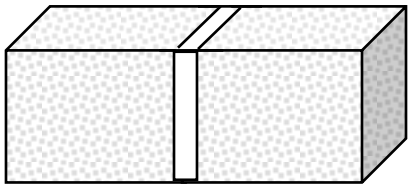
NIST Diffusion Workshop
May 14-15, 2007, Gaithersburg, MD

Single Phase Layer Formation at the Initial Interface of Multiphase Diffusion Couples



John E. Morral
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The Ohio State University
Columbus, Ohio

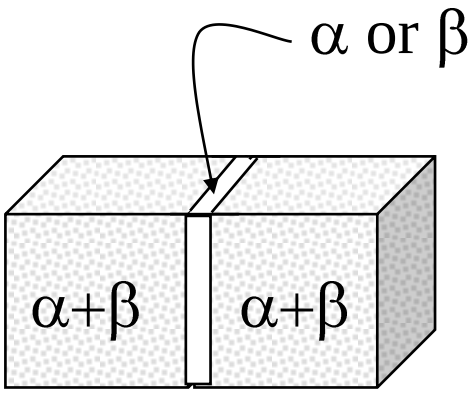
OUTLINE

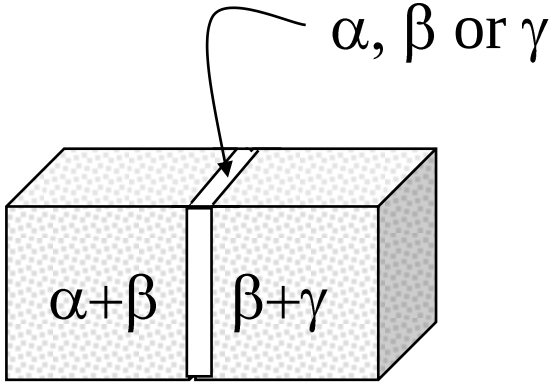
- Introduction
- Binary (Sekerka et. al. 1975) and pseudo binary
- Horns (Schwind et. al. 2001)
- Strange attractors (Carol 1985)
- Gas-solid reactions (Li 2002)
- Conclusions

also for discussion

- Notation
- Terminology

Introduction
Two Types of Multiphase Diffusion Couples

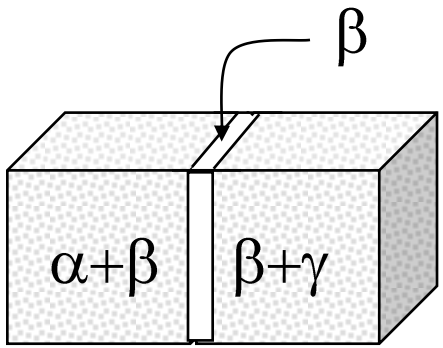


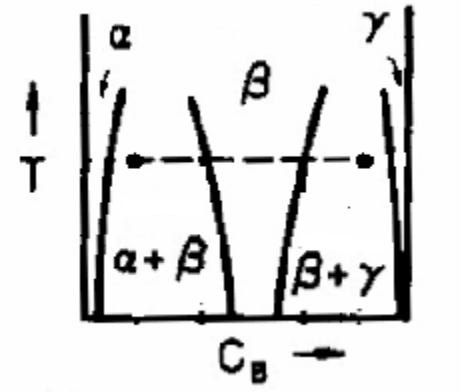


Created by
- Horns
- Gas-solid reactions

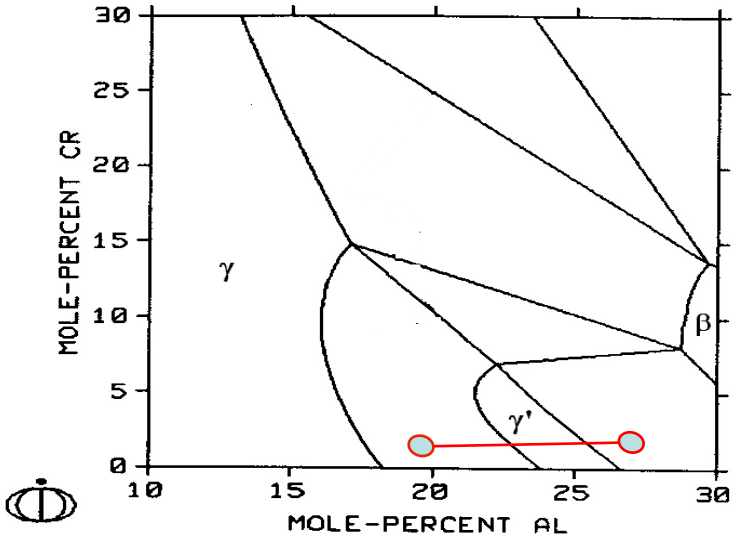
Created by
- Binary and pesudo-binary systems
- Strange attractors

