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Transformation: lamella - rod within oriented eutectic Al-Si

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IMMS PAS

Education and Culture

Criterion for the formation lamellae or rods Jackson-Hunt theory

relation: undercooling – growth rate

lamellar growth

$$\frac{(\Delta T)^2}{v} = 4m^2 a^L Q^L$$

rod-like growth

$$\frac{(\Delta T)^2}{v} = 4m^2 a^R Q^R$$

criterion for the formation lamellae or rods is given by Jackson – Hunt (J-H) theory

J-H criterion

$$\frac{\left(\frac{a_\alpha^L}{m_\alpha} + \frac{a_\beta^L}{\xi\, m_\beta}\right)}{\left(\frac{a_\alpha^R}{m_\alpha} + \frac{a_\beta^R}{\xi\, m_\beta}\right)} > \frac{4E}{P^*}\frac{1}{(1+\xi)^{1.5}}$$

when free energies for s / l interface are isotropic
then l.h.s. of criterion is equal to one

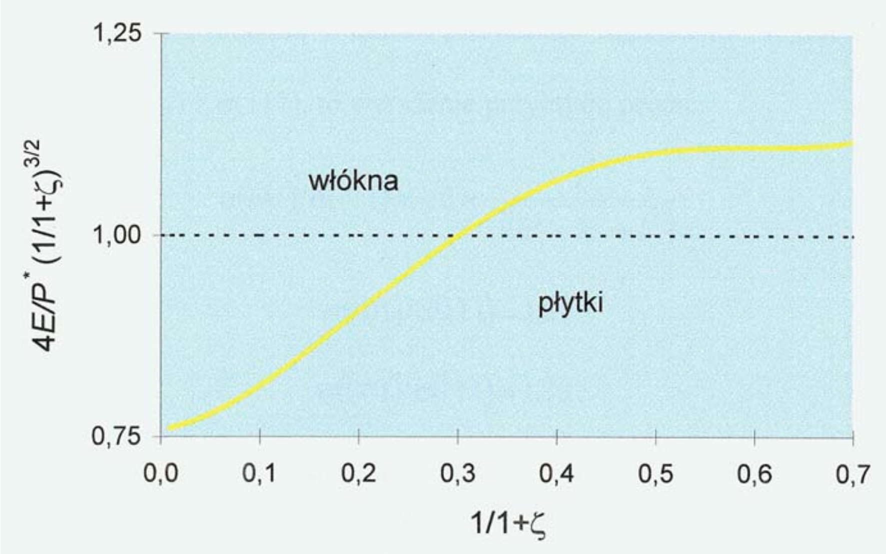
K.A. Jackson, J.D. Hunt, Trans. AIME, **236**, 1129-1142, (1966)

Criterion for the formation lamellae or rods

some constants
typical for a given phase diagram
are introduced into r.h.s. of J-H criterion

J-H inequality (criterion) changes at f(ζ) = 0.32 FIG. 1

f(ζ) = 0.114 for Al-Si phase diagram thus, rod-like structure should be expected



J-H criterion

$$\frac{\left(\frac{a_\alpha^L}{m_\alpha}+\frac{a_\beta^L}{\xi\, m_\beta}\right)}{\left(\frac{a_\alpha^R}{m_\alpha}+\frac{a_\beta^R}{\xi\, m_\beta}\right)} > \frac{4E}{P^*}\frac{1}{(1+\xi)^{1.5}}$$

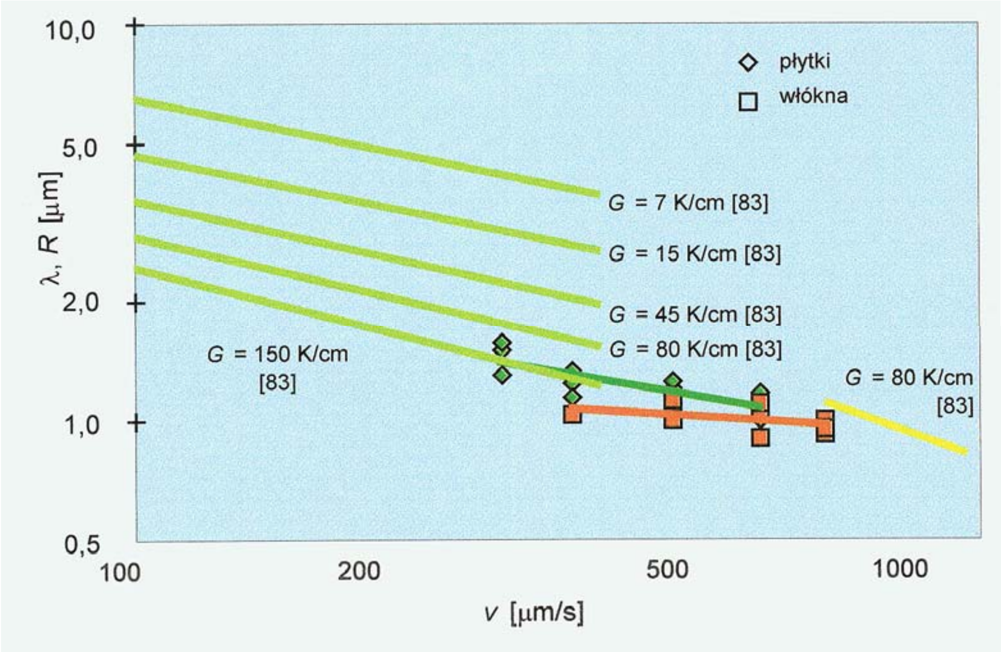
FIG. 1 r.h.s of the J-H criterion versus f(ζ)

włókna = rods płytki = lamellae

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

Lamellar or rod-like spacing measurements

since some constants typical for a given phase diagram are introduced into r.h.s. of J-H criterion the J-H criterion is not adequate to describe the lamella / rod transformation occurring at critical growth rate



it is expected that:
lamellae are stable form below critical growth rate
rods are stable form over critical growth rate
(within oriented Al-Si eutectic morphology)

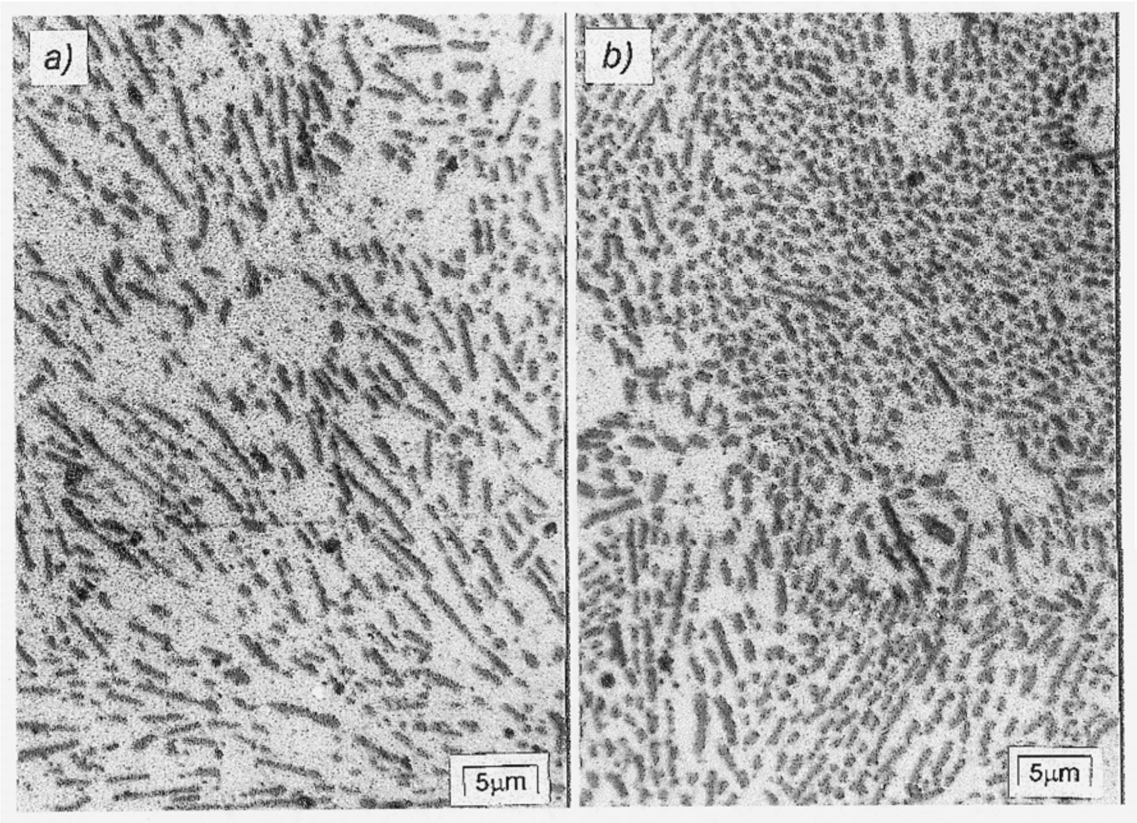
inter-lamellar, λ or inter-rod, R, spacing versus growth rate, v, as measured
płytki = lamellae **włókna = rods**

FIG. 2

[83] = B. Toloui, A. Hellawell, Acta Met. **24**, 565, (1976)

lamella ➔ rod transformation
Oriented growth by *Bridgman* system

FIG. 3



a/ v = 370 μm/s, G = 100 K/cm   b/ v = 500 μm/s, G = 40 K/cm

lamella ➔ rod transformation
Oriented growth by *Bridgman* system

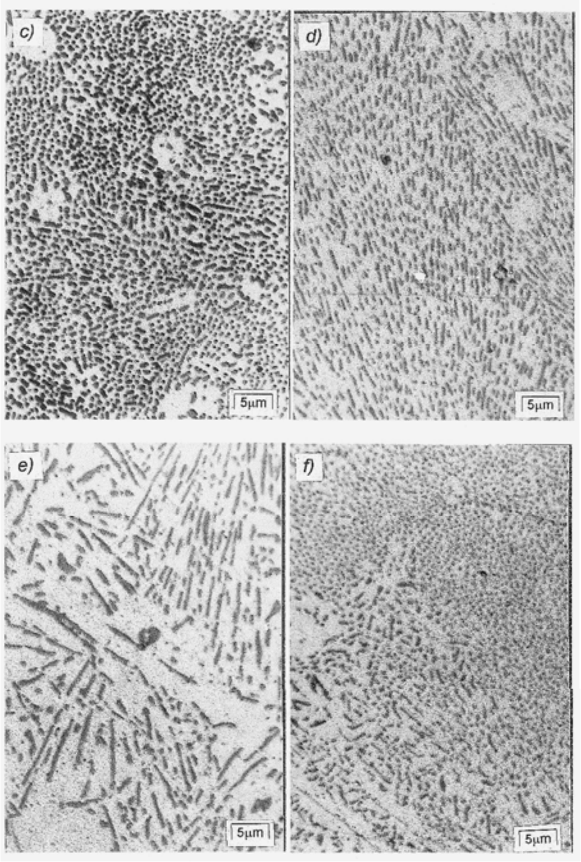
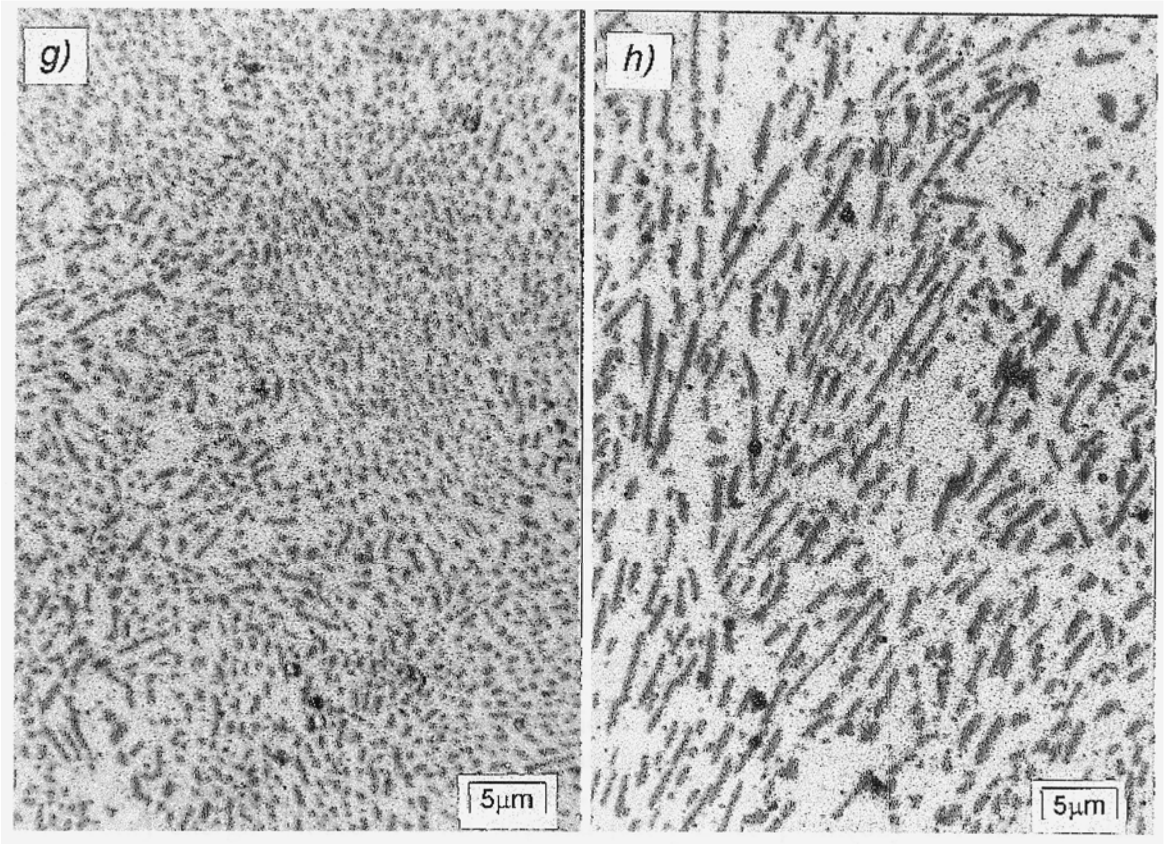


FIG. 4

c/ v = 790 μm/s, G = 40 K/cm   d/ v = 790 μm/s, G = 250 K/cm
e/ v = 370 μm/s, G = 250 K/cm   f/ v = 500 μm/s, G = 250 K/cm

lamella ➔ rod transformation
Oriented growth by *Bridgman* system

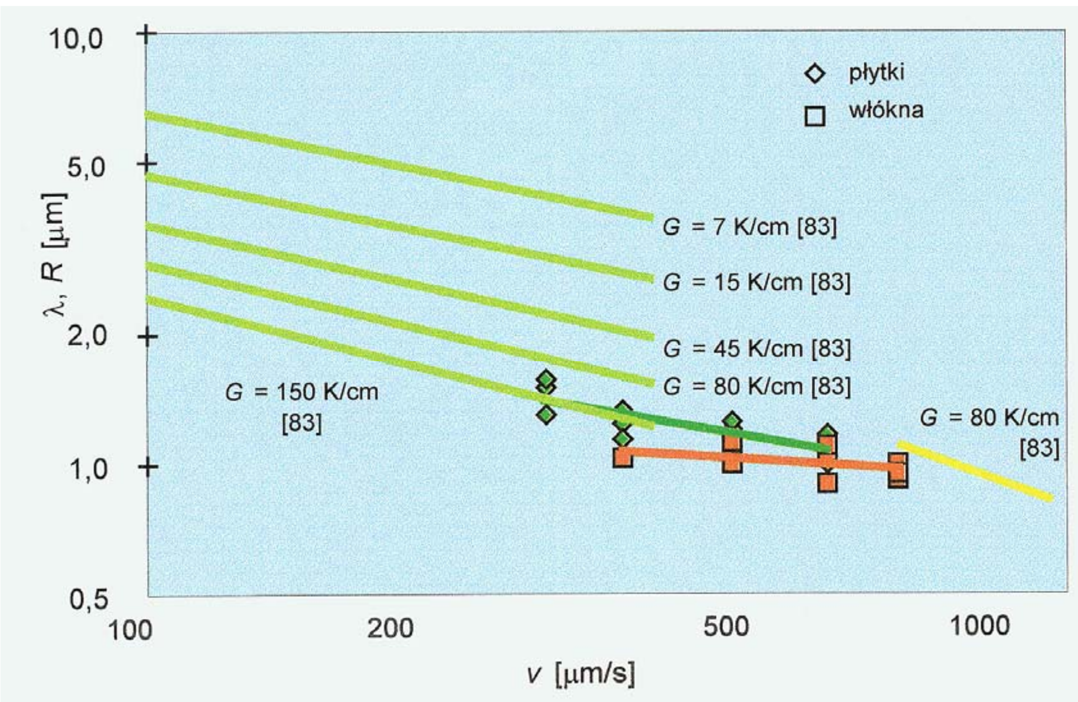
FIG. 5



g/ v = 790 μm/s, G = 250 K/cm   h/ v = 370 μm/s, G = 100 K/cm

lamella ➔ rod transformation
Oriented growth by *Bridgman* system

no threshold rate for transformation: lamella ➔ rod !
contribution of rods increases along with growth rate
within the range of: 400 μm/s - 700 μm/s
lamellae and rods coexist within this range of rates !



