* - T^\alpha(x,0)$$

$$\delta T_R^\beta(x,0) = T_\beta^* - T^\beta(x,0)$$

undercooling – phase diagram

$$\delta T^\alpha(x,0) + \delta T_R^\alpha(x,0) = \Delta T_\alpha^*$$

$$\delta T^\beta(x,0) + \delta T_D^\beta(x,0) = \Delta T_\beta^*$$

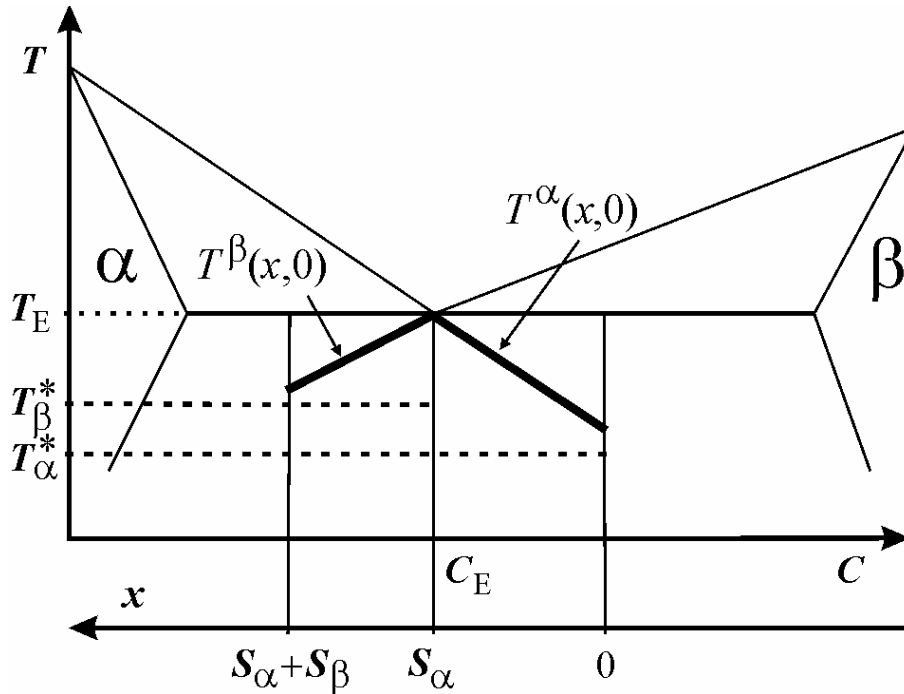
total undercooling



FIG. 11



Solute concentration due to the concept of *coupled growth*



$$\delta C^\alpha(x,0) = C^\alpha(x,0) - C_E$$

$$\delta C^\beta(x,0) = C^\beta(x,0) - C_E$$

undercooling – phase diagram

$$C_0^\alpha(S_\alpha,0) = C_S^\alpha(S_\alpha,0) - C_E < 0$$

$$C_0^\beta(S_\alpha,0) = C_S^\beta(S_\alpha,0) - C_E > 0$$

consequentially



FIG. 12



Fundamentals of the new solution due to the concept of *coupled growth*

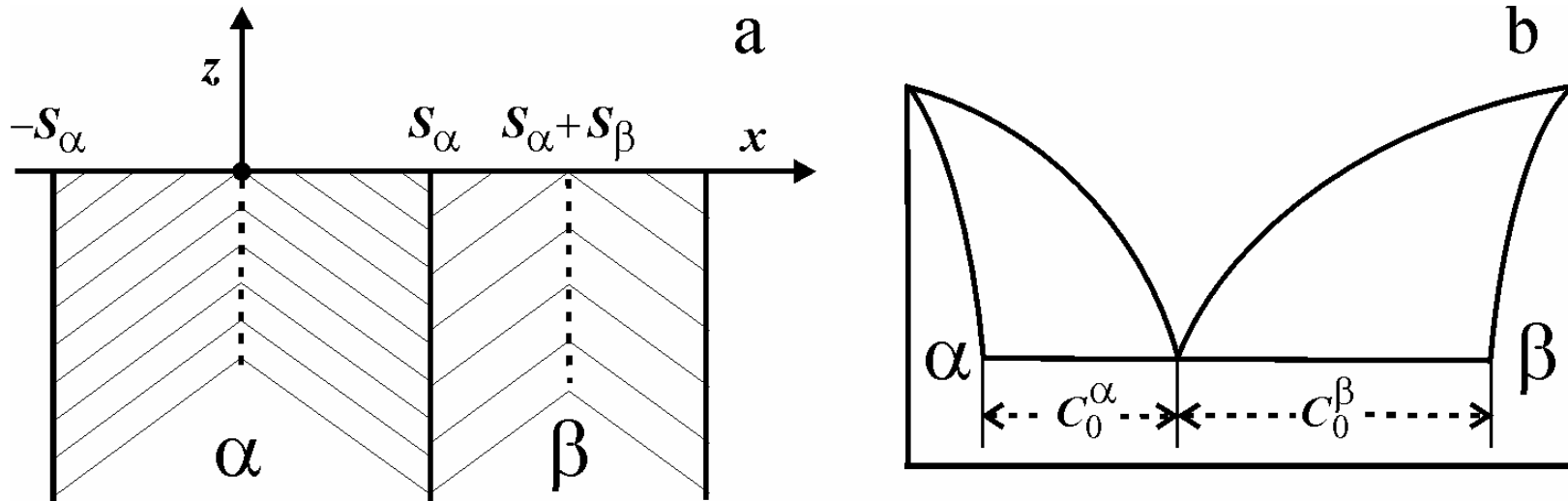
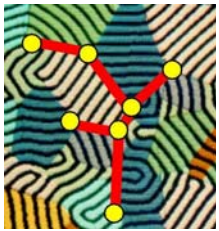