Binary and Pseudo-Binary





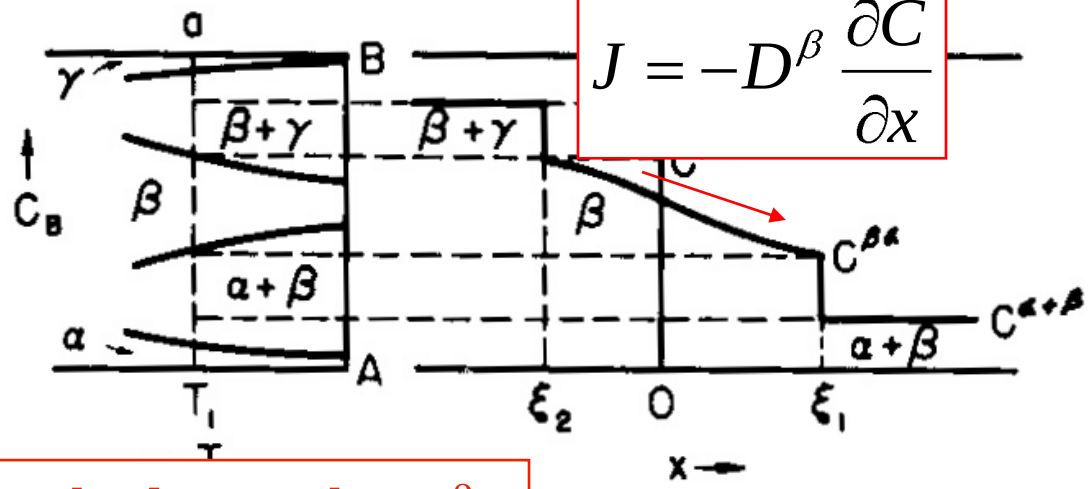
Binary



Pseudo Binary

Binary Diffusion Couples

$$J = -D^{\beta}\frac{\partial C}{\partial x}$$

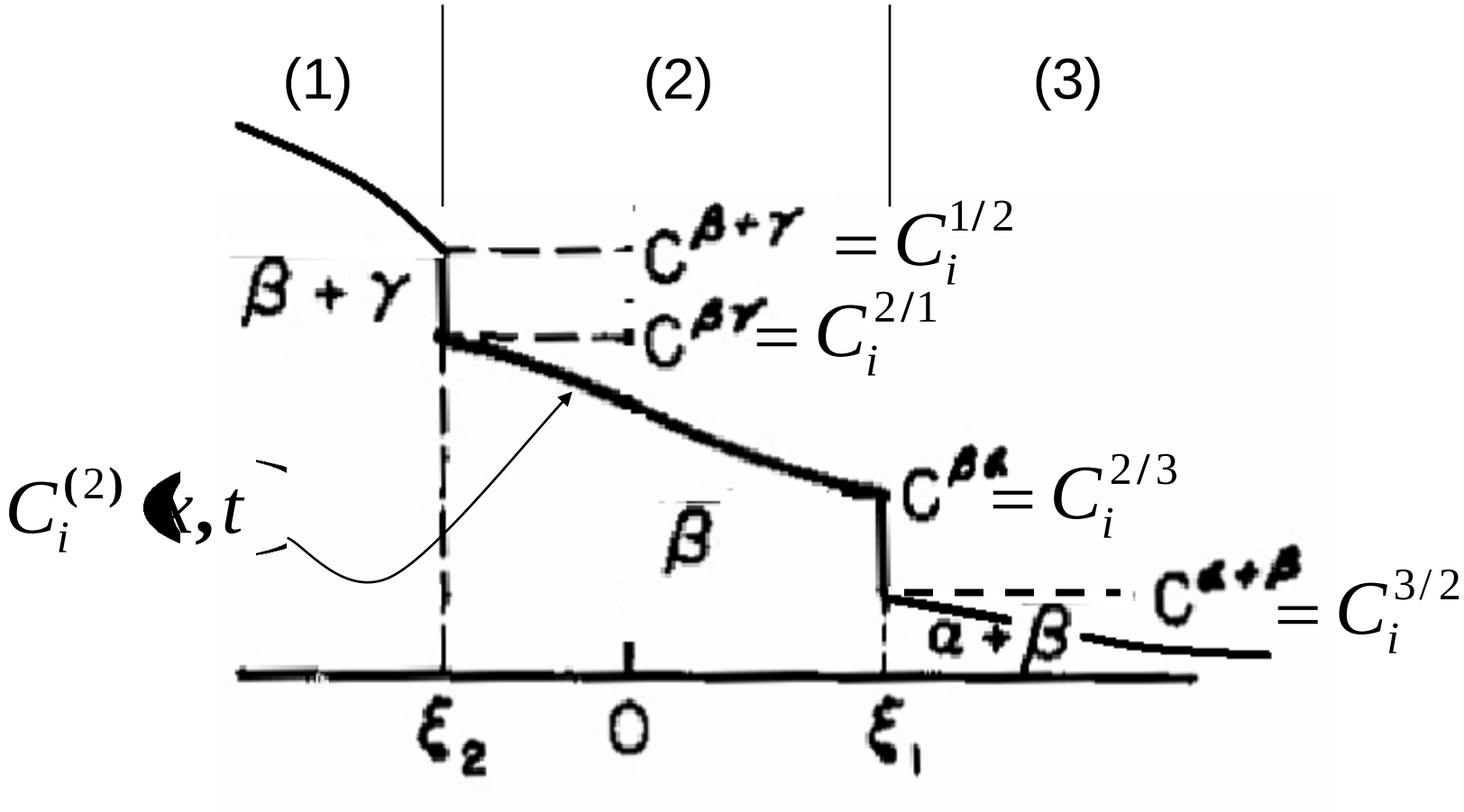


(b) for a system of infinite ex-
the α+β and β+γ fields of the