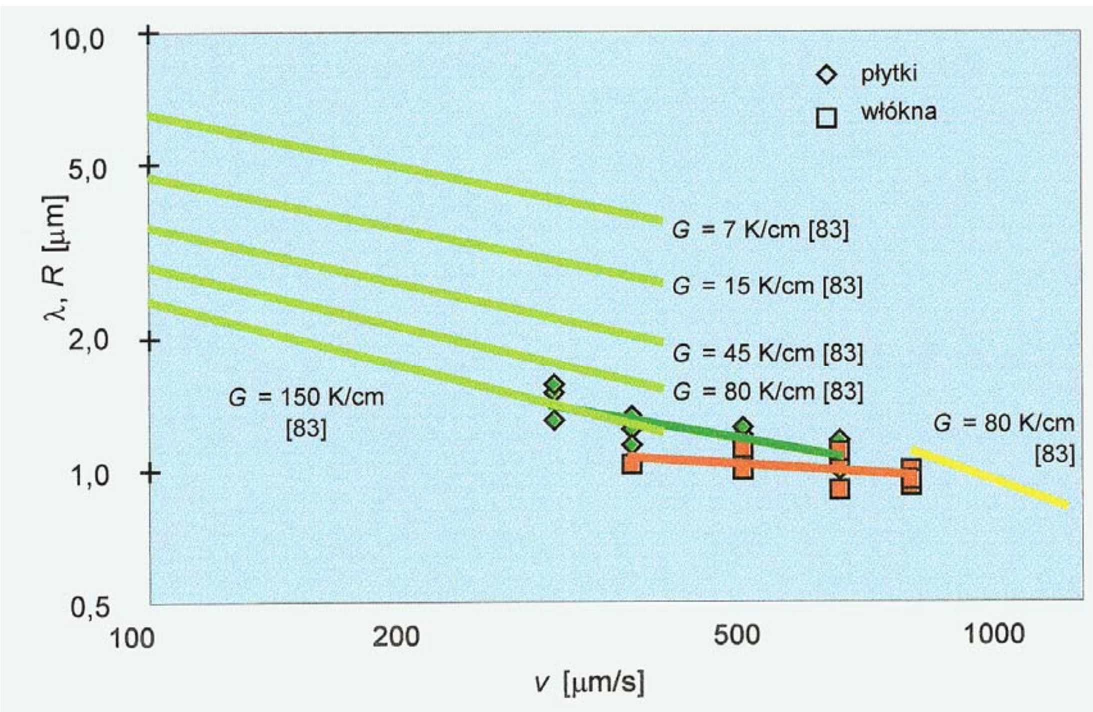
operating range
for transformation
lamella ➔ rod

płytki = lamellae
włókna = rods

FIG. 6

lamella ➔ rod transformation
Oriented growth by *Bridgman* system

not only the description for transformation
lamella ➔ rod is required
but explication of the co-existence
of lamellae and rods within the range of rates



operating range
for transformation
lamella ➔ rod

płytki = lamellae
włókna = rods

FIG. 7

Thermodynamics of the solid / liquid interface

lamellar structure

average undercooling (J-H theory)

$$\Delta T_{\alpha}^{L} = m_{\alpha}\left(B_0 + \frac{2v}{D} N_0 \frac{\left(S_{\alpha} + S_{\beta}\right)^2}{S_{\alpha}} P^{*} \right) + \frac{T_E}{L_{\alpha}} \sigma_{\alpha}^{L} \frac{1}{S_{\alpha}} \sin \theta_{\alpha}^{L}$$

$$\Delta T_{\beta}^{L} = m_{\beta}\left(-B_0 + \frac{2v}{D} N_0 \frac{\left(S_{\alpha} + S_{\beta}\right)^2}{S_{\beta}} P^{*} \right) + \frac{T_E}{L_{\beta}} \sigma_{\beta}^{L} \frac{1}{S_{\beta}} \sin \theta_{\beta}^{L}$$

rod-like structure

$$\Delta T_{\alpha}^{R} = m_{\alpha}\left(A_0 + \frac{4v}{D} N_0 \left(r_{\alpha} + r_{\beta}\right) E \right) + \frac{T_E}{L_{\alpha}} \sigma_{\alpha}^{R} \frac{2}{r_{\alpha}} \sin \theta_{\alpha}^{R}$$

$$\Delta T_{\beta}^{R} = m_{\beta}\left(-A_0 + \frac{4v}{D} N_0 \left(r_{\alpha} + r_{\beta}\right) \frac{r_{\alpha}^{2}}{\left(r_{\alpha} + r_{\beta}\right)^2 - r_{\alpha}^{2}} E \right) + \frac{T_E}{L_{\beta}} \sigma_{\beta}^{R} \frac{2 r_{\alpha}}{\left(r_{\alpha} + r_{\beta}\right)^2 - r_{\alpha}^{2}} \sin \theta_{\beta}^{R}$$

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

average undercooling can be recalculated into average free energy:

$\Delta T \rightarrow \Delta G^{*}$

Structure geometry

average undercooling (J-H theory)

lamellar structure

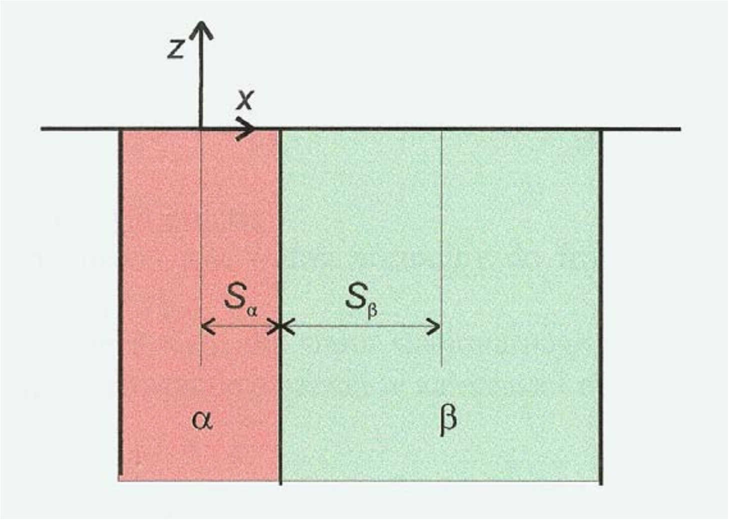
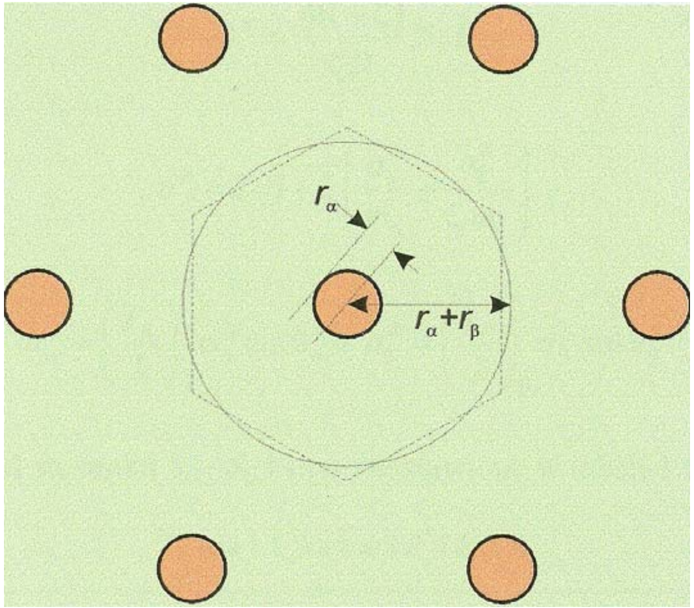


FIG. 8

rod-like structure

FIG. 9



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

average undercooling can be recalculated into average free energy:

$$\Delta T \rightarrow \Delta G^*$$

Thermodynamics of s / l interface and α / β inter-phase boundary

average undercooling recalculated into average free energy:

ΔT ➔ ΔG*

lamellar structure

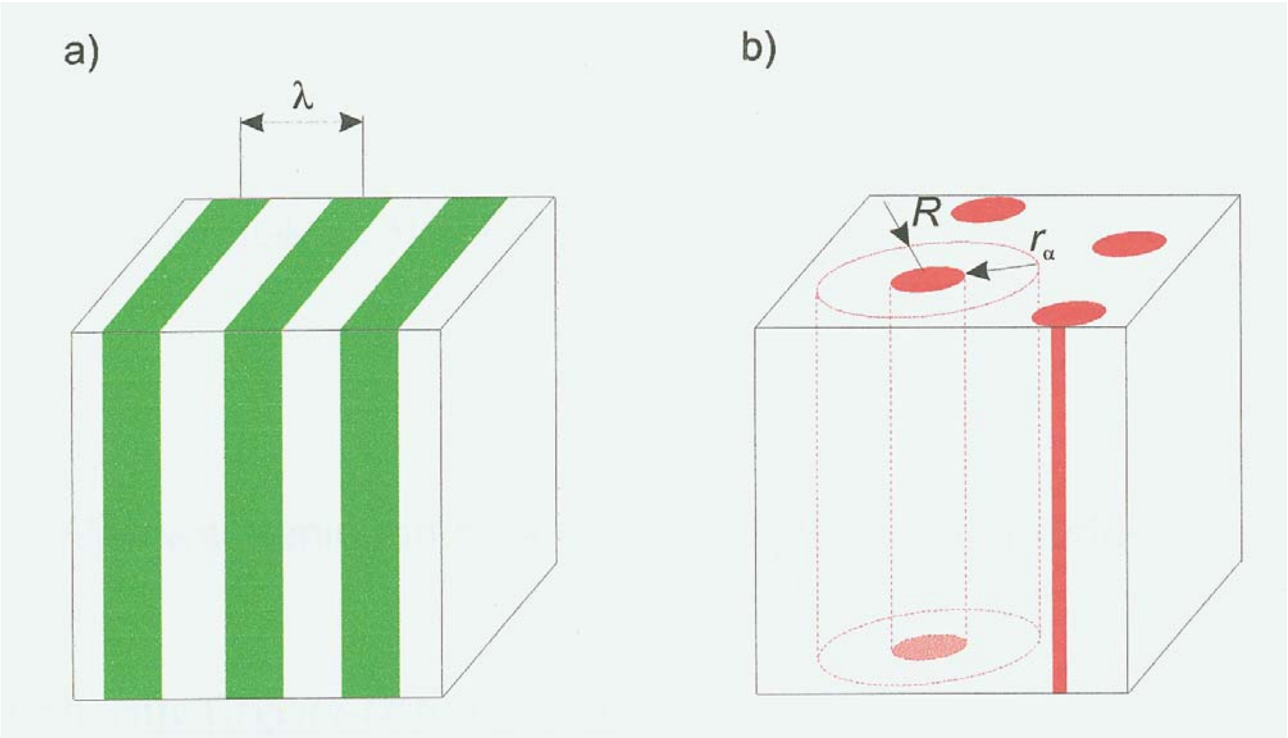
$$\Delta G_L^* = \left\{ m \frac{\left(L_\alpha \zeta + L_\beta\right)}{T_E} \frac{v}{D} \lambda \frac{P^*\left(1+\zeta\right)N_0}{\zeta} + m \frac{2\left(1+\zeta\right)}{\lambda} \left(\frac{\sigma_\alpha^L \sin\theta_\alpha^L}{m_\alpha} + \frac{\sigma_\beta^L \sin\theta_\beta^L}{\zeta m_\beta} \right) \right\} + \frac{2\sigma_{\alpha-\beta}^L}{\lambda}$$

rod-like structure

$$\Delta G_R^* = \left\{ m \frac{\left(L_\alpha \zeta + L_\beta\right)}{T_E} \frac{4v}{D} R \frac{EN_0}{\zeta} + m \frac{2\sqrt{1+\zeta}}{R} \left(\frac{\sigma_\alpha^R \sin\theta_\alpha^R}{m_\alpha} + \frac{\sigma_\beta^R \sin\theta_\beta^R}{\zeta m_\beta} \right) \right\} + \frac{2\sigma_{\alpha-\beta}^R}{R\sqrt{1+\zeta}}$$

where $$\frac{1}{m} = \frac{1}{m_\alpha} + \frac{1}{m_\beta}$$

Geometry of the α / β inter-phase boundary



$$\zeta = \frac{S_\beta}{S_\alpha}$$

$$\lambda = 2\left(S_\alpha + S_\beta\right)$$

$$r_\alpha = \frac{R}{\sqrt{1+\zeta}}$$

$$R = r_\alpha + r_\beta$$

FIG. 10

a/ lamellar structure
b/ rod-like structure

Mechanical equilibrium at a triple point

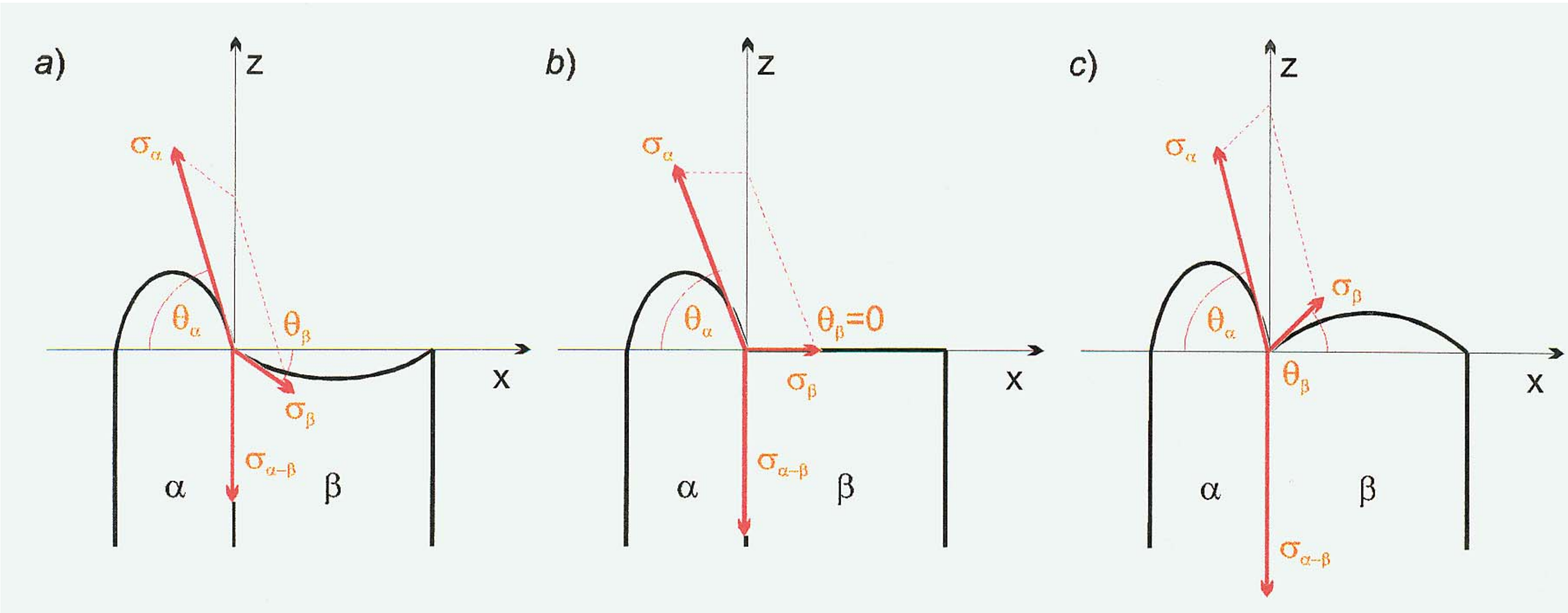


FIG. 11

a/ convex / concave interface
b/ convex / planar interface
c/ convex / convex interface

$$\sigma_{\alpha}^{L} \sin\theta_{\alpha}^{L} + \sigma_{\beta}^{L} \sin\theta_{\beta}^{L} - \sigma_{\alpha-\beta}^{L} = 0$$

$$\sigma_{\alpha}^{R} \sin\theta_{\alpha}^{R} + \sigma_{\beta}^{R} \sin\theta_{\beta}^{R} - \sigma_{\alpha-\beta}^{R} = 0$$