FIG. 13

a/ planar s/l interface
b/ corresponding
arbitrary phase diagram

$$C_0^\alpha(S_\alpha, 0) = C_S^\alpha(S_\alpha, 0) - C_E < 0$$

$$C_0^\beta(S_\alpha, 0) = C_S^\beta(S_\alpha, 0) - C_E > 0$$



Diffusion equation due to the concept of *coupled growth*



FIG. 14

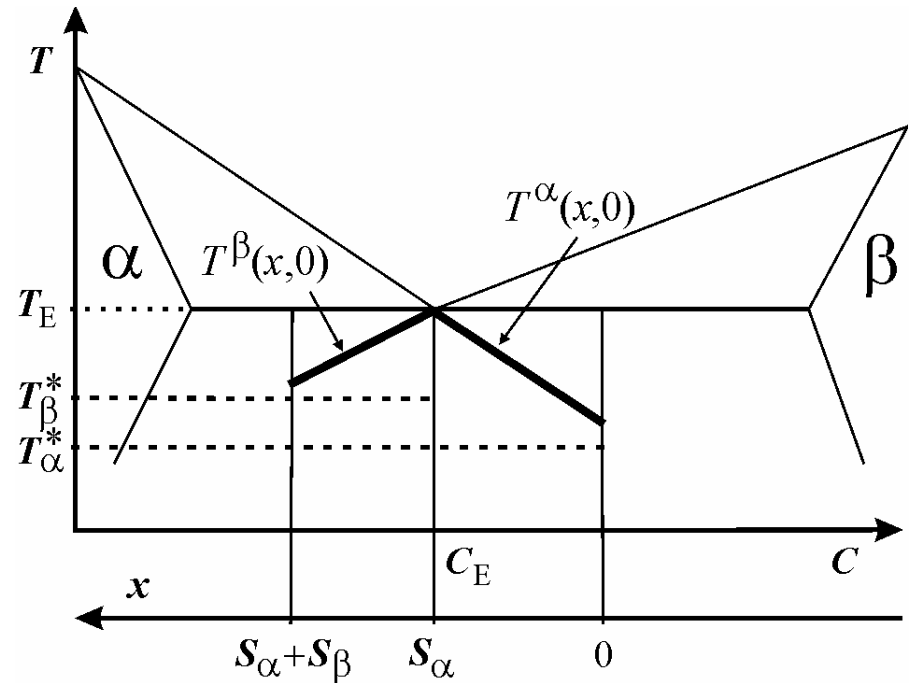
undercooling – phase diagram

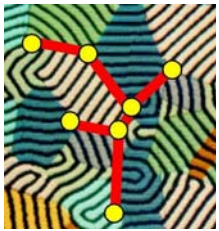
diffusion equation is:

$$\frac{\partial^2 \delta C}{\partial x^2} + \frac{\partial^2 \delta C}{\partial z^2} + \frac{v}{D} \frac{\partial \delta C}{\partial z} = 0$$

with

$$\delta C(S_\alpha, z) = C(S_\alpha, z) - C_E = 0$$





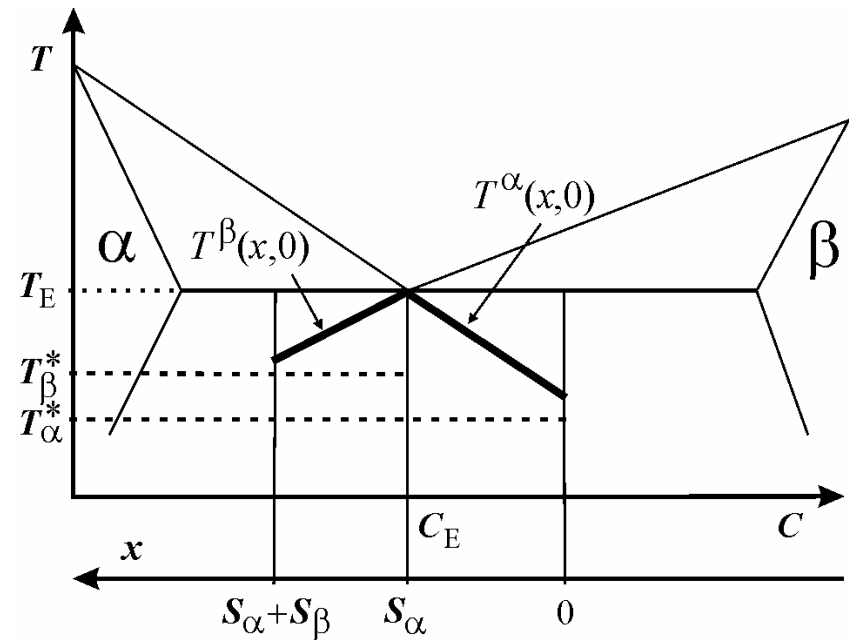
Assumptions for the new solution to diffusion equation



undercooling – phase diagram

diffusion equation is:

$$\frac{\partial^2 \delta C}{\partial x^2} + \frac{\partial^2 \delta C}{\partial z^2} + \frac{v}{D} \frac{\partial \delta C}{\partial z} = 0$$



it is required to solve the diffusion equation in such a way to:

- a/ satisfy the solid / liquid interface undercooling behaviour defined in FIG. 15*
- b/ obtain the solution separately for the α – phase lamella and β – phase lamella*

FIG. 15



General solution to the diffusion equation

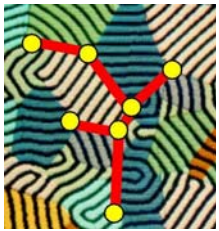


diffusion equation is:

$$\frac{\partial^2 \delta C}{\partial x^2} + \frac{\partial^2 \delta C}{\partial z^2} + \frac{v}{D} \frac{\partial \delta C}{\partial z} = 0$$

*general solution to diffusion equation formulated in accordance with the concept of **coupled growth** is as follows:*

$$\delta C(x, z) = X(x) Z(z)$$



Solution to the diffusion equation

Detailed formulations



*general solution to diffusion equation formulated in accordance with the concept of **coupled growth** is as follows:*

where

$$\delta C(x, z) = X(x) Z(z)$$

$$X(x) = A \cos(\omega x) + B \sin(\omega x)$$

$$Z(z) = \exp \left[\left(-\frac{v}{2D} - \sqrt{\frac{v^2}{4D^2} + \omega^2} \right) z \right]$$

A, B, ω - parameters are to be defined



Definition of the unknown parameters



A, B, ω - parameters are to be defined

definitions are to be given separately

a/ for the α phase lamella $x \in [0, S_\alpha]$ $z \geq 0$

the values of B and ω parameter yield from conditions a/ and b/:

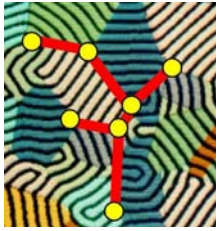
$$\text{a/ } \left. \frac{\partial \delta C(x, z)}{\partial x} \right|_{x=0} = 0 \quad \text{and} \quad \text{b/ } \delta C(S_\alpha, z) = 0$$

from a/ $-\omega A \sin(\omega \cdot 0) + \omega B \cos(\omega \cdot 0) = 0$ it yields $B = 0$

from a/ and b/ $A \cos(\omega S_\alpha) = 0$

and

$$\omega = \omega_{2n-1} = \frac{(2n-1)\pi}{2S_\alpha}, \quad n = 1, 2, \dots$$



Detailed solution to the diffusion equation



a/ for the α phase lamella $x \in [0, S_\alpha]$ $z \geq 0$

the detailed solution to diffusion equation is:

$$\delta C(x, z) = \sum_{n=1}^{\infty} A_{2n-1} \cos\left(\frac{(2n-1)\pi x}{2S_\alpha}\right) \exp\left[\left(-\frac{v}{2D} - \sqrt{\frac{v^2}{4D^2} + \left(\frac{(2n-1)\pi}{2S_\alpha}\right)^2}\right) z\right]$$

where

A_{2n-1}

are constants



Slow solidification

Solution to diffusion equation



it is evident that for slow solidification:

$$\frac{(2n-1)\pi}{2S_\alpha} \gg \frac{v}{2D}$$

a/ for the α phase lamella

$$x \in [0, S_\alpha] \quad z \geq 0$$

$$\delta C(x, z) = \sum_{n=1}^{\infty} A_{2n-1} \cos\left(\frac{(2n-1)\pi x}{2S_\alpha}\right) \exp\left[\left(-\frac{v}{2D} - \sqrt{\frac{v^2}{4D^2} + \left(\frac{(2n-1)\pi}{2S_\alpha}\right)^2}\right)z\right]$$

reduces to

$$\delta C(x, z) = \sum_{n=1}^{\infty} A_{2n-1} \cos\left(\frac{(2n-1)\pi x}{2S_\alpha}\right) \exp\left(-\frac{(2n-1)\pi}{2S_\alpha} z\right)$$



A_{2n-1} parameters



the values of A_{2n-1} parameters are calculated applying the condition:

$$\left. \frac{\partial \delta C(x, z)}{\partial z} \right|_{z=0} = f_{\alpha}(x); \quad f_{\alpha}(x) < 0, \quad x \in [0, S_{\alpha}]$$

for

a/ micro-filed of solute concentration for rapid solidification

$$\left. \frac{\partial \delta C(x, z)}{\partial z} \right|_{z=0} = \sum_{n=1}^{\infty} A_{2n-1} \left(-\frac{v}{2D} - \sqrt{\frac{v^2}{4D^2} + \left(\frac{(2n-1)\pi}{2S_{\alpha}} \right)^2} \right) \cos \left(\frac{(2n-1)\pi x}{2S_{\alpha}} \right)$$

b/ micro-filed of solute concentration for slow solidification

$$\left. \frac{\partial \delta C(x, z)}{\partial z} \right|_{z=0} = \sum_{n=1}^{\infty} A_{2n-1} \left(-\frac{(2n-1)\pi}{2S_{\alpha}} \right) \cos \left(\frac{(2n-1)\pi x}{2S_{\alpha}} \right)$$



Application of the $f(x)$ function



additionally, new function $f(x)$ is to be introduced:

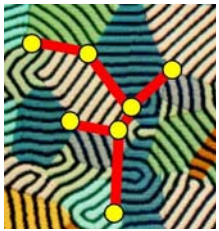
$$f(x), \quad -2S_\alpha \leq x \leq 2S_\alpha, \quad f(-x) = f(x), \quad f(x + 2S_\alpha) = -f(x)$$

the following property of the $f(x)$ is to be applied

$$f(x) \approx \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi x}{2S_\alpha}\right)$$

where

$$a_n = \frac{1}{S_\alpha} \int_0^{2S_\alpha} f(x) \cos\left(\frac{n\pi x}{2S_\alpha}\right) dx$$



$f(x)$



since:

$$f(x + 2S_\alpha) = -f(x)$$

for

$$n = 2k$$

$$k = 0, 1, 2, \dots$$

it yields:

$$\begin{aligned}
 a_{2k} &= \frac{1}{S_\alpha} \int_0^{2S_\alpha} f(x) \cos\left(\frac{2k\pi x}{2S_\alpha}\right) dx = \\
 &= \frac{1}{S_\alpha} \left(\int_0^{S_\alpha} f(x) \cos\left(\frac{2k\pi x}{2S_\alpha}\right) dx + \int_{S_\alpha}^{2S_\alpha} f(x) \cos\left(\frac{2k\pi x}{2S_\alpha}\right) dx \right) = \\
 &= \frac{1}{S_\alpha} \left(\int_0^{S_\alpha} f(x) \cos\left(\frac{2k\pi x}{2S_\alpha}\right) dx + \int_{-S_\alpha}^0 f(x + 2S_\alpha) \cos\left(\frac{2k\pi(x + 2S_\alpha)}{2S_\alpha}\right) dx \right) = \\
 &= \frac{1}{S_\alpha} \left(\int_0^{S_\alpha} f(x) \cos\left(\frac{2k\pi x}{2S_\alpha}\right) dx - \int_{-S_\alpha}^0 f(x) \cos\left(\frac{2k\pi x}{2S_\alpha}\right) dx \right) = \\
 &= \frac{1}{S_\alpha} \left(\int_0^{S_\alpha} f(x) \cos\left(\frac{2k\pi x}{2S_\alpha}\right) dx + \int_0^{-S_\alpha} f(x) \cos\left(\frac{2k\pi x}{2S_\alpha}\right) dx \right) = \\
 &= \frac{1}{S_\alpha} \left(\int_0^{S_\alpha} f(x) \cos\left(\frac{2k\pi x}{2S_\alpha}\right) dx + \int_0^{S_\alpha} f(-x) \cos\left(\frac{-2k\pi x}{2S_\alpha}\right) d(-x) \right) = \\
 &= \frac{1}{S_\alpha} \left(\int_0^{S_\alpha} f(x) \cos\left(\frac{2k\pi x}{2S_\alpha}\right) dx - \int_0^{S_\alpha} f(x) \cos\left(\frac{2k\pi x}{2S_\alpha}\right) dx \right) = 0
 \end{aligned}$$