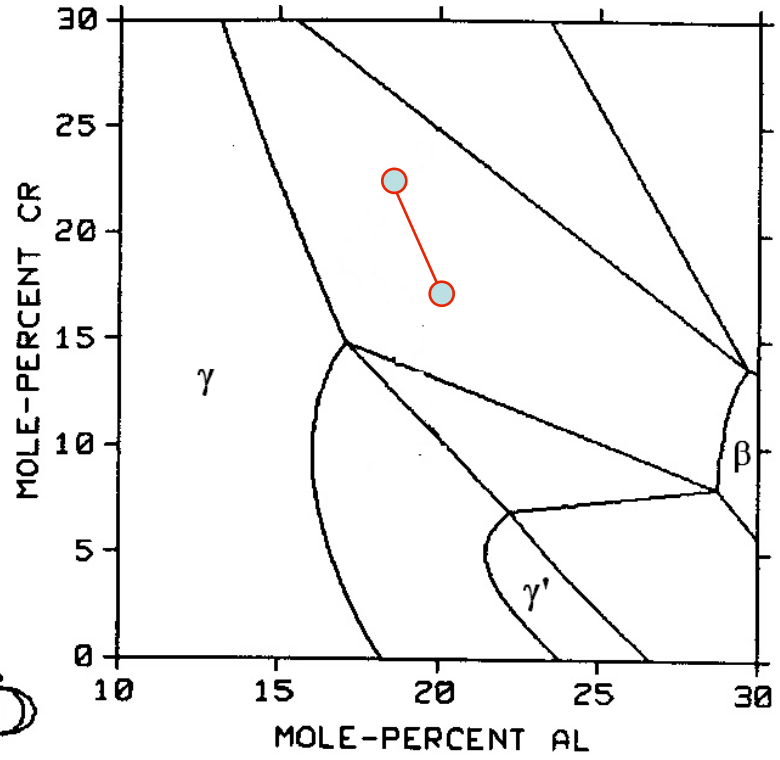
Take Away: The larger the D^{β}, the larger the layer

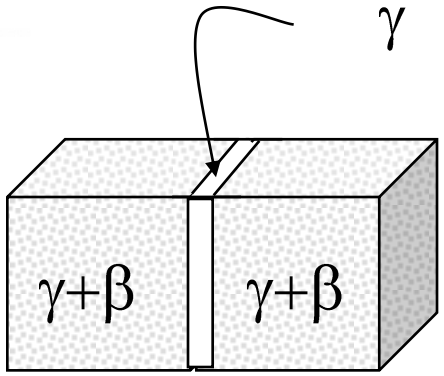
R.F. Sekerka, C.L. Jeanfils, and R.W. Heckel, The moving boundary problem, Lectures on the Theory of Phase Transformations, ed. H.I. Aaronson (1975, AIME).