Thermodynamics of s / l interface and α / β inter-phase boundary

final definitions

lamellar structure

$$\Delta G_L^* = v\lambda Q_{C-W}^L + \frac{a_{C-W}^L}{\lambda}$$

$$Q_{C-W}^L = m\frac{L_\alpha \zeta + L_\beta}{T_E}\frac{P^*(1+\zeta)N_0}{\zeta D}$$

$$a_{C-W}^L = 2\left[m(1+\zeta)\left(\frac{\sigma_\alpha^L \sin\theta_\alpha^L}{m_\alpha} + \frac{\sigma_\beta^L \sin\theta_\beta^L}{\zeta m_\beta}\right) + \sigma_{\alpha-\beta}^L\right]$$

rod-like structure

$$\Delta G_R^* = vRQ_{C-W}^R + \frac{a_{C-W}^R}{R}$$

$$Q_{C-W}^R = m\frac{L_\alpha \zeta + L_\beta}{T_E}\frac{4EN_0}{\zeta D}$$

$$a_{C-W}^R = 2\left[m\sqrt{1+\zeta}\left(\frac{\sigma_\alpha^R \sin\theta_\alpha^R}{m_\alpha} + \frac{\sigma_\beta^R \sin\theta_\beta^R}{\zeta m_\beta}\right) + \frac{\sigma_{\alpha-\beta}^R}{\sqrt{1+\zeta}}\right]$$

Use of the phase diagram

final definitions

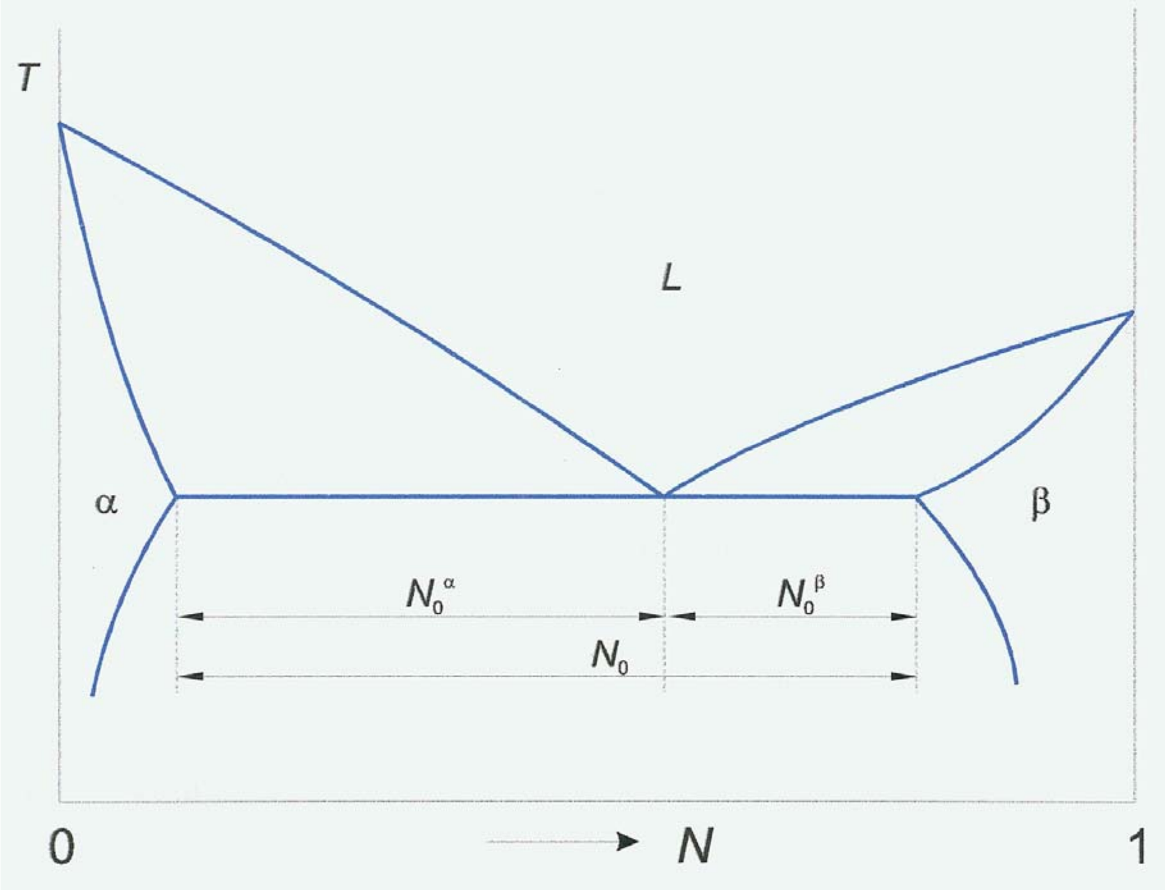
lamellar structure

$$Q_{C-W}^{L} = m\frac{L_\alpha\zeta + L_\beta}{T_E}\frac{P^*(1+\zeta)N_0}{\zeta D}$$

rod-like structure

$$Q_{C-W}^{R} = m\frac{L_\alpha\zeta + L_\beta}{T_E}\frac{4EN_0}{\zeta D}$$

FIG. 12



arbitrary phase diagram

New criterion for the formation lamellae or rods

$$\frac{m\left(\dfrac{\sigma_{\alpha}^{L}\sin\theta_{\alpha}^{L}}{m_{\alpha}}+\dfrac{\sigma_{\beta}^{L}\sin\theta_{\beta}^{L}}{\zeta m_{\beta}}\right)+\dfrac{\sigma_{\alpha-\beta}^{L}}{1+\zeta}}{m\left(\dfrac{\sigma_{\beta}^{R}\sin\theta_{\beta}^{R}}{m_{\alpha}}+\dfrac{\sigma_{\beta}^{R}\sin\theta_{\beta}^{R}}{\zeta m_{\beta}}\right)+\dfrac{\sigma_{\alpha-\beta}^{R}}{1+\zeta}} > 4\frac{E}{P^{*}}\left(\frac{1}{1+\zeta}\right)^{1.5}$$

when specific surface free energy of s / l interface and free energy of α / β inter-phase boundary are isotropic then l.h.s. of criterion is equal to one

since some constants typical for a given phase diagram are introduced into r.h.s. of C-W criterion the C-W criterion is not adequate to describe the lamella / rod transformation occurring within operating range FIG. 7

C-W inequality (criterion) changes at f(ζ) = 0.32
f(ζ) = 0.114 for Al-Si phase diagram
thus, rod-like structure should be expected

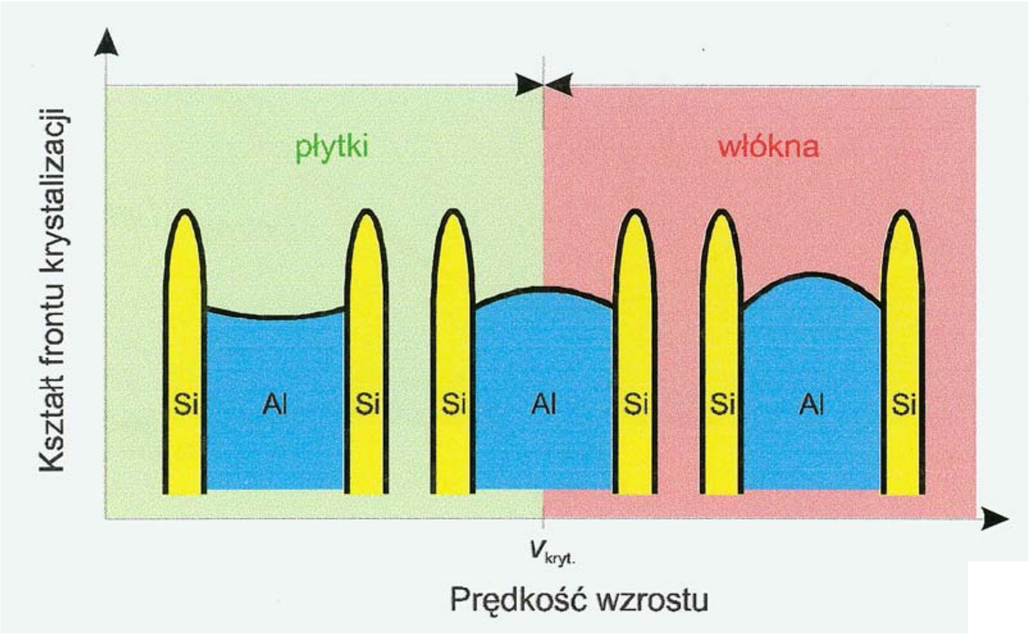
R.Cupryś, PhD Thesis, University of Science and Technology, Kraków 2000

New criterion for the formation lamellae or rods Growth rate

since f(ζ) = 0.114 for Al-Si phase diagram and the beginning of transformation appears at v = 400 μm/s the l.h.s. of the new criterion should be equal to 0.81 this would be satisfied if adequate changes of the specific surface free energy were possible; thus, a model for the s / l interface shape varying along with growth rate is introduced; a suggested behaviour of the specific surface free energy (surface tension) has already been shown, FIG. 11

FIG. 13

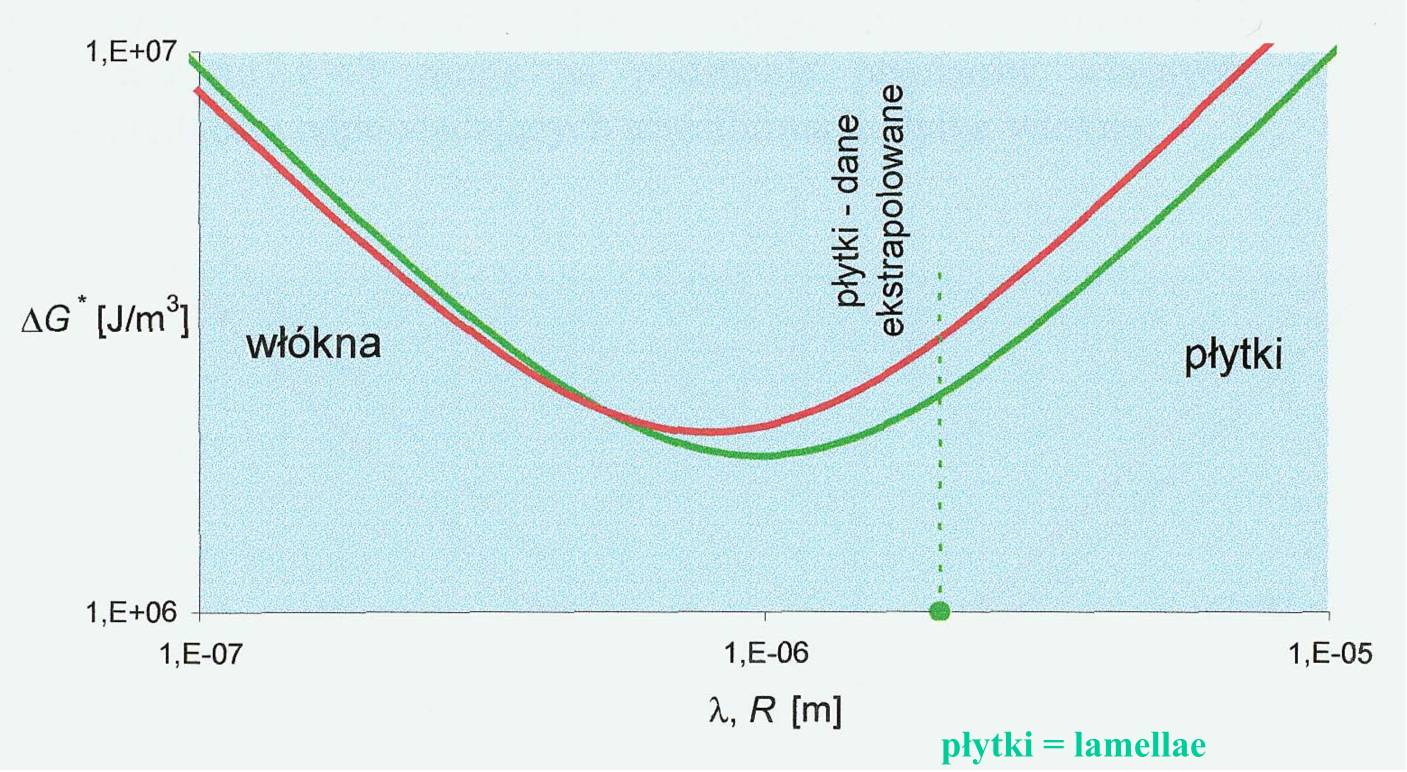
varying curvature of the s / l interface resulting in some changes of the specific surface free energy with an adequate behaviour of mechanical equilibrium at a triple point



New criterion for the formation lamellae or rods Growth of lamellae

FIG. 14

ΔG^*_L and ΔG^*_R calculated for v = 100 μm/s and adequate mechanical equilibrium defined at triple point, FIG. 13



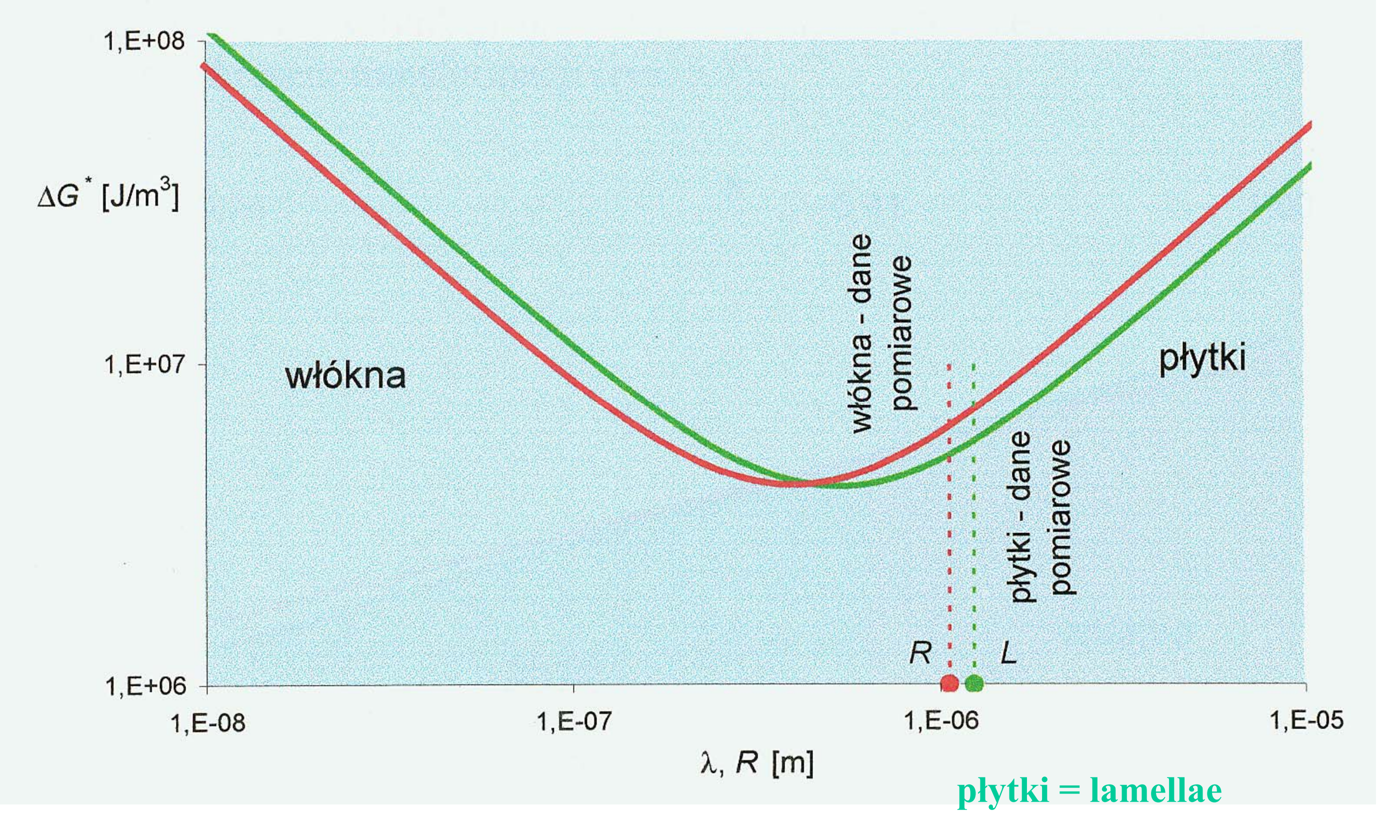
płytki = lamellae
włókna = rods

RESULT - minimum for lamellae is below minimum for rods !