$f(x)$



since:

$$f(x + 2S_\alpha) = -f(x) \quad \text{for}$$

$$n = 2k - 1, k = 1, 2, \dots$$

it yields:

$$\begin{aligned} a_{2k-1} &= \frac{1}{S_\alpha} \int_0^{2S_\alpha} f(x) \cos\left(\frac{(2k-1)\pi x}{2S_\alpha}\right) dx = \\ &= \frac{1}{S_\alpha} \left(\int_0^{S_\alpha} f(x) \cos\left(\frac{(2k-1)\pi x}{2S_\alpha}\right) dx + \int_{S_\alpha}^{2S_\alpha} f(x) \cos\left(\frac{(2k-1)\pi x}{2S_\alpha}\right) dx \right) = \\ &= \frac{1}{S_\alpha} \left(\int_0^{S_\alpha} f(x) \cos\left(\frac{(2k-1)\pi x}{2S_\alpha}\right) dx + \int_{-S_\alpha}^0 f(x+2S_\alpha) \cos\left(\frac{(2k-1)\pi(x+2S_\alpha)}{2S_\alpha}\right) dx \right) = \\ &= \frac{1}{S_\alpha} \left(\int_0^{S_\alpha} f(x) \cos\left(\frac{(2k-1)\pi x}{2S_\alpha}\right) dx - \int_{-S_\alpha}^0 f(x) \cos\left(\frac{(2k-1)\pi x}{2S_\alpha} + 2k\pi + \pi\right) dx \right) = \\ &= \frac{1}{S_\alpha} \left(\int_0^{S_\alpha} f(x) \cos\left(\frac{(2k-1)\pi x}{2S_\alpha}\right) dx + \int_{-S_\alpha}^0 f(x) \cos\left(\frac{(2k-1)\pi x}{2S_\alpha}\right) dx \right) = \\ &= \frac{1}{S_\alpha} \left(\int_0^{S_\alpha} f(x) \cos\left(\frac{(2k-1)\pi x}{2S_\alpha}\right) dx - \int_0^{-S_\alpha} f(x) \cos\left(\frac{(2k-1)\pi x}{2S_\alpha}\right) dx \right) = \\ &= \frac{1}{S_\alpha} \left(\int_0^{S_\alpha} f(x) \cos\left(\frac{(2k-1)\pi x}{2S_\alpha}\right) dx - \int_0^{S_\alpha} f(-x) \cos\left(\frac{-(2k-1)\pi x}{2S_\alpha}\right) d(-x) \right) = \\ &= \frac{2}{S_\alpha} \int_0^{S_\alpha} f(x) \cos\left(\frac{(2k-1)\pi x}{2S_\alpha}\right) dx \end{aligned}$$



Result of the application of the $f(x)$ function

assuming: $f(x + 2S_\alpha) = -f(x)$

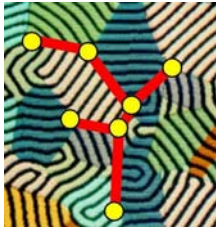
it yields $a_{2k} = 0$ $k = 0, 1, 2, \dots$ for $n = 2k$

and

$$a_{2k-1} = \frac{2}{S_\alpha} \int_0^{S_\alpha} f(x) \cos\left(\frac{(2k-1)\pi x}{2S_\alpha}\right) dx \quad \text{for } n = 2k - 1, k = 1, 2, \dots$$

finally, the *Fourier* series of the $f(x)$ is:

$$f(x) \approx \sum_{k=1}^{\infty} a_{2k-1} \cos\left(\frac{(2k-1)\pi x}{2S_\alpha}\right)$$



Final definition of the A_{2n-1} parameter



for rapid solidification:

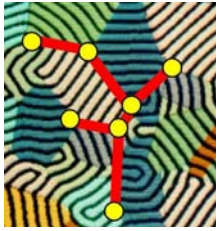
$$A_{2n-1} = \left(-\frac{v}{2D} - \sqrt{\frac{v^2}{4D^2} + \left(\frac{(2n-1)\pi}{2S_\alpha} \right)^2} \right)^{-1} \frac{2}{S_\alpha} \int_0^{S_\alpha} f_\alpha(x) \cos\left(\frac{(2n-1)\pi x}{2S_\alpha} \right) dx$$

$n = 1, 2, \dots$

for slow solidification:

$$A_{2n-1} = -\frac{4}{(2n-1)\pi} \int_0^{S_\alpha} f_\alpha(x) \cos\left(\frac{(2n-1)\pi x}{2S_\alpha} \right) dx$$

$n = 1, 2, \dots$



Properties of the solution to diffusion equation



$$\left. \frac{\partial \delta C(x, z)}{\partial x} \right|_{x=0} = \left. \frac{\partial \delta C(x, z)}{\partial x} \right|_{x=2S_\alpha} = 0$$

$$x \in [0, S_\alpha]$$

$$\left. \frac{\partial \delta C(x, z)}{\partial z} \right|_{z=0} = f_\alpha(x) = f_\alpha(-x) = -f_\alpha(-x + 2S_\alpha) = - \left. \frac{\partial \delta C(-x + 2S_\alpha, z)}{\partial z} \right|_{z=0}$$

according to assumption:

$$f_\alpha(-x) = f_\alpha(x), \quad f_\alpha(x + 2S_\alpha) = -f_\alpha(x)$$



Solution to the diffusion equation



b/ for the β phase lamella

$$x \in [S_\alpha, S_\alpha + S_\beta]$$

$$z \geq 0$$

$\delta C(x, z) =$

$$\sum_{n=1}^{\infty} B_{2n-1} \cos\left(\frac{(2n-1)\pi(x - S_\alpha + S_\beta)}{2S_\beta}\right) \exp\left[\left(-\frac{v}{2D} - \sqrt{\frac{v^2}{4D^2} + \left(\frac{(2n-1)\pi}{2S_\beta}\right)^2}\right)z\right]$$