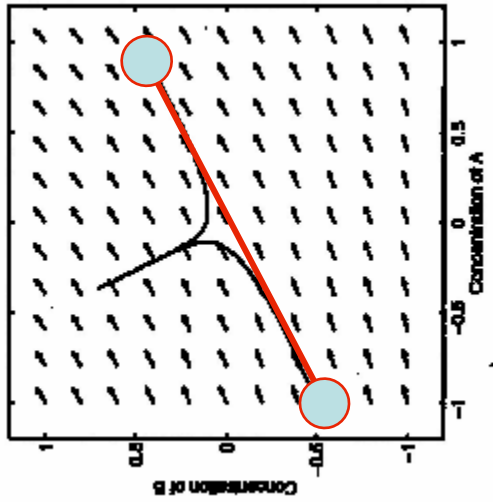
Multicomponent, Multiphase Notation



Single Phase Layers Formed by Horns



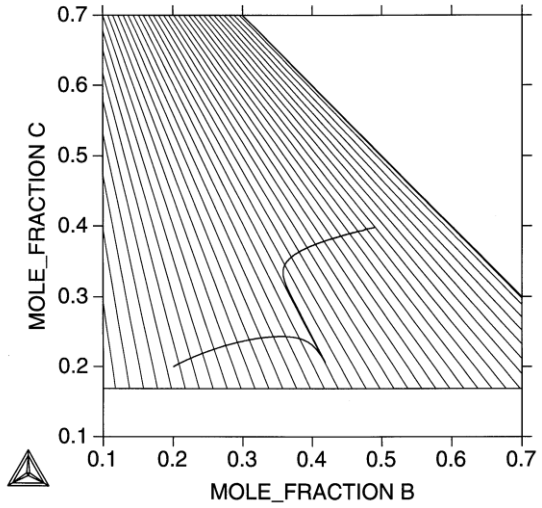


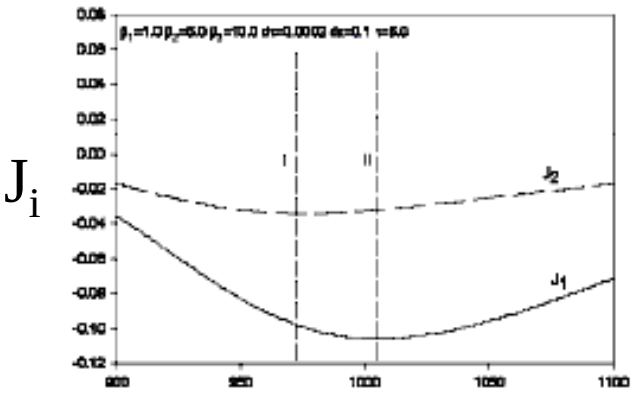


M. Schwind, T. Helander, J. Ågren, Scripta mater. 44 (2001) 415-421.

SINGLE HORNS IN SIMULATIONS

Finite difference simulation of the A-B-C system