New criterion for the formation lamellae or rods Transformation

FIG. 15

ΔG^*_L and ΔG^*_R calculated for v = 400 μm/s and adequate mechanical equilibrium defined at triple point, FIG. 13



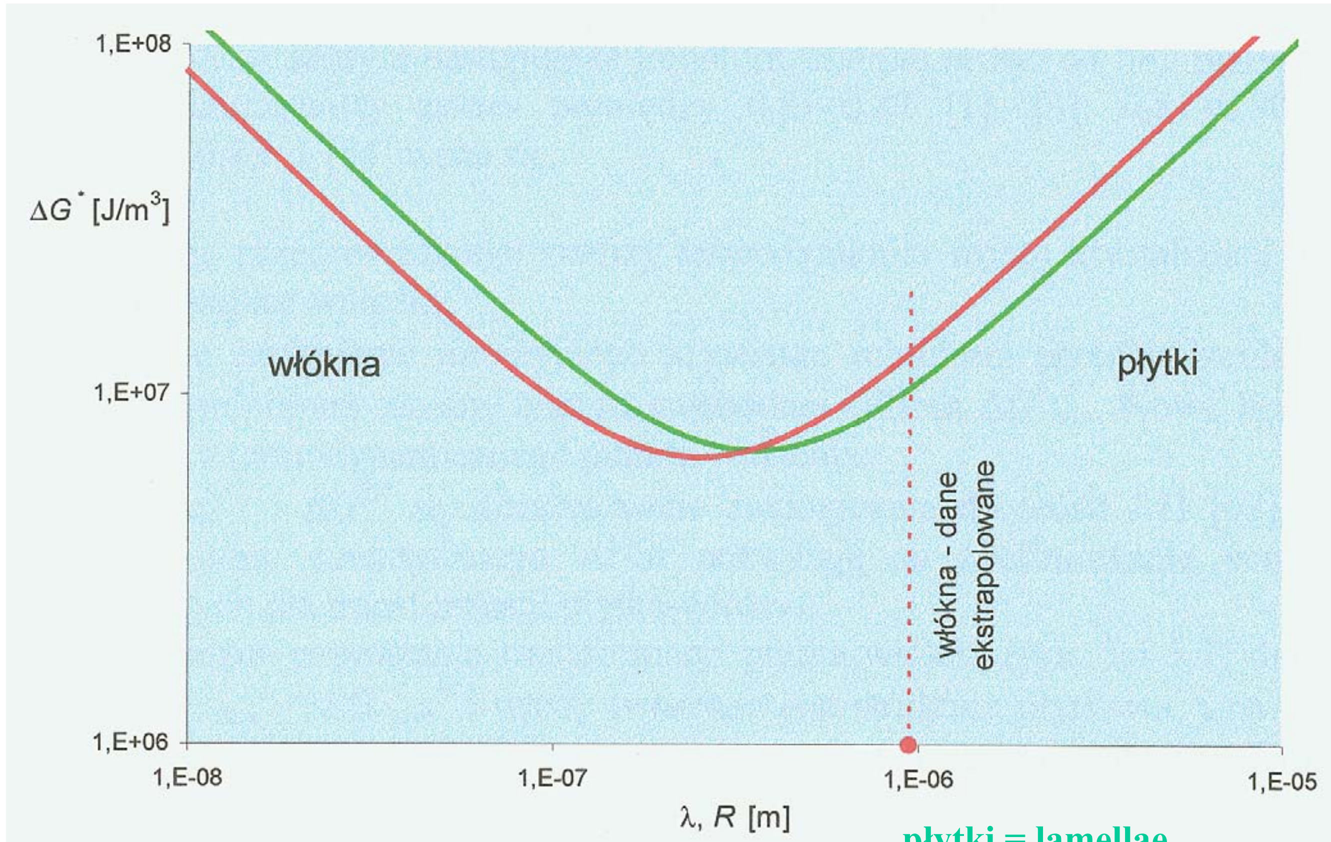
płytki = lamellae
włókna = rods

RESULT - minimum for lamellae is at the same level as minimum for rods !

New criterion for the formation lamellae or rods
Growth of rods

FIG. 16

ΔG^*_L and ΔG^*_R calculated for $v = 1000\ \mu m/s$ and adequate mechanical equilibrium defined at triple point, FIG. 13



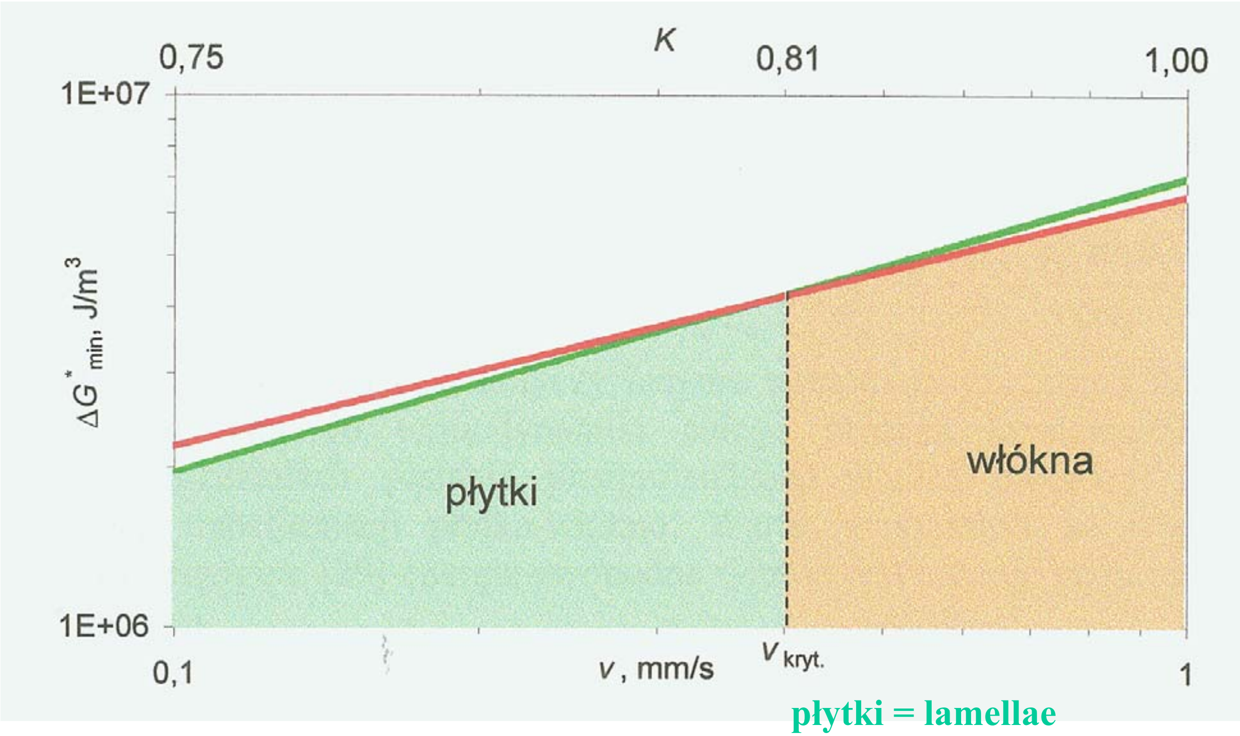
płytki = lamellae
włókna = rods

RESULT - minimum for rods is below minimum for lamellae !

New criterion for the formation lamellae or rods Threshold growth rate

FIG. 17

minima of ΔG^*_L and ΔG^*_R calculated for $v = 100 - 1000\ \mu m/s$ and adequate mechanical equilibrium defined at a triple point, FIG. 13



płytki = lamellae
włókna = rods

RESULT – threshold growth rate v_{kryt} can be estimated, only ! no possibility to determine the operating range !

Thermodynamics of solidification process

global entropy production for stationary growth of the oriented Al-Si eutectic can be referred to the regular structure formed locally inside the generally, irregular structure

$$P = \int_V \sigma_D \, dV$$

for macroscopically isothermal s / l interface ➔

$$\sigma_D = \frac{DR^{*}\varepsilon}{N_i\left(1 - N_i\right)} \left| grad.N_i \right|^2$$

σ_D - entropy production per unit time and per unit volume connected with mass transport within the boundary layer

global entropy, average for:

lamellar structure formation

$$\overline{P}_L = \frac{1}{S_\alpha + S_\beta} \int_{V_L} \sigma_D \, dV$$

rod-like structure formation

$$\overline{P}_R = \frac{1}{\pi (r_\alpha + r_\beta)^2} \int_{V_R} \sigma_D \, dV$$

Volume Regular structure

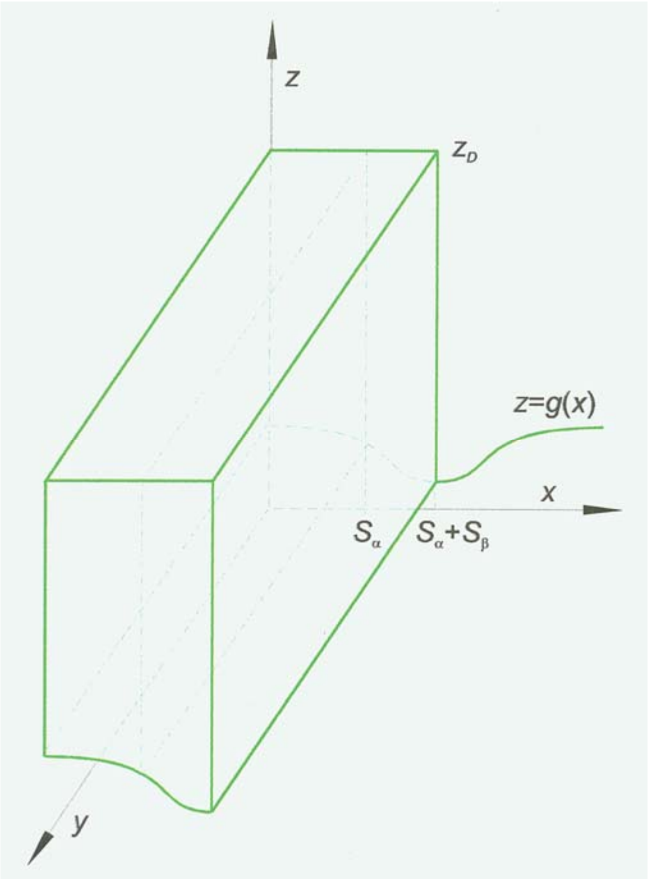


FIG. 18

lamellar growth

geometry of regular structure

volumes required by integral, respectively

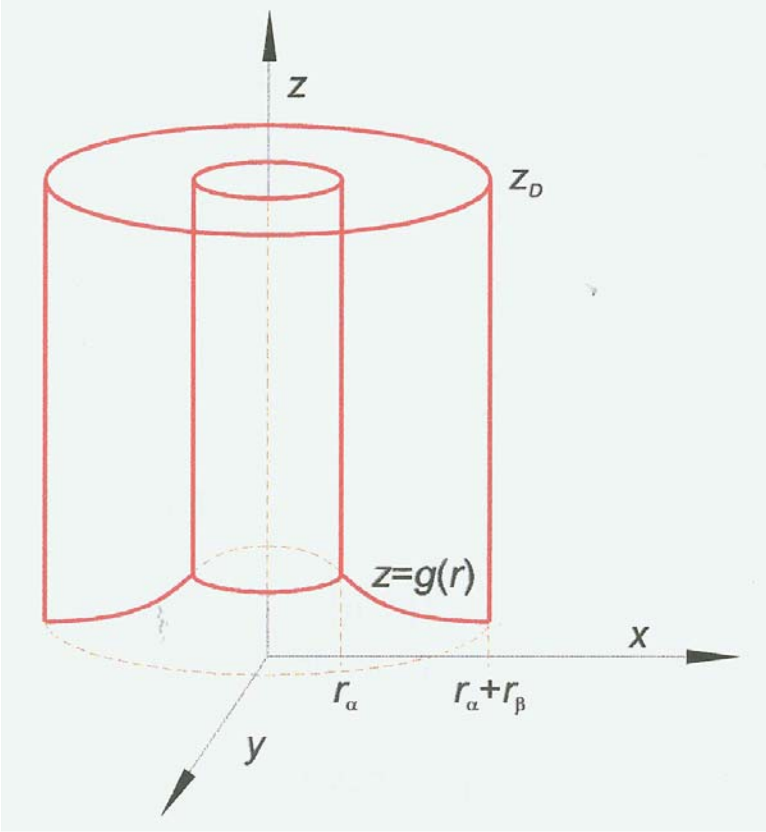


FIG. 19

rod-like growth

Integration

$$\iiint_V \left|grad.N^L(x,z)\right|^2 dV = \iint_A \delta N^L(x,z)\frac{\partial N^L(x,z)}{\partial n}dA + \frac{v}{2D}\iiint_V \delta N^L(x,z)\frac{\partial\left(\delta N^L(x,z)\right)^2}{\partial z}dV$$

lamellar growth

rod-like growth

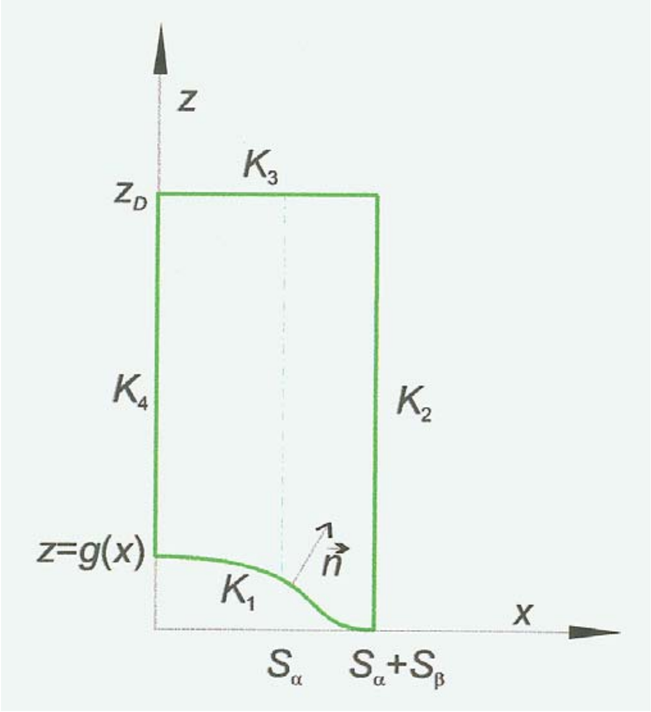


FIG. 20

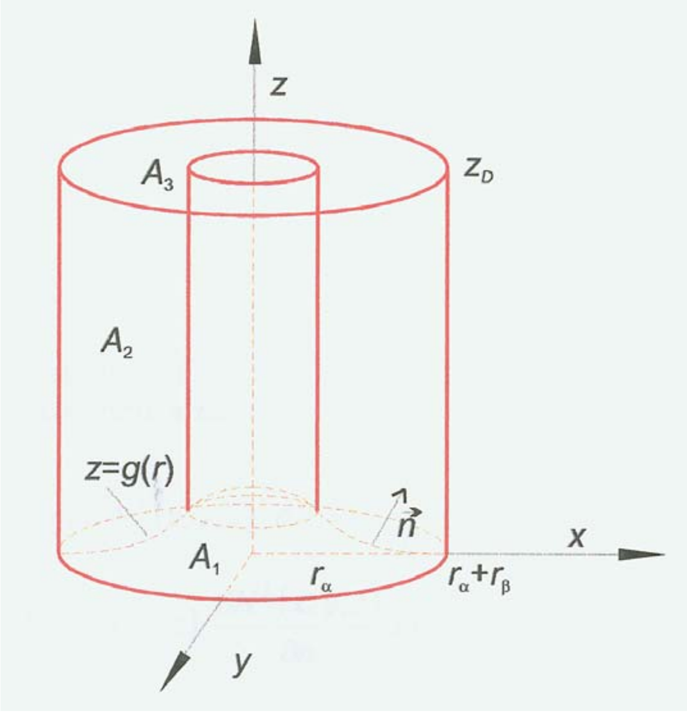


FIG. 21

z – variable Integration

lamellar growth

$$\overline{P}_L = \int_0^{S_\alpha+S_\beta}\int_{g(x)}^{z_D}\left|grad.N^L(x,z)\right|^2 dzdx = -\frac{v}{2D}\int_0^{S_\alpha+S_\beta}\left[\delta N^L(x,g(x))\right]^2 dx$$

$$+\int_0^{S_\alpha}\delta N^L(x,g(x))\frac{v}{D}\left(N^L(x,g(x))-N^\alpha(x,g(x))\right)dx$$

$$+\int_{S_\alpha}^{S_\alpha+S_\beta}\delta N^L(x,g(x))\frac{v}{D}\left(N^\beta(x,g(x))-N^L(x,g(x))\right)dx$$

scheme from FIG. 20 and some conditions given by J-H theory are taken into account