with

$$B_{2n-1} = \left(-\frac{v}{2D} - \sqrt{\frac{v^2}{4D^2} + \left(\frac{(2n+1)\pi}{2S_\beta}\right)^2}\right)^{-1} \frac{2}{S_\beta} \int_{S_\alpha - S_\beta}^{S_\alpha} f_\beta(x) \cos\left(\frac{(2n+1)\pi(x - S_\alpha + S_\beta)}{2S_\beta}\right) dx$$

rapid solidification



Solution to the diffusion equation



b/ for the β phase lamella $x \in [S_\alpha, S_\alpha + S_\beta]$ $z \geq 0$

$$\delta C(x, z) = \sum_{n=1}^{\infty} B_{2n-1} \cos\left(\frac{(2n-1)\pi(x - S_\alpha + S_\beta)}{2S_\beta}\right) \exp\left(-\frac{(2n-1)\pi}{2S_\beta} z\right)$$

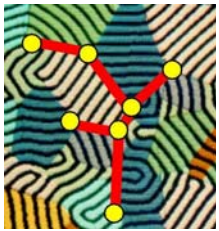
$$B_{2n-1} = -\frac{4}{(2n-1)\pi} \int_{S_\alpha - S_\beta}^{S_\alpha} f_\beta(x) \cos\left(\frac{(2n-1)\pi(x - S_\alpha + S_\beta)}{2S_\beta}\right) dx$$

$$n = 1, 2, \dots$$

and

$$\left. \frac{\partial \delta C(x, z)}{\partial z} \right|_{z=0} = f_\beta(x), \quad x \in [0, S_\beta]$$

slow solidification



Presentation of solution to the diffusion equation



a/ for the α phase lamella

$$x \in [0, S_\alpha] \quad z = 0$$

b/ for the β phase lamella

$$x \in [S_\alpha, S_\alpha + S_\beta] \quad z = 0$$

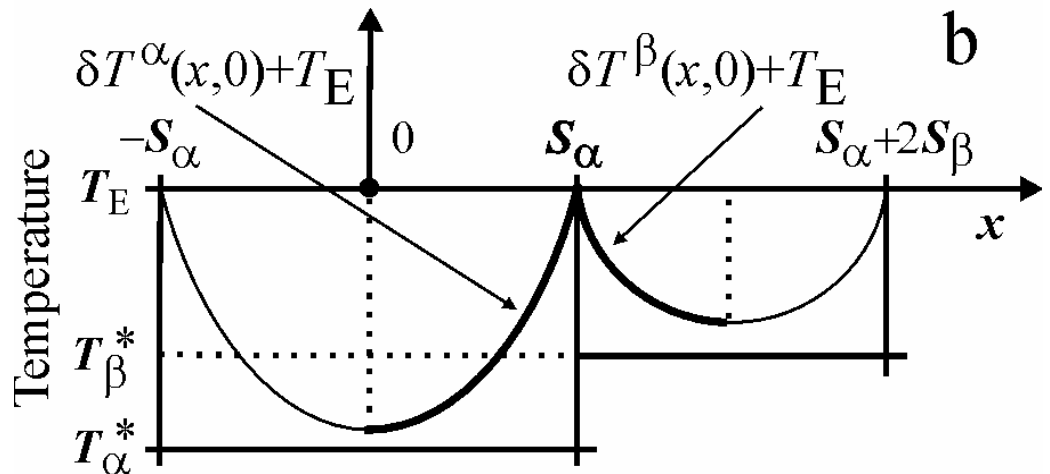
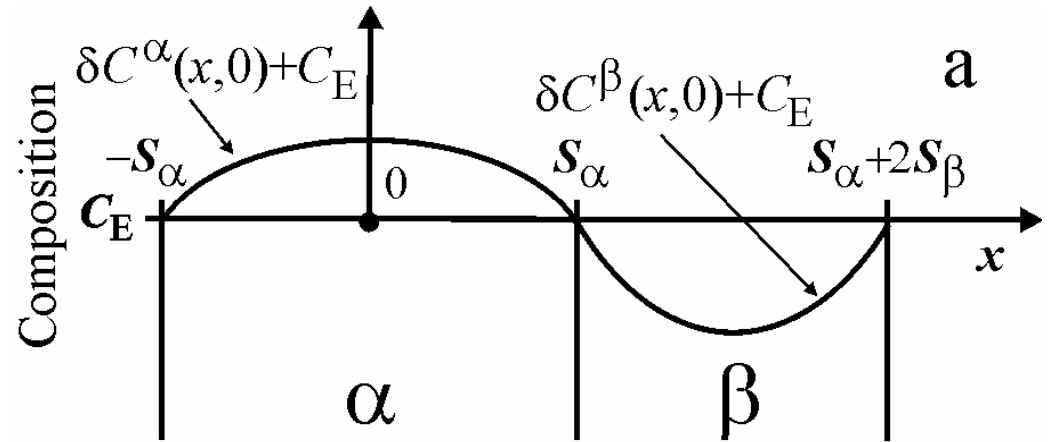


FIG. 16

micro-field
of solute concentration
undercooling



Total mass balance within micro-field of solute concentration



$$\int_0^{\infty} \int_0^{S_\alpha} \delta C(x, z) dx dz + \int_0^{\infty} \int_{S_\alpha}^{S_\alpha + S_\beta} \delta C(x, z) dx dz + = \sum_{n=1}^{\infty} \frac{4(-1)^{n-1} D}{(2n-1)\pi}$$

$$\left(\frac{A_{2n-1} S_\alpha^2}{vS_\alpha + \sqrt{v^2 S_\alpha^2 + (2n-1)^2 D^2 \pi^2}} - \frac{B_{2n-1} S_\beta^2}{vS_\beta + \sqrt{v^2 S_\beta^2 + (2n-1)^2 D^2 \pi^2}} \right) = 0$$

where

$$B_{2n-1} = \frac{A_{2n-1} S_\alpha^2 \left(vS_\beta + \sqrt{v^2 S_\beta^2 + (2n-1)^2 D^2 \pi^2} \right)}{S_\beta^2 \left(vS_\alpha + \sqrt{v^2 S_\alpha^2 + (2n-1)^2 D^2 \pi^2} \right)}, \quad n = 1, 2, \dots$$