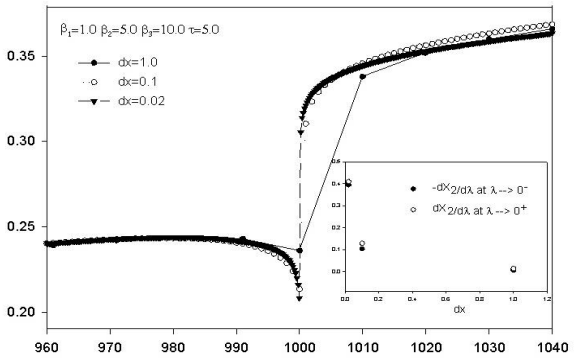


J_i

x

Flux profile

$$\frac{d\overline{C}_i}{d\lambda} = \frac{2}{\lambda}\frac{dJ_i^{\lambda}}{d\lambda}$$



$\overline{C}_i$

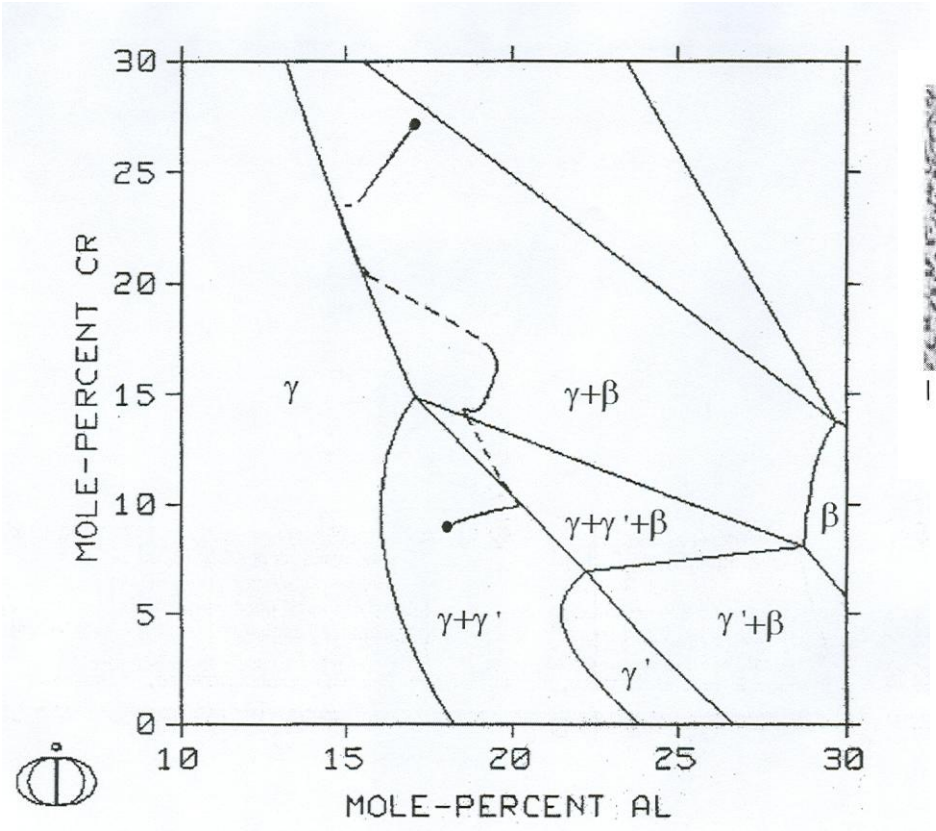
x

Concentration profile

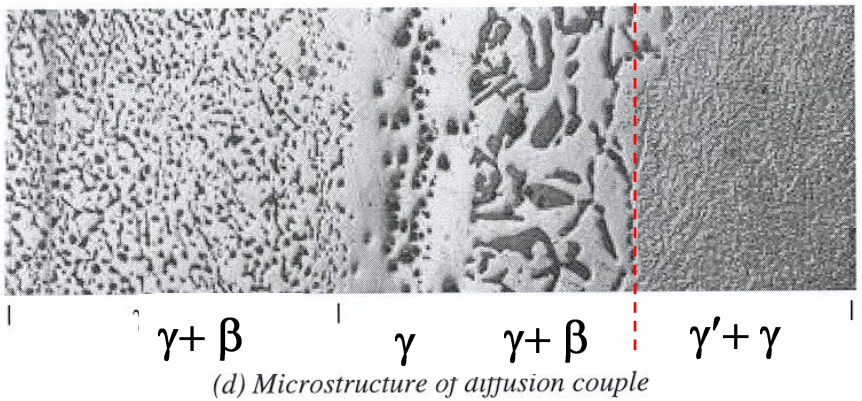
K. Wu, J.E. Morral, and Y. Wang, in press Acta Mater, Oct. 2006