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

Deviation from thermodynamic equilibrium

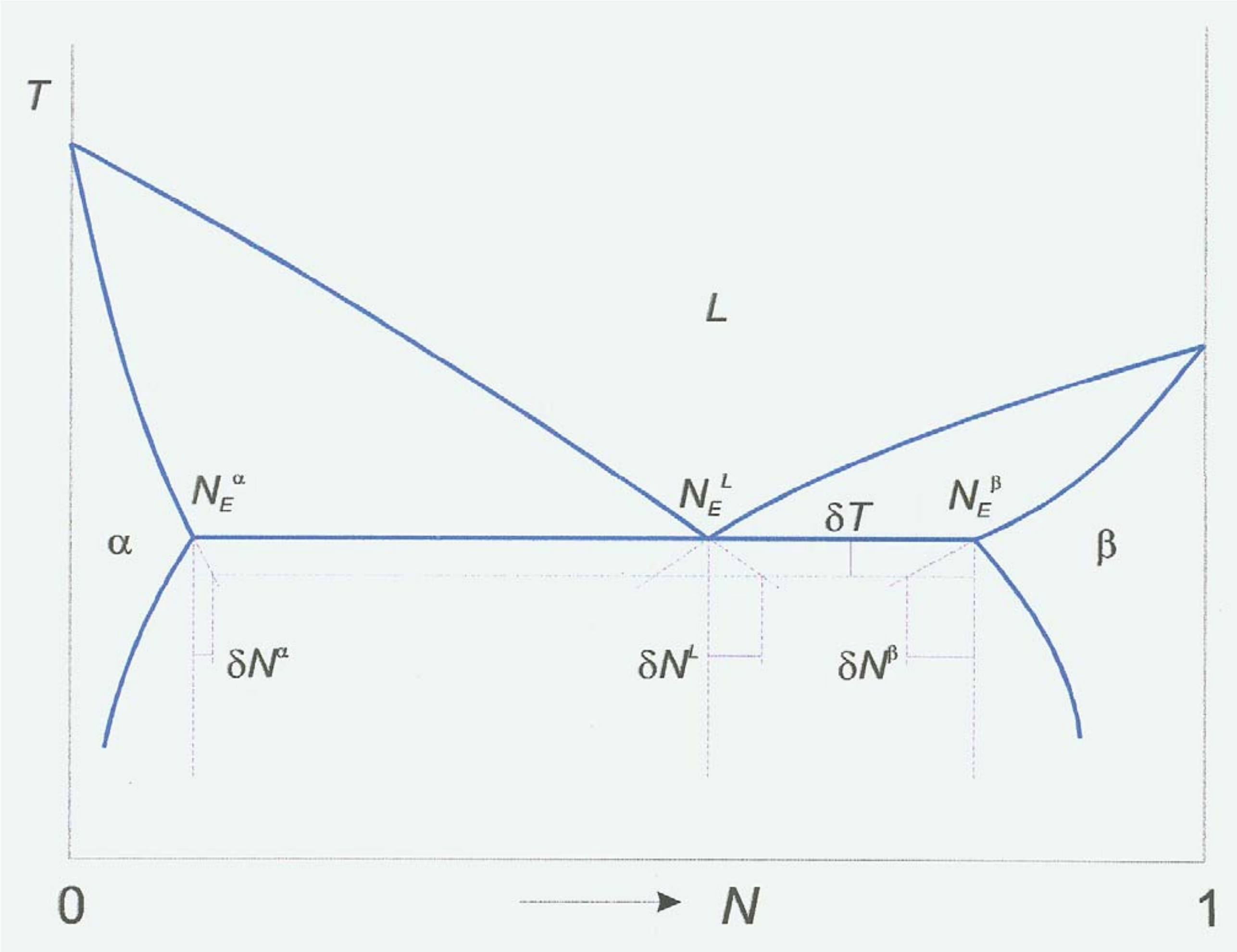
$$N^{L} = N_{E}^{L} \pm \delta N^{L}$$

$$N^{\alpha} = N_{E}^{\alpha} + \delta N^{\alpha}$$

$$N^{\beta} = N_{E}^{\beta} - \delta N^{\beta}$$

FIG. 22

arbitrary
phase diagram



z – variable Integration

lamellar growth

$$\overline{P}_L = \int_0^{S_\alpha+S_\beta}\int_{g(x)}^{z_D}\left|grad.N^L(x,z)\right|^2 dz dx = \frac{v}{2D}\int_0^{S_\alpha+S_\beta}\left[\delta N^L(x,g(x))\right]^2 dx$$

$$+\frac{v}{D}\left[\left(N_E^L - N_E^\alpha\right)\int_0^{S_\alpha}\delta N^L(x,g(x))dx + \left(N_E^\beta - N_E^L\right)\int_{S_\alpha}^{S_\alpha+S_\beta}\delta N^L(x,g(x))dx\right]$$

$$-\frac{v}{D}\left[\int_0^{S_\alpha}\delta N^L(x,g(x))\delta N^\alpha(x,g(x))dx + \int_{S_\alpha}^{S_\alpha+S_\beta}\delta N^L(x,g(x))\delta N^\beta(x,g(x))dx\right]$$

some parameters from FIG. 22 are introduced into integral

z – variable Integration

rod-like growth

$$\overline{P}_R = \iiint_V \left| grad.N^L(x,y,z) \right|^2 dV = -\frac{\pi v}{D} \int_0^{r_\alpha + r_\beta} \left[\delta N^L(r, g(r)) \right]^2 r\, dr$$

$$+ \frac{2\pi v}{D} \int_0^{r_\alpha} \delta N^L(r, g(r)) \left[N^L(r, g(r)) - N^\alpha(r, g(r)) \right] r\, dr$$

$$+ \frac{2\pi v}{D} \int_{r_\alpha}^{r_\alpha + r_\beta} \delta N^L(r, g(r)) \left[N^\beta(r, g(r)) - N^L(r, g(r)) \right] r\, dr$$

scheme from FIG. 21 and some conditions given by J-H theory are taken into account

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

z – variable Integration

rod-like growth

$$\overline{P}_R = \iiint_V \left| grad.N^L(x,y,z) \right|^2 dV = -\frac{\pi v}{D} \int_0^{r_\alpha + r_\beta} \left[\delta N^L(r, g(r)) \right]^2 r\, dr$$

$$+\frac{2\pi v}{D}\left[\left(N_E^L - N_E^\alpha \right) \int_0^{r_\alpha} \delta N^L(r, g(r)) r\, dr + \left(N_E^\beta - N_E^L \right) \int_{r_\alpha}^{r_\alpha + r_\beta} \delta N^L(r, g(r)) r\, dr \right]$$

$$-\frac{2\pi v}{D}\left[\int_0^{r_\alpha} \delta N^L(r, g(r)) \delta N^\alpha(r, g(r)) r\, dr + \int_{r_\alpha}^{r_\alpha + r_\beta} \delta N^L(r, g(r)) \delta N^\beta(r, g(r)) r\, dr \right]$$

some parameters from FIG. 22 are introduced into integral

Capillarity parameters

lamellar growth

definitions of the δN^{α}, δN^{β} parameters, FIG. 22

$$\delta N^{\alpha}(x,g(x)) = k_{\alpha}\delta N^{L}(x,g(x)) + \frac{k_{\alpha}}{m_{\alpha}}\frac{T_E}{L_{\alpha}}\sigma_{\alpha}^{L}(x,g(x))\frac{1}{R_{\alpha}(x,g(x))}$$

simplifications

$$\delta N^{\beta}(x,g(x)) = k_{\beta}\delta N^{L}(x,g(x)) + \frac{k_{\beta}}{m_{\beta}}\frac{T_E}{L_{\beta}}\sigma_{\beta}^{L}(x,g(x))\frac{1}{R_{\beta}(x,g(x))}$$

$$\frac{1}{R_{\alpha}(x,g(x))} = \hat{K}_{\alpha}(x,g(x)) \qquad \hat{K}_{\alpha}(x,g(x)) = \frac{\sin\theta_{\alpha}^{L}}{S_{\alpha}} \qquad \frac{1}{R_{\beta}(x,g(x))} = \hat{K}_{\beta}(x,g(x)) \qquad \hat{K}_{\beta}(x,g(x)) = \frac{\sin\theta_{\beta}^{L}}{S_{\beta}}$$

$$\sigma_{\beta}^{L}(x,g(x)) = \sigma_{\beta}^{L} \qquad \sigma_{\alpha}^{L}(x,g(x)) = \sigma_{\alpha}^{L}$$

additionally

$$\frac{1}{m_{\alpha}}\frac{T_E}{L_{\alpha}}\sigma_{\alpha}^{L} = M_{\alpha}^{L} \qquad \frac{1}{m_{\beta}}\frac{T_E}{L_{\beta}}\sigma_{\beta}^{L} = M_{\beta}^{L}$$

Capillarity parameters
Entropy production

lamellar growth

capillarity parameters are introduced

$$\overline{P}_L = \frac{v}{D}\left[\left(N_E^L - N_E^\alpha\right)\int_0^{S_\alpha} \delta N^L(x,g(x))dx + \left(N_E^\beta - N_E^L\right)\int_{S_\alpha}^{S_\alpha+S_\beta} \delta N^L(x,g(x))dx\right]$$

$$-\frac{v}{D}\left[k_\alpha \int_0^{S_\alpha}\left[\delta N^L(x,g(x))\right]^2 dx + k_\alpha M_\alpha^L \frac{\sin\theta_\alpha^L}{S_\alpha}\int_0^{S_\alpha} \delta N^L(x,g(x))dx\right]$$

$$-\frac{v}{D}\left[k_\beta \int_{S_\alpha}^{S_\alpha+S_\beta}\left[\delta N^L(x,g(x))\right]^2 dx + k_\beta M_\beta^L \frac{\sin\theta_\beta^L}{S_\beta}\int_{S_\alpha}^{S_\alpha+S_\beta} \delta N^L(x,g(x))dx\right]$$

$$+\frac{v}{2D}\left[\int_0^{S_\alpha}\left[\delta N^L(x,g(x))\right]^2 dx + \int_{S_\alpha}^{S_\alpha+S_\beta}\left[\delta N^L(x,g(x))\right]^2 dx\right]$$

Capillarity parameters

rod-like growth

definitions of the δN^{α}, δN^{β} parameters, FIG. 22

$$\delta N^{\alpha}(r,g(r)) = k_{\alpha}\delta N^{L}(r,g(r)) + \frac{k_{\alpha}}{m_{\alpha}}\frac{T_E}{L_{\alpha}}\sigma_{\alpha}^{R}(r,g(r))\frac{1}{R_{\alpha}(r,g(r))}$$

$$\delta N^{\beta}(r,g(r)) = k_{\beta}\delta N^{L}(r,g(r)) + \frac{k_{\beta}}{m_{\beta}}\frac{T_E}{L_{\beta}}\sigma_{\beta}^{R}(r,g(r))\frac{1}{R_{\beta}(r,g(r))}$$

simplifications

↓

$$\frac{1}{R_{\alpha}(r,g(r))} = \hat{K}_{\alpha}(r,g(r))$$

$$\hat{K}_{\alpha}(r,g(r)) = \frac{2\sin\theta_{\alpha}^{L}}{r_{\alpha}}$$

$$\frac{1}{R_{\beta}(r,g(r))} = \hat{K}_{\beta}(r,g(r))$$

$$\hat{K}_{\beta}(r,g(r)) = \frac{2r_{\alpha}\sin\theta_{\beta}^{L}}{(r_{\alpha}+r_{\beta})^{2} - r_{\alpha}^{2}}$$

$$\sigma_{\alpha}^{R}(r,g(r)) = \sigma_{\alpha}^{R} \qquad \sigma_{\beta}^{R}(r,g(r)) = \sigma_{\beta}^{R}$$

additionally

$$\frac{1}{m_{\alpha}}\frac{T_E}{L_{\alpha}}\sigma_{\alpha}^{R} = M_{\alpha}^{R} \qquad \frac{1}{m_{\beta}}\frac{T_E}{L_{\beta}}\sigma_{\beta}^{R} = M_{\beta}^{R}$$

Capillarity parameters
Entropy production

rod-like growth

capillarity parameters are introduced

$$\overline{P}_R = \frac{2\pi v}{D}\left[\left(N_E^L - N_E^\alpha\right)\int_0^{r_\alpha} \delta N^L(r,g(r))rdr + \left(N_E^\beta - N_E^L\right)\int_{r_\alpha}^{r_\alpha+r_\beta}\delta N^L(r,g(r))rdr\right]$$

$$- \frac{2\pi v}{D}\left[k_\alpha \int_0^{r_\alpha}\left[\delta N^L(r,g(r))\right]^2 rdr + k_\alpha M_\alpha^R \frac{2\sin\theta_\alpha^R}{r_\alpha}\int_0^{r_\alpha}\delta N^L(r,g(r))rdr\right]$$

$$- \frac{2\pi v}{D}\left[k_\beta \int_{r_\alpha}^{r_\alpha+r_\beta}\left[\delta N^L(r,g(r))\right]^2 rdr + k_\beta M_\beta^R \frac{2r_\alpha \sin\theta_\beta^R}{\left(r_\alpha + r_\beta\right)^2 - r_\alpha^{\ 2}}\int_{r_\alpha}^{r_\alpha+r_\beta}\delta N^L(r,g(r))rdr\right]$$

$$+ \frac{\pi v}{D}\left[\int_0^{r_\alpha}\left[\delta N^L(r,g(r))\right]^2 rdr + \int_{r_\alpha}^{r_\alpha+r_\beta}\left[\delta N^L(r,g(r))\right]^2 rdr\right]$$

Real shape of the solid / liquid interface

analytical solutions for $\delta N^L(x,g(x))$ and $\delta N^R(r,g(r))$ are unknown but J-H theory gives solution for $\delta N^L(x,0)$ and $\delta N^R(r,0)$ thus, the following equations are introduced

lamellar growth

$$\int_0^{S_\alpha} \delta N^L(x,0)\,dx = \frac{2\left(S_\alpha + S_\beta\right)^2 v N_0 P^*}{D}$$

$$\int_{S_\alpha}^{S_\alpha+S_\beta} \delta N^L(x,0)\,dx = \frac{2\left(S_\alpha + S_\beta\right)^2 v N_0 P^*}{D}$$

$$P^* = \sum_{n=1}^{\infty}\left(\frac{1}{n\pi}\right)^3 \sin^2 \frac{n\pi S_\alpha}{S_\alpha + S_\beta}$$

rod-like growth

$$\int_0^{r_\alpha} \delta N^L(r,0)\,r\,dr = \frac{2\left(r_\alpha + r_\beta\right)^3 V_\alpha v N_0 E}{D}$$

$$\int_{r_\alpha}^{r_\alpha+r_\beta} \delta N^L(r,0)\,r\,dr = \frac{2\left(r_\alpha + r_\beta\right)^3 V_\alpha v N_0 E}{D}$$

$$E = \sum_{n=1}^{\infty} \frac{J_1{}^2\left(\frac{\gamma_n r_\alpha}{r_\alpha + r_\beta}\right)}{\gamma_n{}^3 J_0{}^2\left(\gamma_n\right)}$$