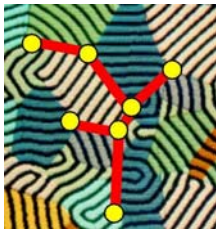
for rapid solidification



for slow solidification



$$B_{2n-1} = A_{2n-1} \left(\frac{S_\alpha}{S_\beta} \right)^2, \quad n = 1, 2, \dots$$

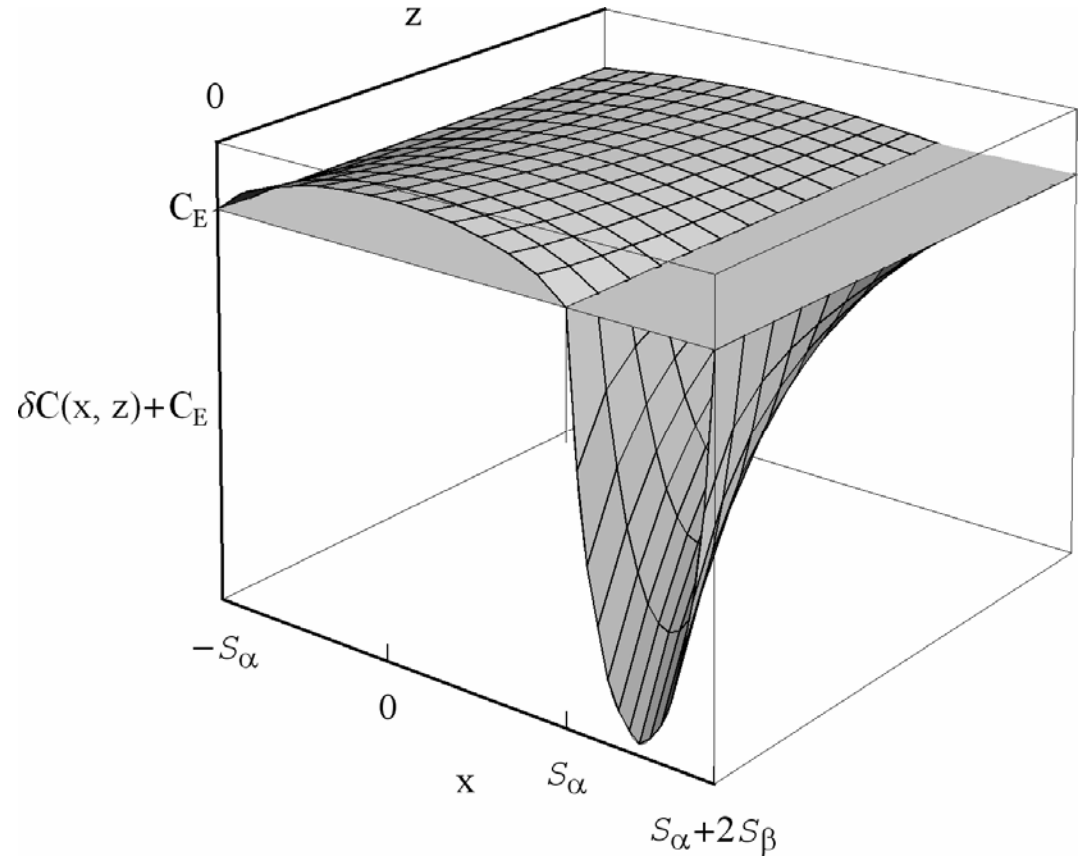


Visualization of total mass balance within micro-field of solute concentration



FIG. 17

mass balance calculated for planar solid / liquid interface





Local mass balance within micro-field of solute concentration



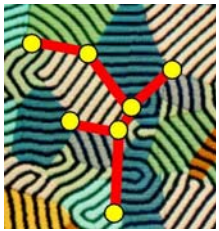
local mass balance is satisfied at $z = 0$ for α phase lamella and $z = d$ for β phase lamella

$$\int_0^{S_\alpha} \delta C(x, 0) dx + \int_{S_\alpha}^{S_\alpha + S_\beta} \delta C(x, d) dx = 0$$

after some rearrangements

$$\sum_{n=1}^{\infty} A_{2n-1} \frac{2S_\alpha (-1)^{n-1}}{(2n-1)\pi} - \sum_{n=1}^{\infty} B_{2n-1} \frac{2S_\beta (-1)^{n-1}}{(2n-1)\pi} \exp\left(-\frac{vS_\beta + \sqrt{v^2 S_\beta^2 + (2n-1)^2 D^2 \pi^2}}{2DS_\beta} d\right) = 0$$