Single Phase Layers formed by Horns

Predicted by DICTRA



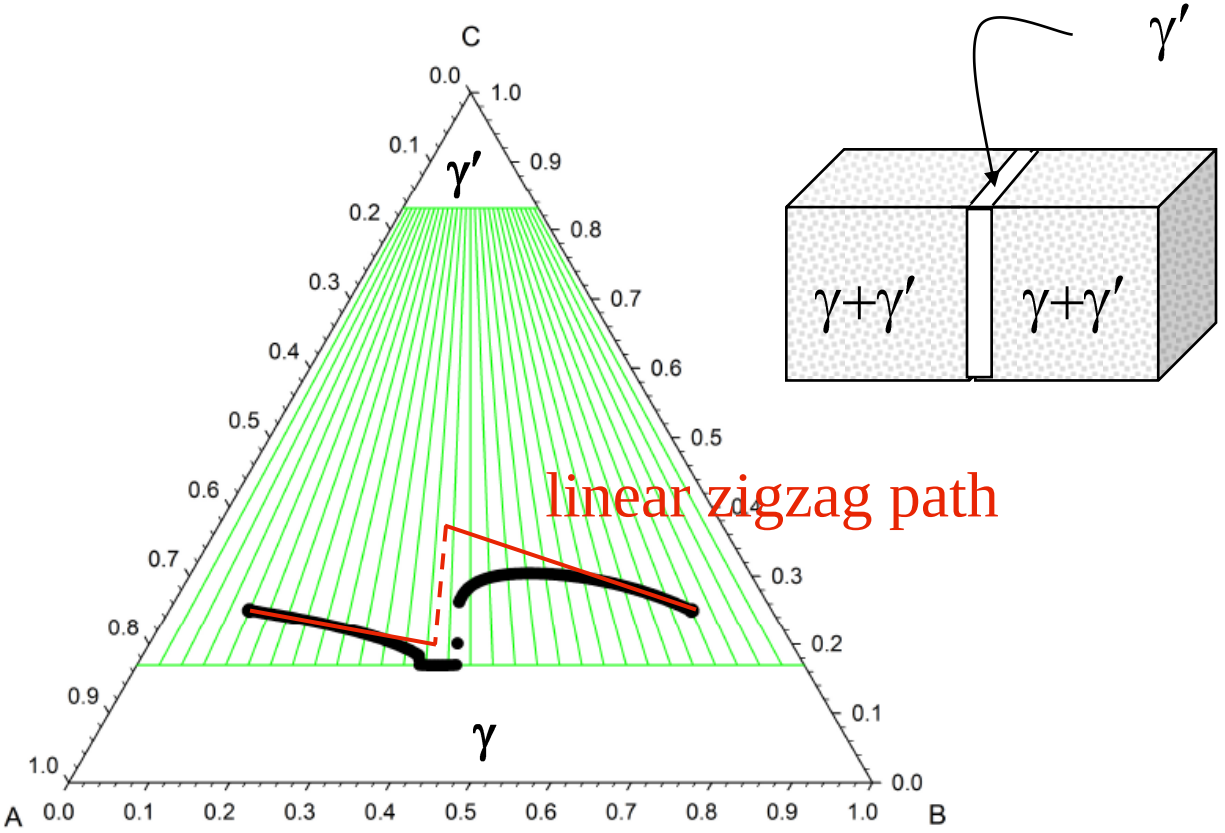
Diffusion Couple results



(d) Microstructure of diffusion couple

Single Phase Layers formed by Horns

Predicted by an in-house 1D finite difference programs



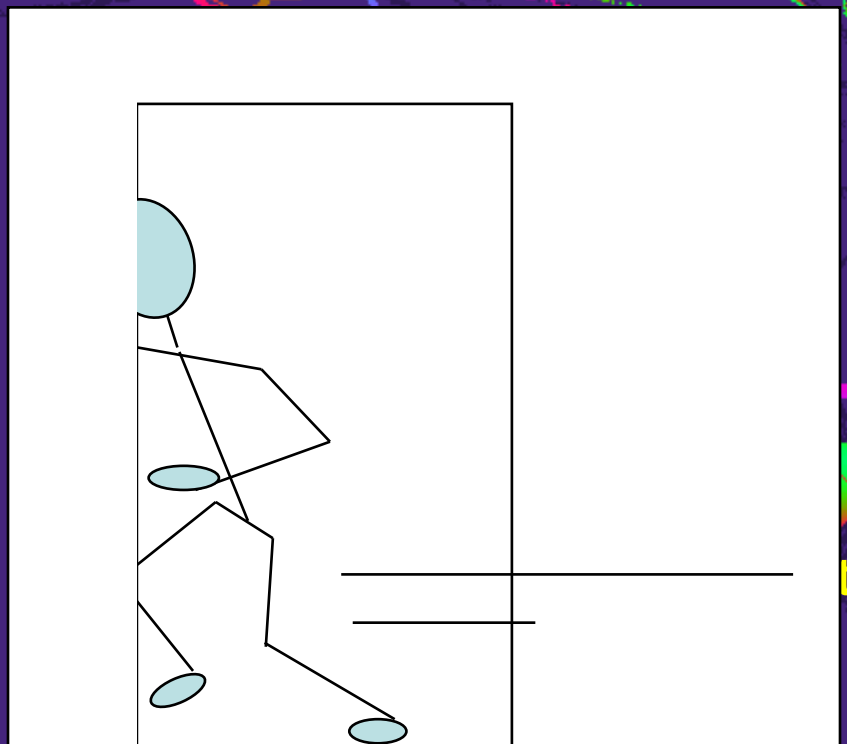
TMS Annual Meeting, Orlando, FL, Feb. 25-28, 2007