Real shape of the solid / liquid interface

analytical solutions for $\delta N^{L}(x,g(x))$ and $\delta N^{R}(r,g(r))$ are unknown
but J-H theory gives solution for $\delta N^{L}(x,0)$ and $\delta N^{R}(r,0)$
thus, the following equations are introduced

lamellar growth

$$\int_0^{S_\alpha}\left[\delta N^{L}(x,0)\right]^2 dx=\frac{4\left(S_\alpha+S_\beta\right)^3 v^2 N_0^{\,2}}{D^2}\left[\frac{V_\alpha\Theta}{2}+T^*\right]$$

$$\int_{S_\alpha}^{S_\alpha+S_\beta}\left[\delta N^{L}(x,0)\right]^2 dx=\frac{4\left(S_\alpha+S_\beta\right)^3 v^2 N_0^{\,2}}{D^2}\left[\frac{V_\beta\Theta}{2}-T^*\right]$$

$$\Theta=\sum_{n=1}^{\infty}\left(\frac{1}{n\pi}\right)^4 \sin^2\left(\frac{n\pi S_\alpha}{S_\alpha+S_\beta}\right)$$

rod-like growth

$$\int_0^{r_\alpha}\left[\delta N^{L}(r,0)\right]^2 r\,dr=\frac{2\left(r_\alpha+r_\beta\right)^4 V_\alpha v^2 N_0^{\,2}}{D^2}\left[V_\alpha U+4\sqrt{V_\alpha}\,H^*\right]$$

$$\int_{r_\alpha}^{r_\alpha+r_\beta}\left[\delta N^{L}(r,0)\right]^2 r\,dr=\frac{2\left(r_\alpha+r_\beta\right)^4 V_\alpha v^2 N_0^{\,2}}{D^2}\left[S^*-V_\alpha U-4\sqrt{V_\alpha}\,H^*\right]$$

$$S^*=\sum_{n=1}^{\infty}\frac{J_1^{\,2}\left(\frac{\gamma_n r_\alpha}{r_\alpha+r_\beta}\right)}{\gamma_n^{\,4} J_0^{\,2}\left(\gamma_n\right)}$$

Real shape of the solid / liquid interface

the following equations are introduced

lamellar growth

$$T^* = \sum_{n=2}^{\infty}\sum_{k=1}^{n-1}\left(\frac{1}{n}\right)^2\left(\frac{1}{k}\right)^2\left(\frac{1}{\pi}\right)^5 \sin\frac{n\pi S_\alpha}{S_\alpha+S_\beta}\sin\frac{k\pi S_\alpha}{S_\alpha+S_\beta}\left[\frac{1}{n+k}\sin\frac{(n+k)\pi S_\alpha}{S_\alpha+S_\beta}+\frac{1}{n-k}\sin\frac{(n-k)\pi S_\alpha}{S_\alpha+S_\beta}\right] + 0.5\sum_{n=1}^{\infty}\left(\frac{1}{n\pi}\right)^5\sin^3\frac{n\pi S_\alpha}{S_\alpha+S_\beta}\cos\frac{n\pi S_\alpha}{S_\alpha+S_\beta}$$

rod-like growth

$$U = \sum_{n=1}^{\infty}\frac{J_1^{\,2}\left(\frac{\gamma_n r_\alpha}{r_\alpha+r_\beta}\right)}{\gamma_n^{\,4}J_0^{\,4}(\gamma_n)}\left[J_1^{\,2}\left(\frac{\gamma_n r_\alpha}{r_\alpha+r_\beta}\right)+J_0^{\,2}\left(\frac{\gamma_n r_\alpha}{r_\alpha+r_\beta}\right)+J_0^{\,2}\left(\frac{\gamma_n r_\alpha}{r_\alpha+r_\beta}\right)\right]$$

$$H^* = \sum_{n=2}^{\infty}\sum_{k=1}^{n-1}\frac{J_1\left(\frac{\gamma_n r_\alpha}{r_\alpha+r_\beta}\right)J_1\left(\frac{\gamma_k r_\alpha}{r_\alpha+r_\beta}\right)}{\gamma_n^{\,2}J_0^{\,2}(\gamma_n)\gamma_k^{\,2}J_0^{\,2}(\gamma_k)}\;\frac{\gamma_n J_0\left(\frac{\gamma_k r_\alpha}{r_\alpha+r_\beta}\right)J_1\left(\frac{\gamma_n r_\alpha}{r_\alpha+r_\beta}\right)-\gamma_k J_0\left(\frac{\gamma_n r_\alpha}{r_\alpha+r_\beta}\right)J_1\left(\frac{\gamma_k r_\alpha}{r_\alpha+r_\beta}\right)}{\gamma_n^{\,2}-\gamma_k^{\,2}}$$

Entropy production

lamellar growth

after some rearrangements

$$\overline{P}_L = W_1 \frac{v}{S_\alpha + S_\beta} + W_2 \frac{v}{\left(S_\alpha + S_\beta\right)^2} + W_3 v^2 + W_4 v^2 \left(S_\alpha + S_\beta\right) + W_5 v^3 \left(S_\alpha + S_\beta\right)^2$$

where ➔

$$W_1 = \left(N_E^L - N_E^\alpha\right)\frac{M_\alpha^L}{D}\sin\theta_\alpha^L + \left(N_E^\beta - N_E^L\right)\frac{M_\beta^L}{D}\sin\theta_\beta^L$$

$$W_2 = \left(0.5 - 2k_\alpha\right)\frac{\left(M_\alpha^L\right)^2 \sin^2\theta_\alpha^L}{DV_\alpha} + \left(0.5 - 2k_\beta\right)\frac{\left(M_\beta^L\right)^2 \sin^2\theta_\beta^L}{DV_\beta}$$

$$W_3 = \left\{\left(1 - 3k_\alpha\right)\frac{M_\alpha^L \sin\theta_\alpha^L}{V_\alpha} - \left(1 - 3k_\beta\right)\frac{M_\beta^L \sin\theta_\beta^L}{V_\beta}\right\}\frac{2N_0 P^*}{D^2}$$

$$W_4 = \left(N_E^\beta - N_E^\alpha\right)\frac{2N_0 P^*}{D^2}$$

$$W_5 = \left\{0.25\Theta - 0.5\left(k_\alpha V_\alpha + k_\beta V_\beta\right)\Theta - \left(k_\alpha - k_\beta\right)T^*\right\}\frac{4N_0^2}{D^2}$$

Entropy production

rod-like growth

after some rearrangements

$$\overline{P}_R = V_1 \frac{v}{r_\alpha + r_\beta} + V_2 \frac{v}{\left(r_\alpha + r_\beta\right)^2} + V_3 v^2 + V_4 v^2 \left(r_\alpha + r_\beta\right) + V_5 v^3 \left(r_\alpha + r_\beta\right)^2$$

where ➔

$$V_1 = \left(N_E^L - N_E^\alpha\right) \frac{2M_\alpha^R \sqrt{V_\alpha}}{D} \sin\theta_\alpha^R + \left(N_E^\beta - N_E^L\right) \frac{2M_\beta^R \sqrt{V_\alpha}}{D} \sin\theta_\beta^R$$

$$V_2 = \left(1 - 4k_\alpha\right) \frac{2\left(M_\alpha^R\right)^2 \sin^2\theta_\alpha^R}{D} + \left(1 - 4k_\beta\right) \frac{2\left(M_\beta^R\right)^2 \sin^2\theta_\beta^R}{D}$$

$$V_3 = 2N_0 E \sqrt{V_\alpha} \left\{ 4\left(1 - 3k_\alpha\right) \frac{M_\alpha^R \sin\theta_\alpha^R}{D^2} - 4\left(1 - 3k_\beta\right) \frac{M_\beta^R \sin\theta_\beta^R}{D^2} \right\}$$

$$V_4 = \left(N_E^\beta - N_E^\alpha\right) \frac{4V_\alpha N_0 E}{D^2}$$

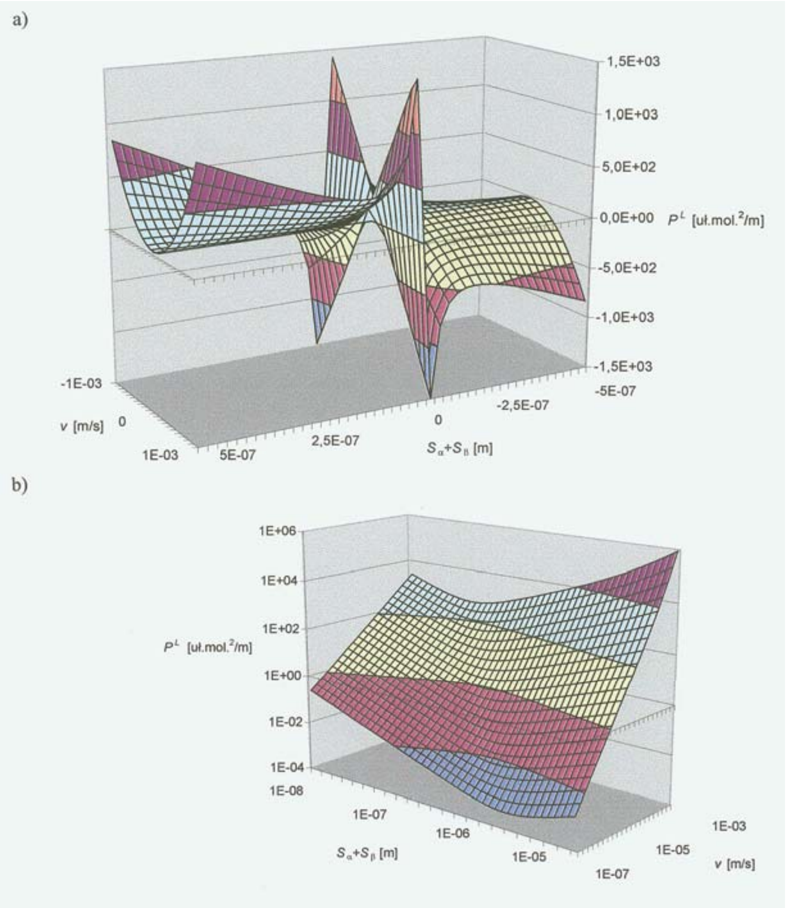
$$V_5 = \left\{ 0.5S^* - k_\beta S^* - \left(k_\alpha - k_\beta\right)\left(V_\alpha U + 4\sqrt{V_\alpha} H^*\right) \right\} \frac{4V_\alpha N_0^{\ 2}}{D^3}$$

Entropy production Visualization

entropy production calculated as a function of v and ($S_\alpha + S_\beta$)

lamellar growth

$$\overline{P}_L(v,(S_\alpha + S_\beta))$$



entropy production
a/ general view
b/ for real range of growth rates, v

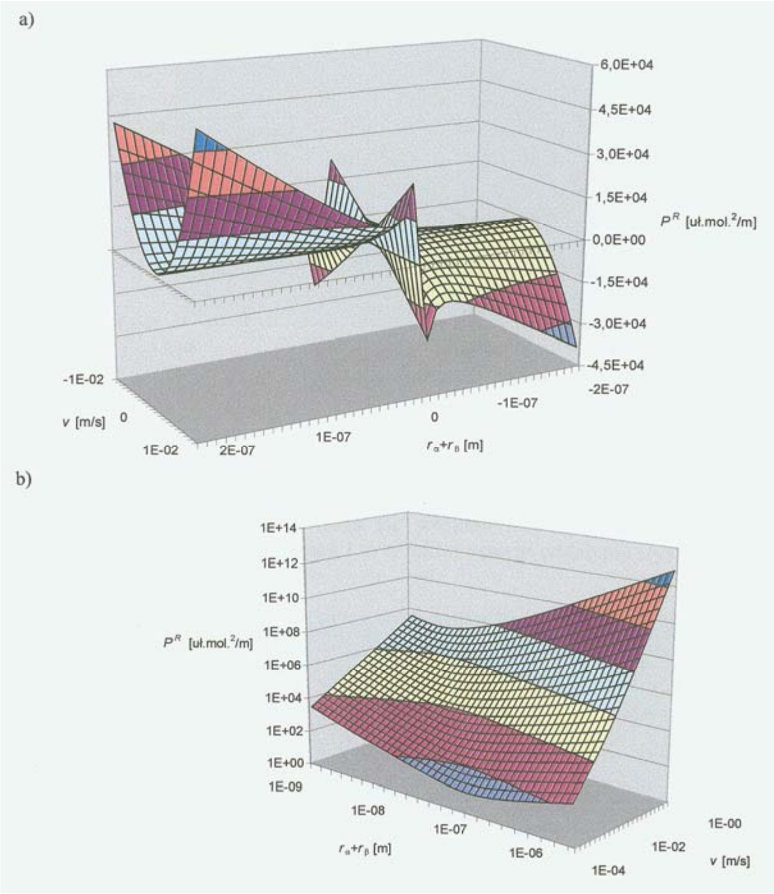
FIG. 23

Entropy production Visualization

entropy production calculated as a function of v and $(r_\alpha + r_\beta)$

rod-like growth

$$\overline{P}_R(v,(r_\alpha + r_\beta))$$

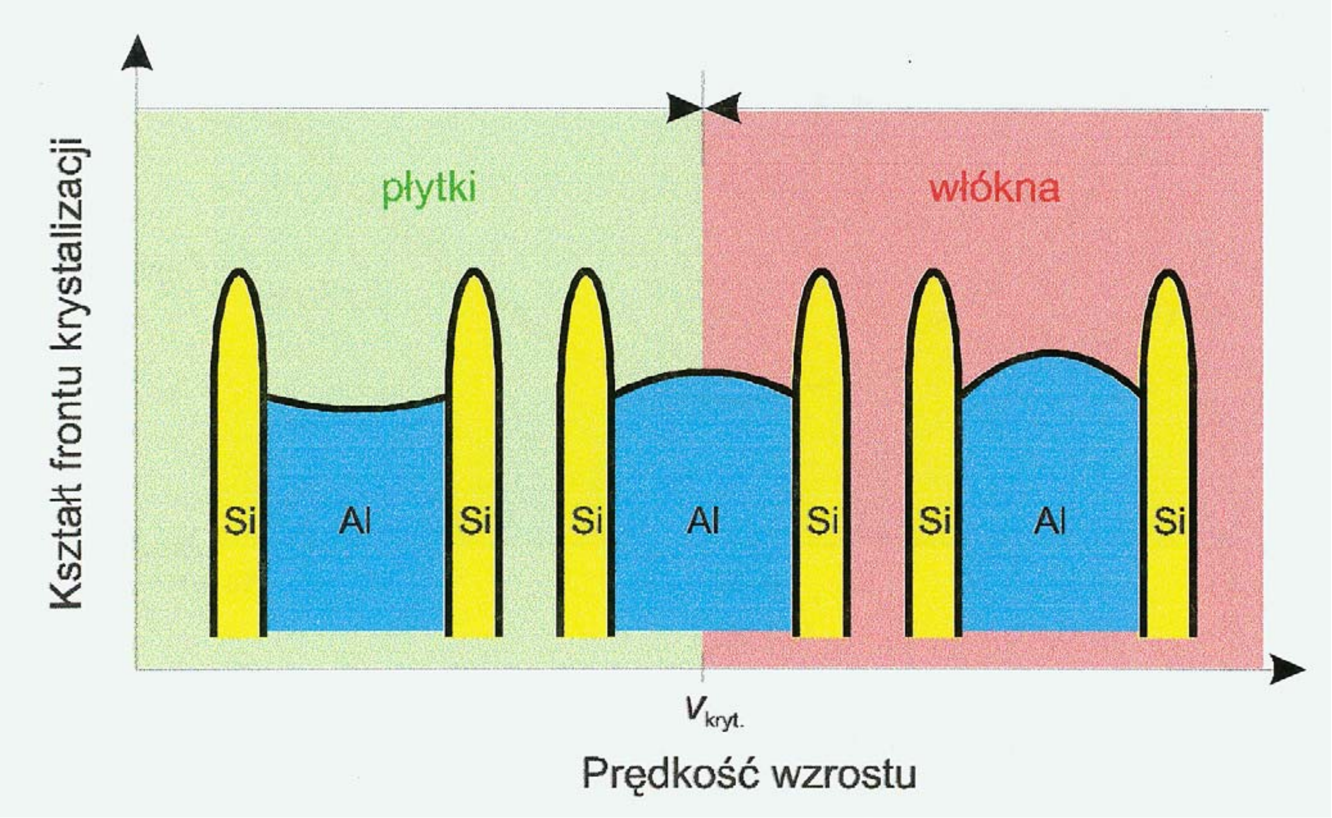


entropy production
a/ general view
b/ for real range of growth rates, v

FIG. 24

Transformation: lamella-rod
Shape of the s / l interface

varying curvature of the s / l interface resulting in some changes of specific surface free energy (surface tension) with an adequate behaviour of mechanical equilibrium at a triple point



płytki = lamellae
włókna = rods
kształt = shape
prędkość = rate

FIG. 25

Entropy production minimum
Lamellae

solidification occurs at the entropy production minimum

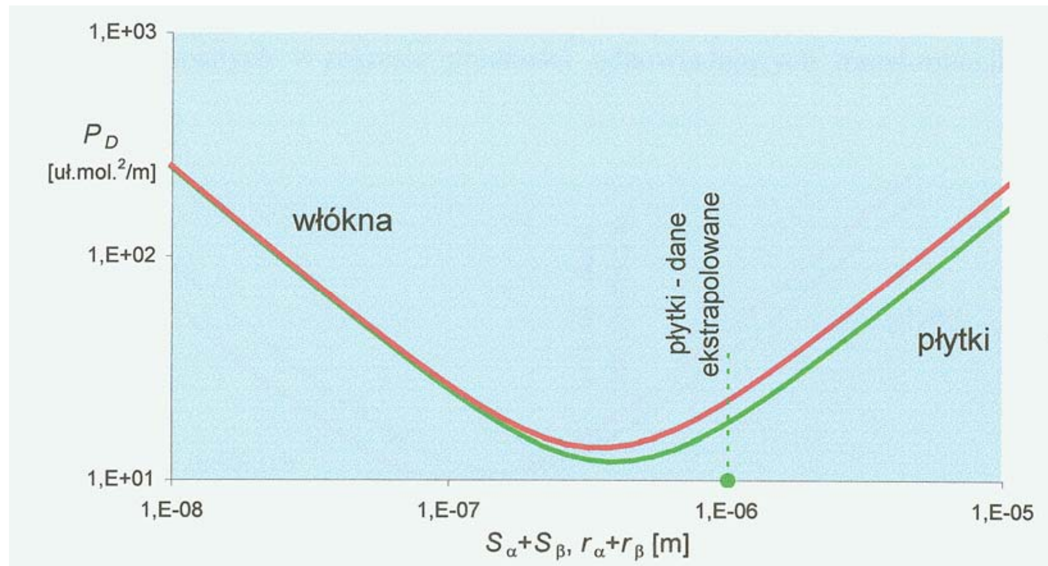
FIG. 26

lamellar growth

rod-like growth

- green point:
  average lamellar spacing
  as measured

płytki = lamellae
włókna = rods



entropy production calculated for a range of inter-lamellar or inter-rod spacing and adequate mechanical equilibrium defined at a triple point, FIG. 25, v = 100 μm/s

RESULT - minimum for lamellae is below minimum for rods !