d - phase protrusion

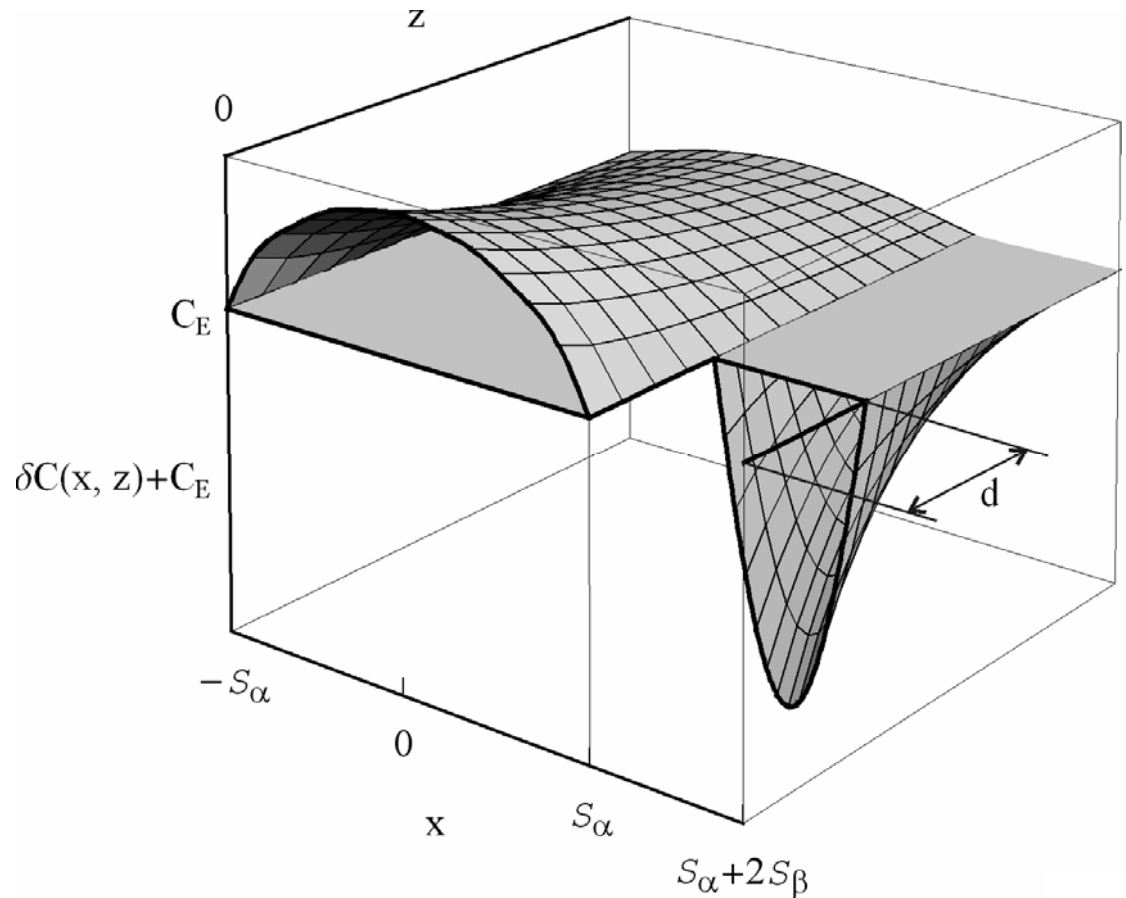


Visualization of local mass balance within micro-field of solute concentration



FIG. 18

protrusion, d ,
is the transient phase;
it has property of the liquid
but structure of the solid





Definition of the phase protrusion



rapid solidification

$$\sum_{n=1}^{\infty} A_{2n-1} \frac{(-1)^{n-1}}{(2n-1)} \times \left(1 - \frac{S_{\alpha} \left(vS_{\beta} + \sqrt{v^2 S_{\beta}^2 + (2n-1)^2 D^2 \pi^2} \right)}{S_{\beta} \left(vS_{\alpha} + \sqrt{v^2 S_{\alpha}^2 + (2n-1)^2 D^2 \pi^2} \right)} \right) \exp \left(- \frac{vS_{\beta} + \sqrt{v^2 S_{\beta}^2 + (2n-1)^2 D^2 \pi^2}}{2DS_{\beta}} d \right) = 0$$

slow solidification

$$\sum_{n=1}^{\infty} A_{2n-1} \frac{(-1)^{n-1}}{(2n-1)} \left(1 - \frac{S_{\alpha}}{S_{\beta}} \exp \left(- \frac{(2n-1)\pi}{2S_{\beta}} d \right) \right) = 0$$



Confirmation for the existence of the phase protrusion

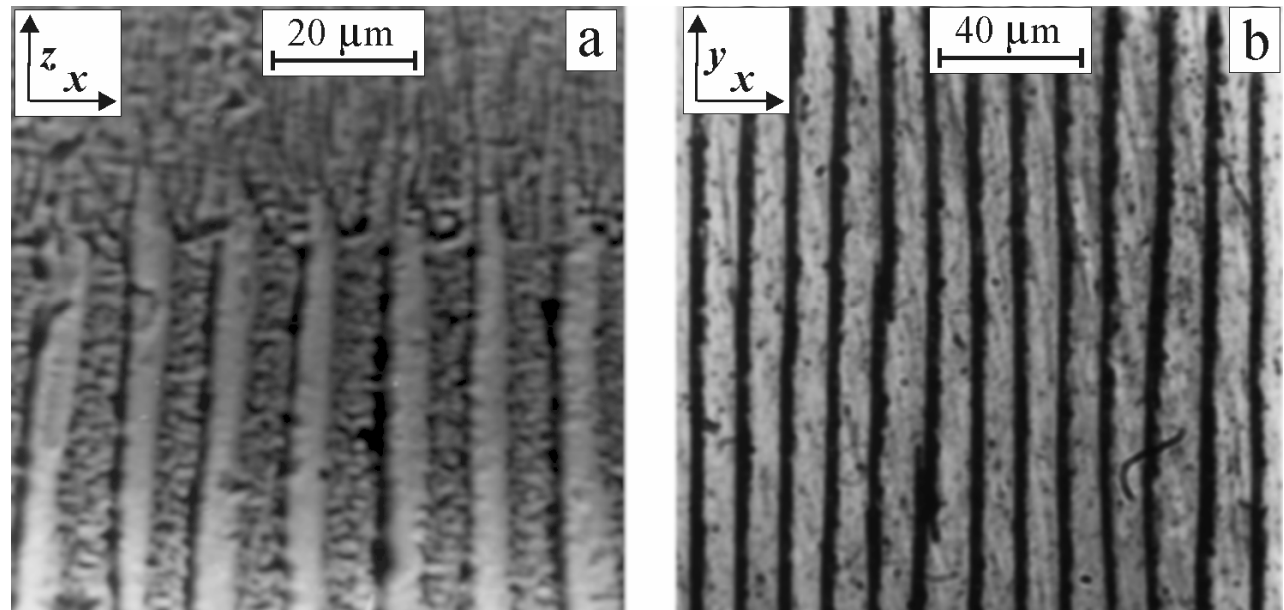


FIG. 19

oriented growth of the (Pb) – (Cd) composite *in situ*

phase protrusion visible for (Cd) - leading phase, FIG. 19a



α / β inter-phase mass balance



the s / l interface mass balance requires

$$S_{\alpha} \frac{\partial \delta C^{\alpha}(x,0)}{\partial z} = S_{\alpha} \frac{v}{D} (1 - k_{\alpha}) C^{\alpha}(x,0)$$