Terminology: Should the name of this effect be changed?

Strange Attractors are not strange

Bill Boettinger 2006

Strange At[illegible]ors



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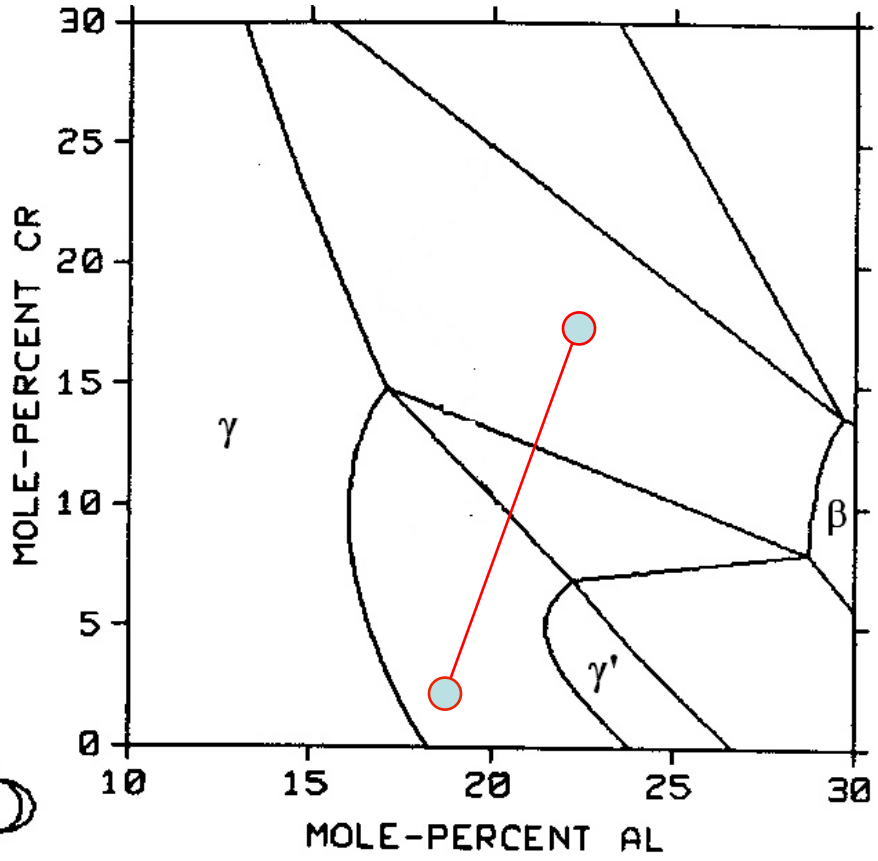
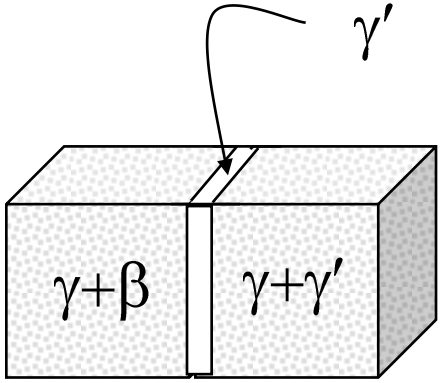
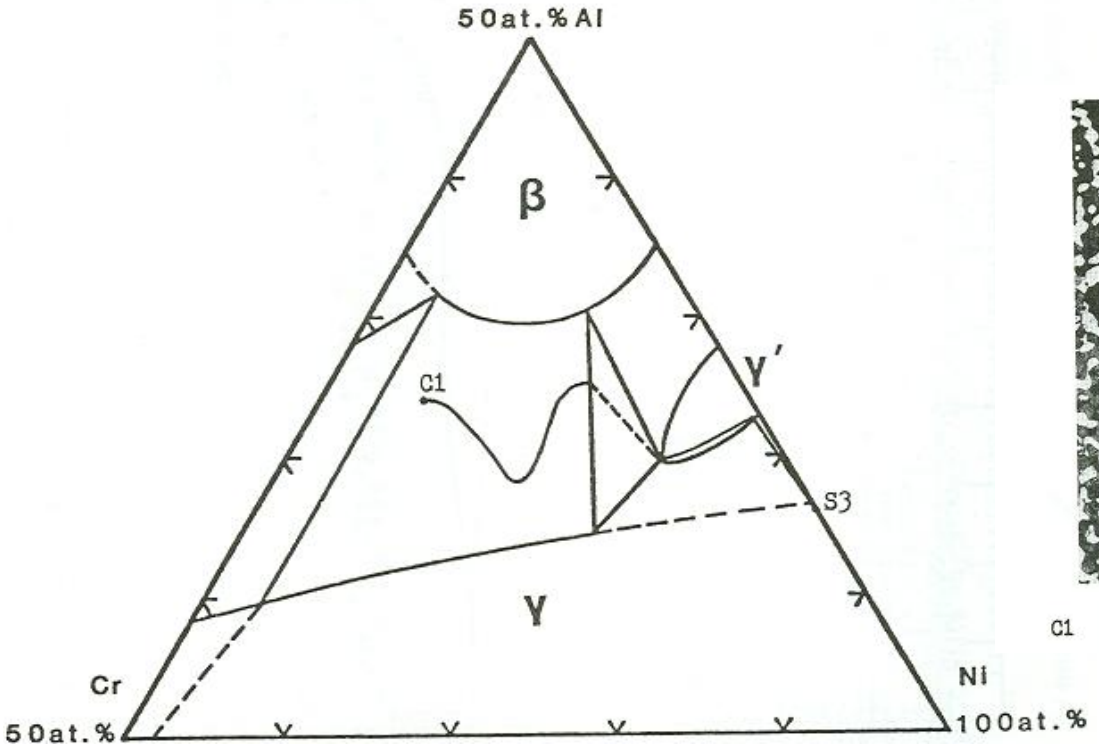
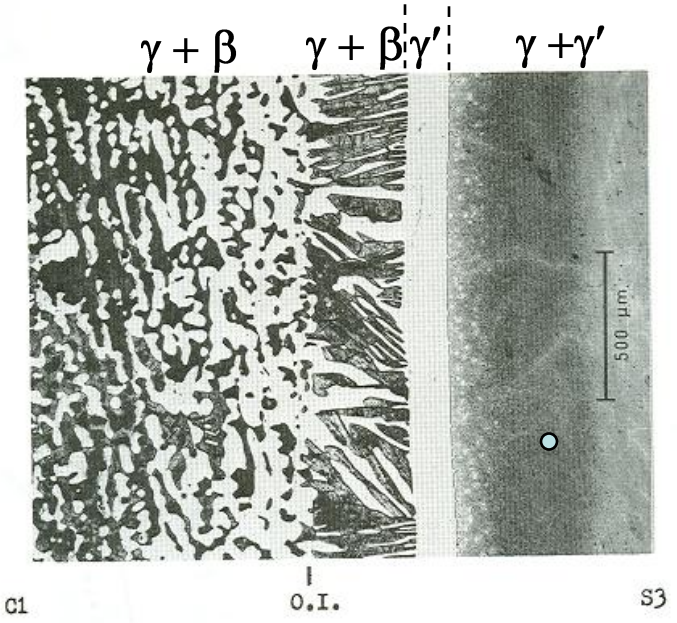
Single Phase Layers formed by Strange Attractors