Entropy production minimum Transformation

solidification occurs at the entropy production minimum

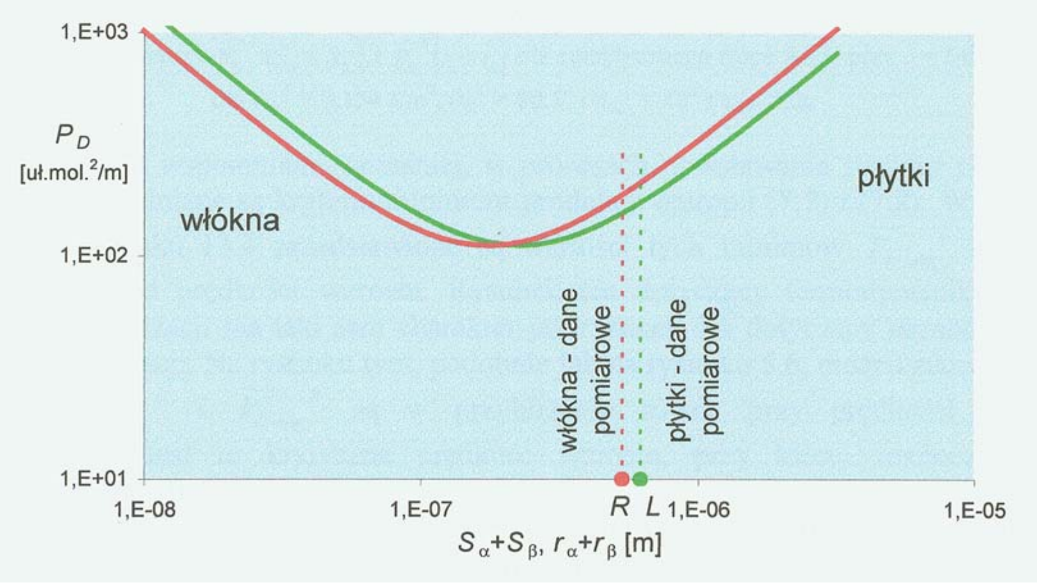
FIG. 27

lamellar growth

rod-like growth

płytki = lamellae
włókna = rods

- green point:
  average lamellar spacing
- red point
  average rod-like spacing
  as measured



entropy production calculated for a range of inter-lamellar or inter-rod spacing and adequate mechanical equilibrium defined at a triple point, FIG. 25, v = 400 μm/s

RESULT - minimum for lamellae is at the same level as minimum for rods !

Entropy production minimum
Rods

solidification occurs at the entropy production minimum

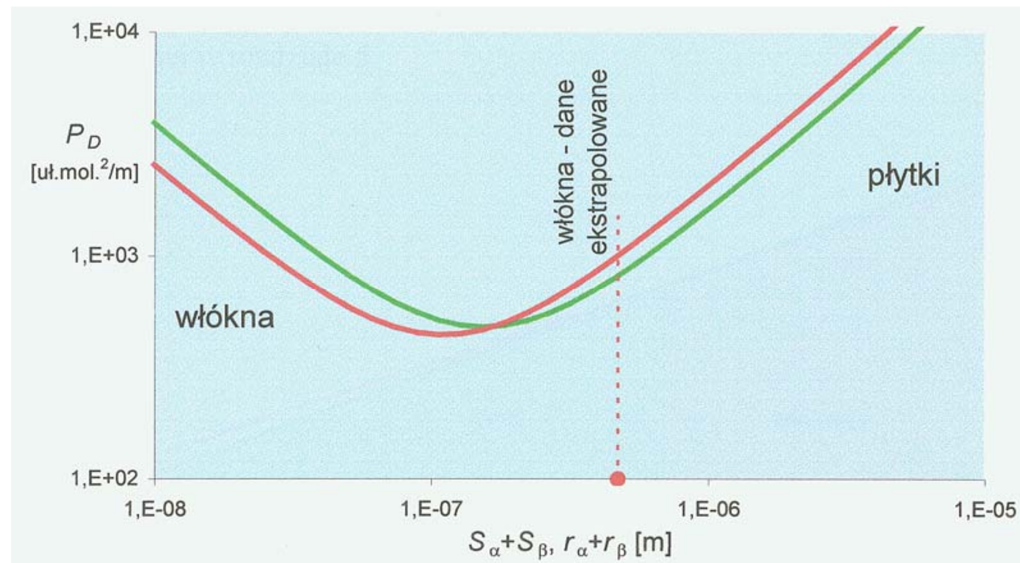
FIG. 28

lamellar growth

rod-like growth

- red point:
average rod-like spacing
as measured

płytki = lamellae
włókna = rods



entropy production calculated for a range of inter-lamellar or inter-rod spacing and adequate mechanical equilibrium defined at a triple point, FIG. 25, v = 1000 μm/s

RESULT - minimum for rods is below minimum for lamellae !

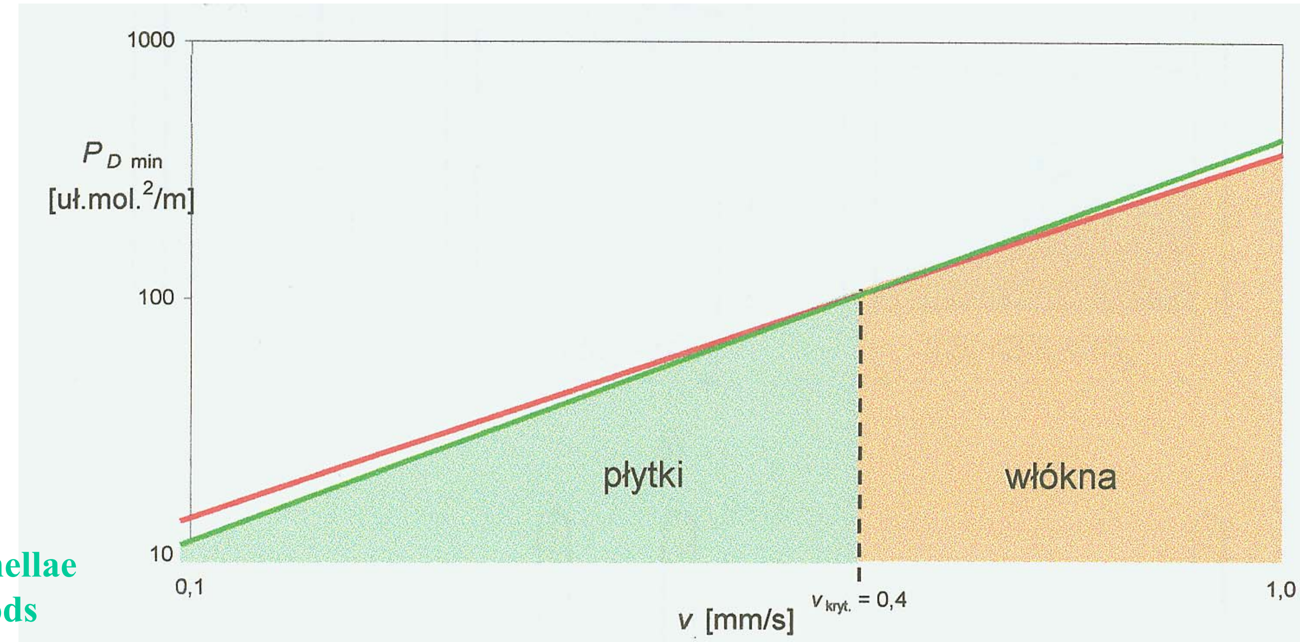
Threshold growth rate

lamellar growth

rod-like growth

FIG. 29

płytki = lamellae
włókna = rods



minima of entropy production for a range of growth rates 100 – 1000 μm/s and adequate mechanical equilibrium defined at a triple point, FIG. 25

RESULT – threshold growth rate v_{kryt} is estimated !
operating range is not yet placed

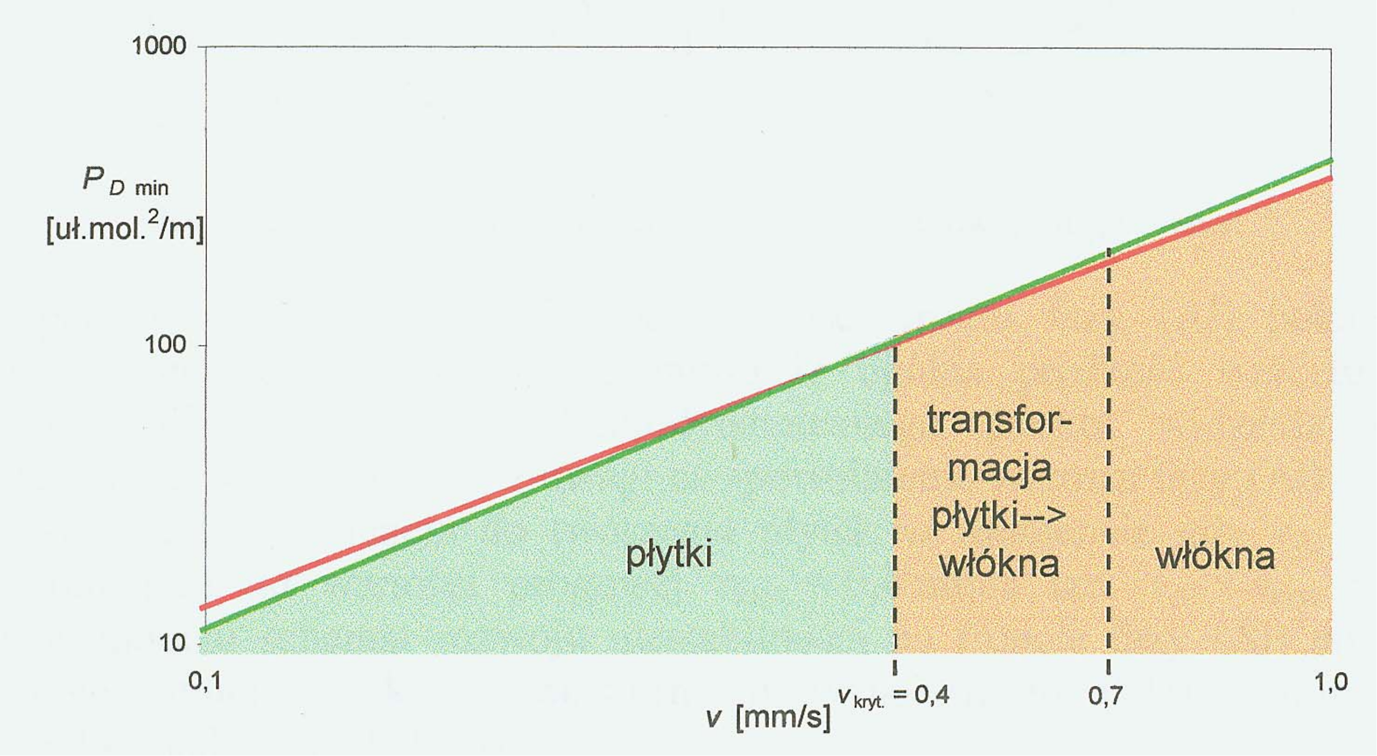
Range of growth rates Transformation: lamella - rod

Experimentally confirmed range of growth rates for transformation (operating range)

lamellar growth

rod-like growth

FIG. 30



minima of entropy production for a range of growth rates of 100 – 1000 μm/s and adequate mechanical equilibrium defined at a triple point, FIG. 25

Range of growth rates for transformation Irregular structure

destabilization of s / l interface of the (Al) – phase for irregular structure formation

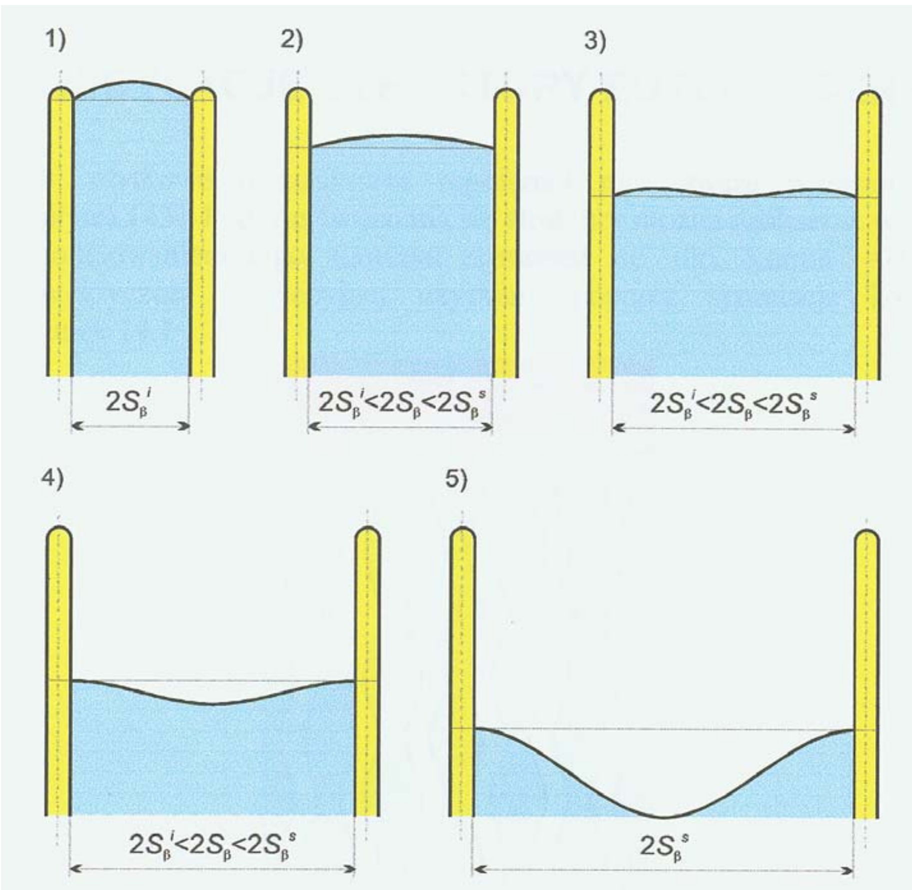


FIG. 31

explanation for the coexistence of **lamellae** and **rods** within the operating range

locally, the structure has slower growth rate where destabilization is greater
this promotes the formation of lamellae

Irregular+regular structure formation Scheme

destabilization of s/l interface of the (Al) – phase (β) for irregular structure formation