$$x \in [0, S_{\alpha}]$$

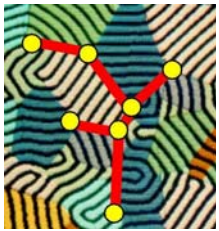
$$S_{\beta} \frac{\partial \delta C^{\beta}(x,d)}{\partial z} = S_{\beta} \frac{v}{D} (1 - k_{\beta}) C^{\beta}(x,d)$$

$$x \in [S_{\alpha}, S_{\alpha} + S_{\beta}]$$

mass balance at the α / β inter-phase

$$\lim_{x \rightarrow S_{\alpha}^{-}} S_{\alpha} \frac{\partial \delta C^{\alpha}(x,0)}{\partial z} + \lim_{x \rightarrow S_{\alpha}^{+}} S_{\beta} \frac{\partial \delta C^{\beta}(x,d)}{\partial z} =$$

$$S_{\alpha} \frac{v}{D} C_0^{\alpha}(S_{\alpha},0) + S_{\beta} \frac{v}{D} C_0^{\beta}(S_{\alpha},d) = \frac{v}{D} \left(S_{\alpha} C_0^{\alpha}(S_{\alpha},0) + S_{\beta} C_0^{\beta}(S_{\alpha},d) \right) = 0$$



Triple point of the s / l interface



not only mechanical equilibrium but thermodynamic equilibrium at the triple point is satisfied as well

solute concentration micro-field exists within the transition phase, d, (over leading phase) as if it was the liquid phase

solute concentration undercooling

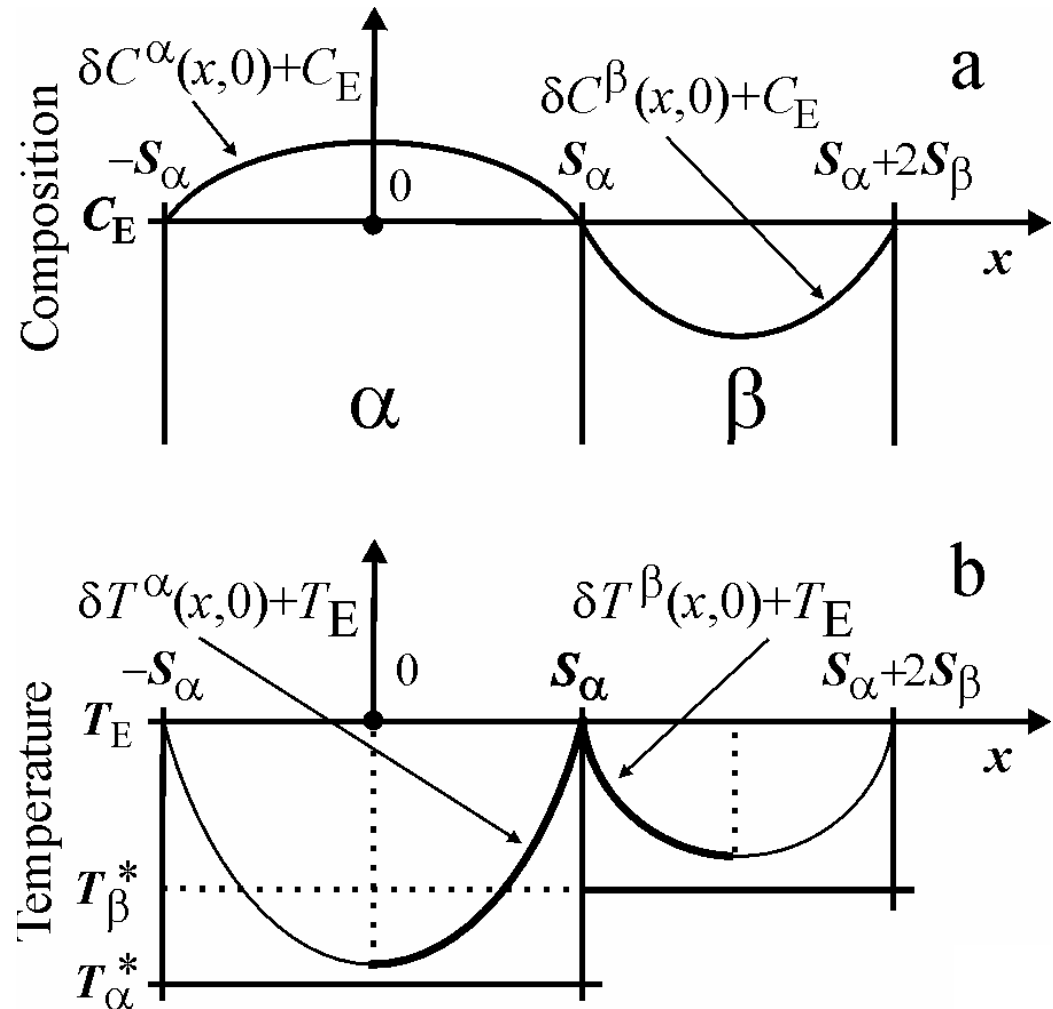


FIG. 20



Concluding remarks



at slow solidification, typical for composite *in situ* growth

$$B_{2n-1} = A_{2n-1} \left(\frac{S_\alpha}{S_\beta} \right)^2, \quad n = 1, 2, \dots$$

$$\left| f_\beta \left(x \frac{S_\beta}{S_\alpha} \right) \right| = |f_\alpha(x)| \left(\frac{S_\alpha}{S_\beta} \right)^2$$

the current description of micro-structure of solute concentration can be mathematically reduced to the J-H equation, however under condition that phase diagram would be symmetrical one that is $C_0^\alpha = C_0^\beta$ and consequentially $S_\alpha = S_\beta$, additionally, phase protrusion becomes $d = 0$, C_E comes back to the α / β inter-phase boundary and mass balance is satisfied at each co-ordinate, z



METRO
MEtallurgical TRaining On-line



Mass transport at the solid/liquid interface of
growing composite *in situ*

End of the lecture



Education and Culture