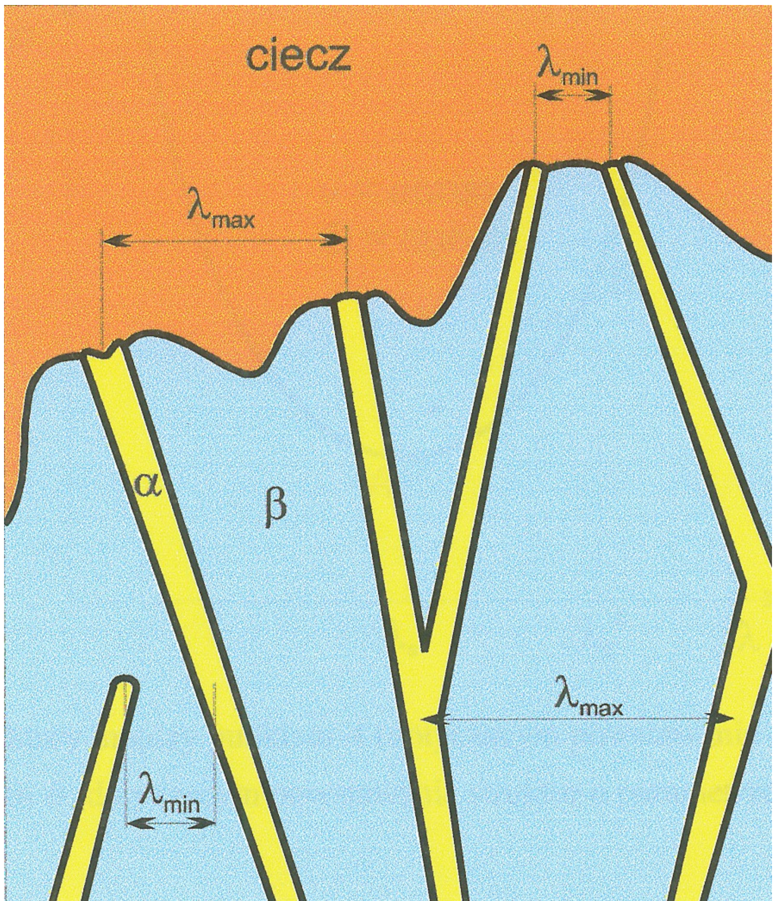


FIG. 32

two parameters are distinguished
λ_{min} referred to regular structure formation
and entropy production minimum
λ_{max} referred to maximum destabilization
of the s / l interface
of the (Al) – phase, (β)
and marginal stability

RESULT – oscillations of spacing

Oscillations of spacing
Entropy production

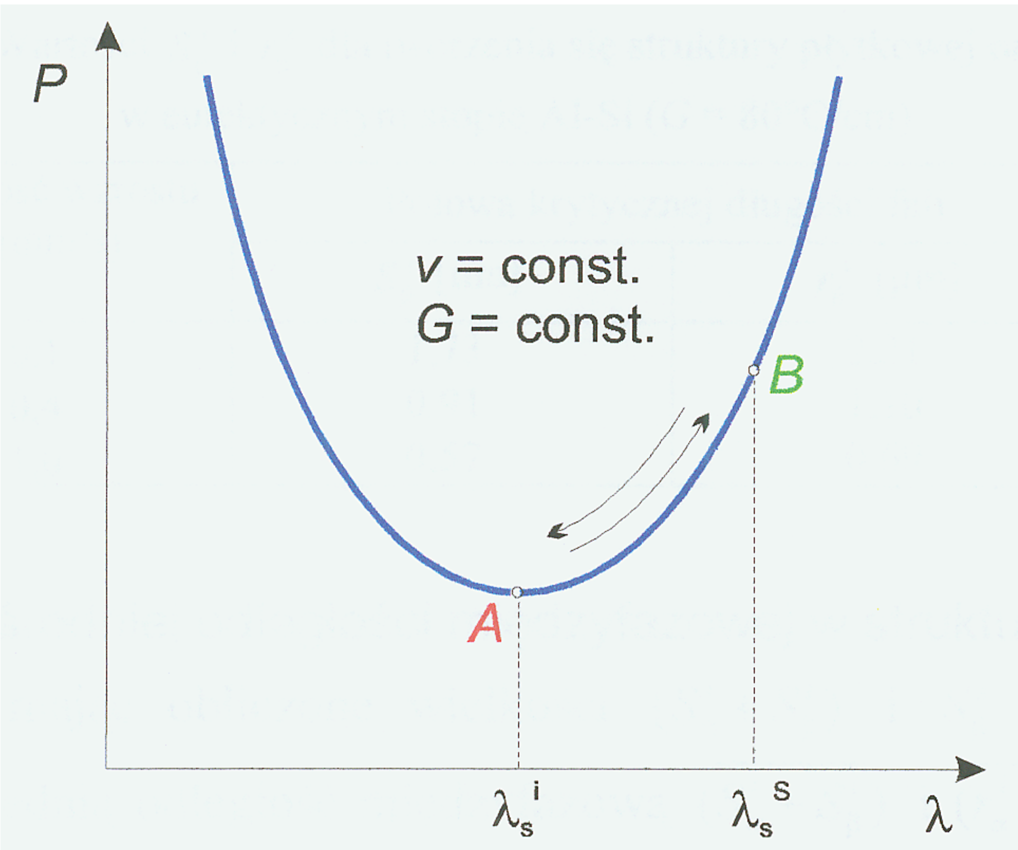


FIG. 33

two parameters are distinguished

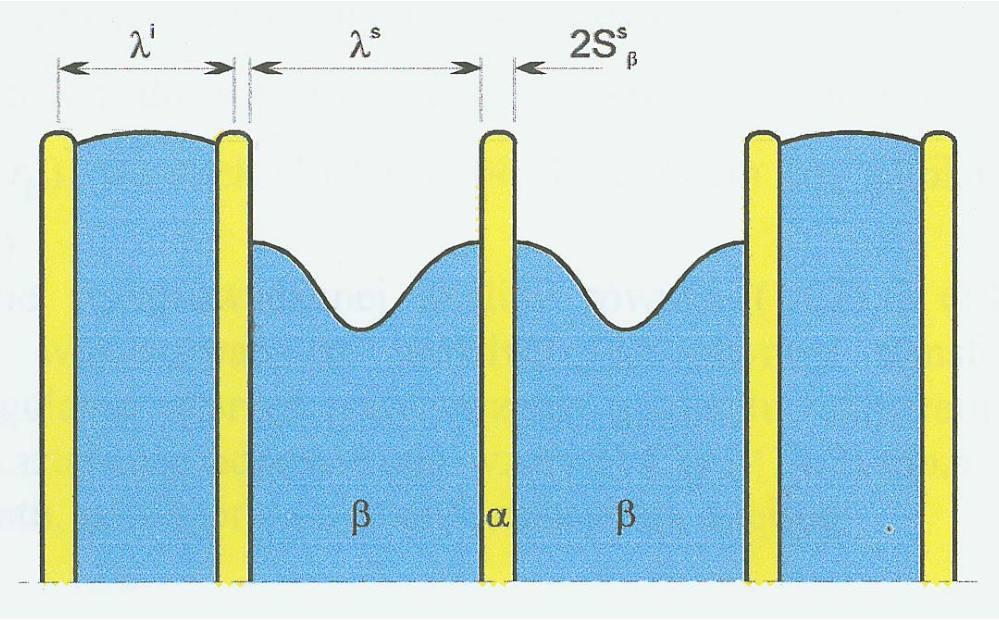
$\lambda_{min} = \lambda_s^i$ referred to regular structure formation and entropy production minimum – point **A**

$\lambda_{max} = \lambda_s^S$ referred to maximum destabilization of s / l interface of the (Al) – phase, (β), and criterion of marginal stability – point **B**

average lamellar spacing λ, is measured within the real structure, FIG. 26

Oscillations of spacing
Simplified scheme of structure

destabilization of s / l interface of the (Al) – phase for irregular structure formation



two parameters are distinguished
$\lambda_{min} = \lambda^{i}$ referred to regular structure formation
and minimum entropy production
$\lambda_{max} = \lambda^{S}$ referred to maximum destabilization
of s / l interface of the (Al) – phase, (β)
and criterion of marginal stability

FIG. 34

RESULT – oscillations of spacing are responsible for local changes of growth rates and finally for replacing the threshold growth rate by the operating range

Entropy production Scheme

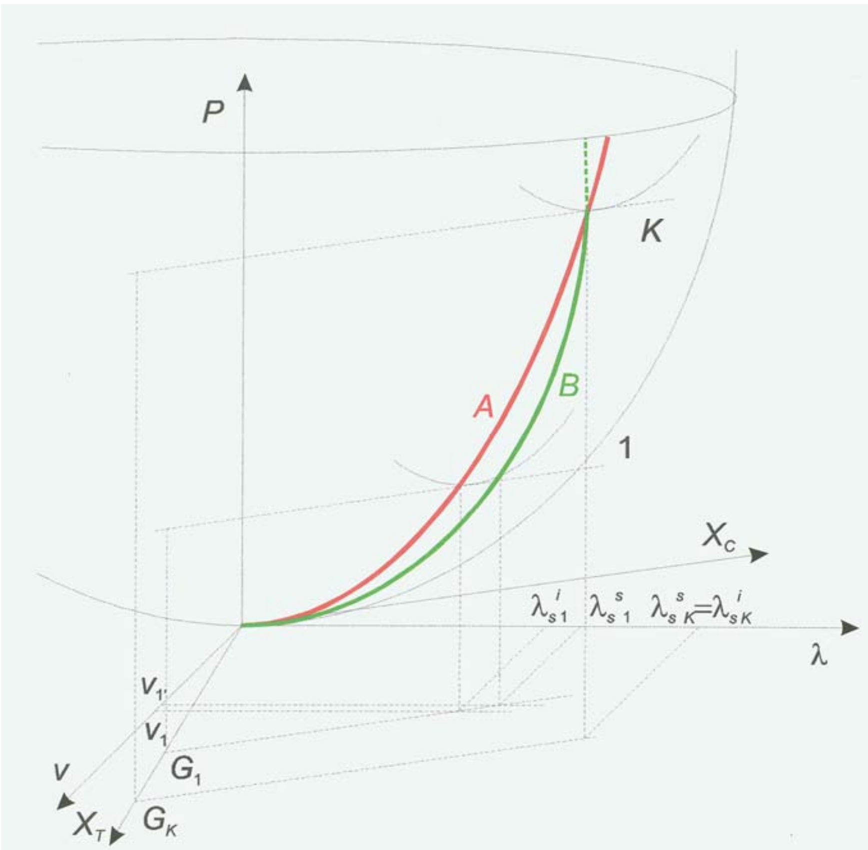


FIG. 35

A – trajectory of entropy production minima
B – trajectory of points of marginal stability

entropy production versus growth rate, v and temperature gradient, G and simultaneously in function of two thermodynamic forces: X_C, X_T

when, formation of irregular structure vanishes for v ➔ 0 or for G ➔ G_K then, only regular structure can be obtained and oscillation between trajectories vanishes

Growth laws

growth law as a result of the application of criterion of minimum undercooling
Jackson-Hunt theory

lamellar growth

$$\lambda^2 v = const_{J-H}{}^{L}$$

rod-like growth

$$R^2 v = const_{J-H}{}^{R}$$

growth law as a result of the application of criterion of entropy production minimum
current model

lamellar growth

$$2W_5\, v^2 \left(S_\alpha + S_\beta\right)^4 + W_4\, v\left(S_\alpha + S_\beta\right)^3 - W_1 \left(S_\alpha + S_\beta\right) = 2W_2$$

rod-like growth

$$2V_5\, v^2 \left(r_\alpha + r_\beta\right)^4 + V_4\, v\left(r_\alpha + r_\beta\right)^3 - V_1 \left(r_\alpha + r_\beta\right) = 2V_2$$

Growth laws
Generalization

growth law as a result of the application of criterion of minimum undercooling Jackson-Hunt theory

lamellar growth

$$\lambda^2 v = const_{J-H}{}^{L}$$

rod-like growth

$$R^2 v = const_{J-H}{}^{R}$$

growth law as a result of the application of criterion of entropy production minimum current model – simplifications justified (W$_2$, W$_5$ and V$_2$, V$_5$ are neglected)

lamellar growth

$$v\left(S_\alpha + S_\beta\right)^2 = \frac{W_1}{W_4} = const_{C-W}{}^{L}$$

rod-like growth

$$v\left(r_\alpha + r_\beta\right)^2 = \frac{V_1}{V_4} = const_{C-W}{}^{R}$$

RESULT – l.h.s. of growth laws are identical !

Criteria

r.h.s. of adequate growth laws should also be identical

lamellar growth

$$const_{J-H}{}^{L} = const_{C-W}{}^{L}$$

rod-like growth

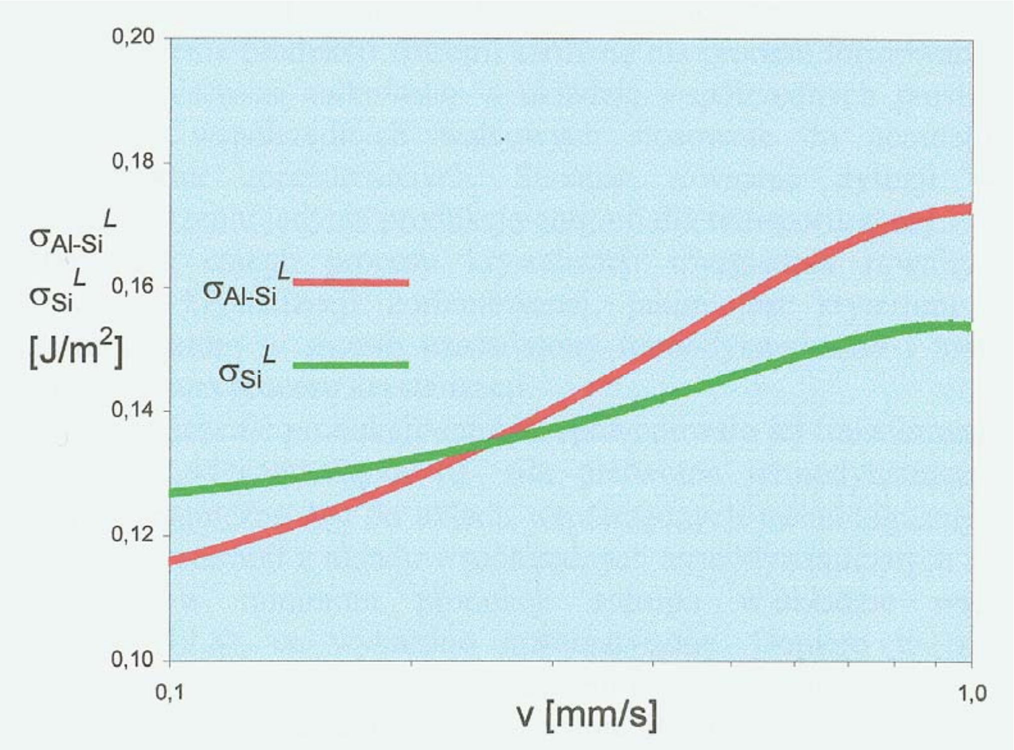
$$const_{J-H}{}^{R} = const_{C-W}{}^{R}$$

RESULT – r.h.s. of growth laws are identical but some simplifications introduced into definitions of W_1, W_4 and V_1, V_4 are necessary

CONCLUSION – the criterion of entropy production minimum is more general than the criterion of minimum undercooling the criterion of free energy minimum seems to be more adequate for the analysis than the criterion of minimum undercooling

Anisotropy

varying mechanical equilibrium is a result of changes of curvature, FIG. 11
but first of all, a result of changes of contribution of crystallographic orientations of s / l interface and α / β inter-phase boundary
CONCLUSION – changes of the specific surface free energy appear, FIG. 11



specific surface free energy of (Si) / liquid interface (surface tension) and free energy of (Al)-(Si) inter-phase boundary versus growth rate as this results from the current model considerations

FIG. 36

Concluding remarks

criterion for the transformation lamella ➔ rod
analogous to the so-called *new criterion for the formation: lamellae or rods*
but origination
from solidification's thermodynamics
(calculation of the entropy production) is required

the criterion (required) should define
the operating range for transformation
but not predict the type of structure
being formed for a given phase diagram: lamellae or rods

an influence of the temperature gradient
on the transformation lamella ➔ rod has not yet been revealed

METRO
MEtallurgical TRaining On-line

Transformation: lamella - rod within oriented eutectic Al-Si

End of the lecture

Education and Culture