Single Phase Layers formed by Strange Attractors





From: Lawrence A. Carol, NASA Contractor Report 174852, 1985.

Single Phase Layers formed by Strange Attractors

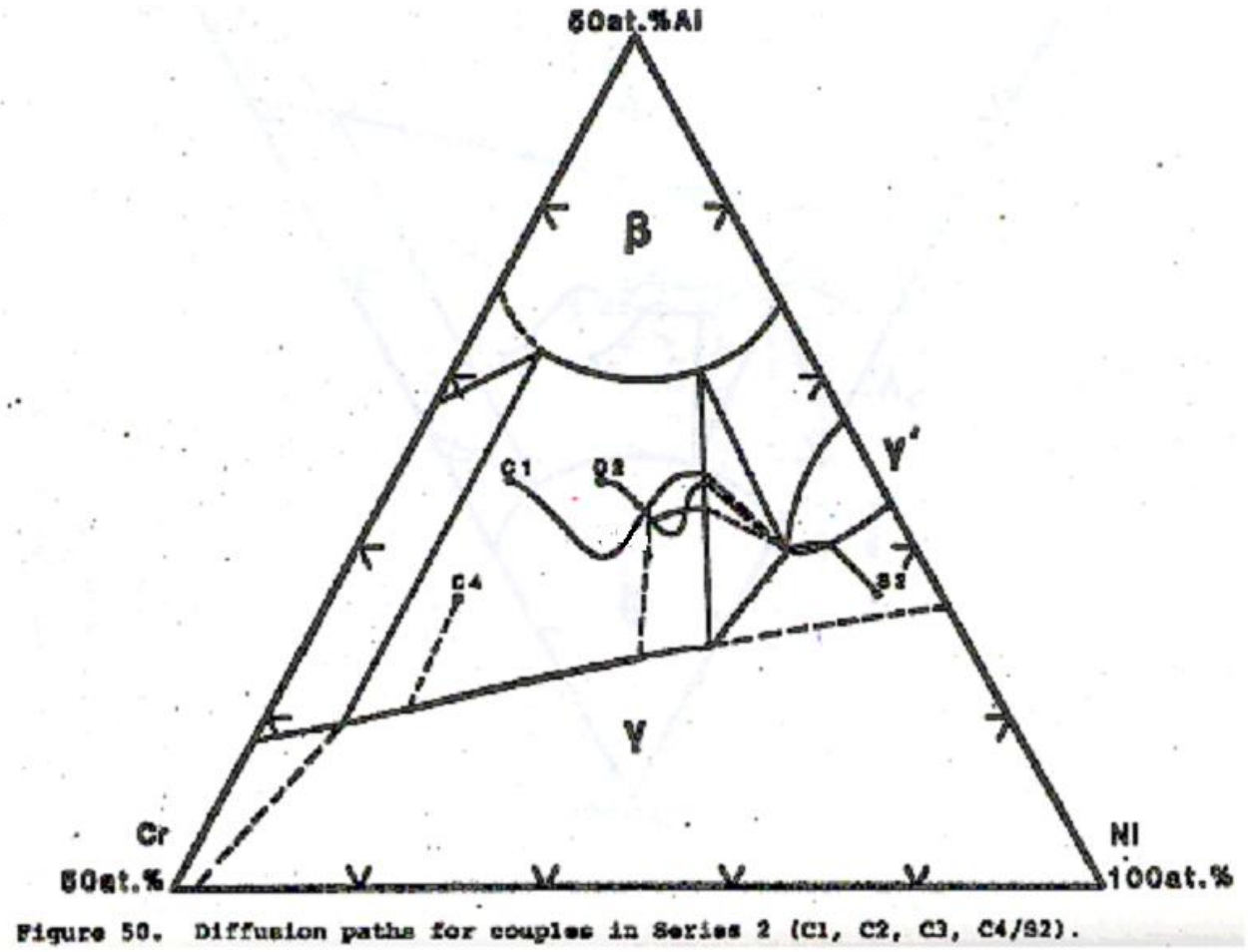
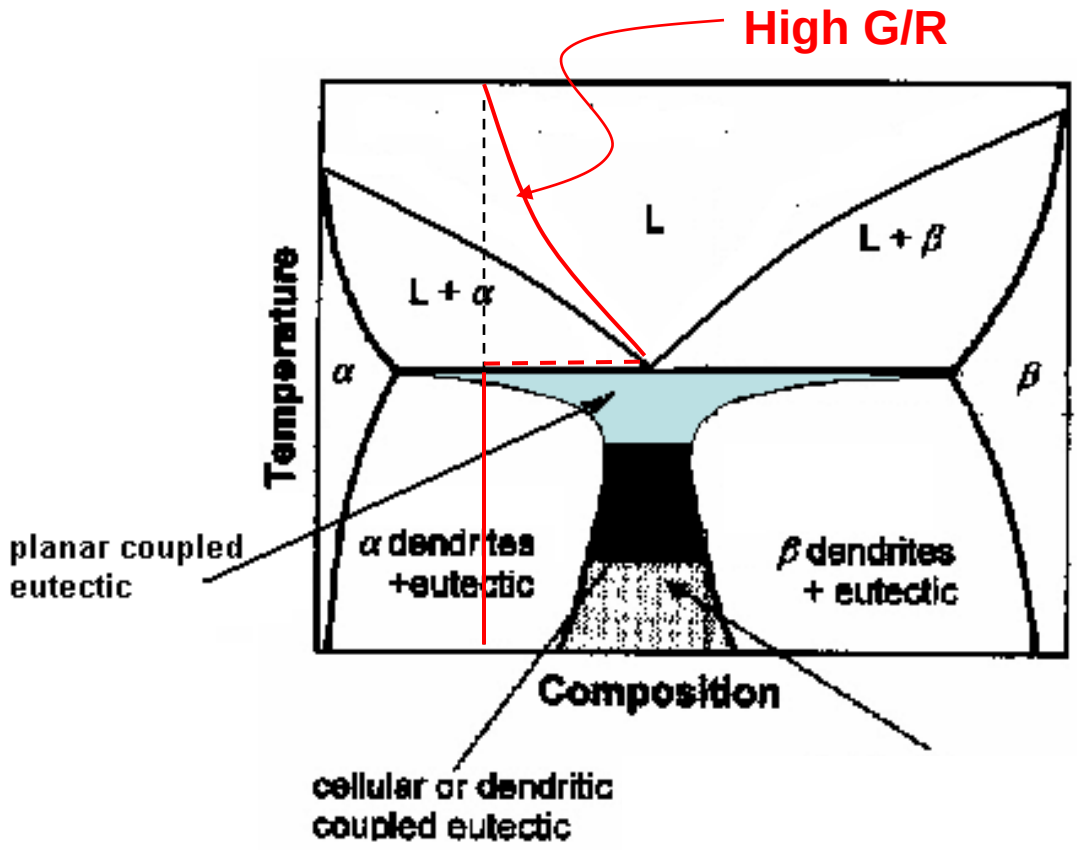


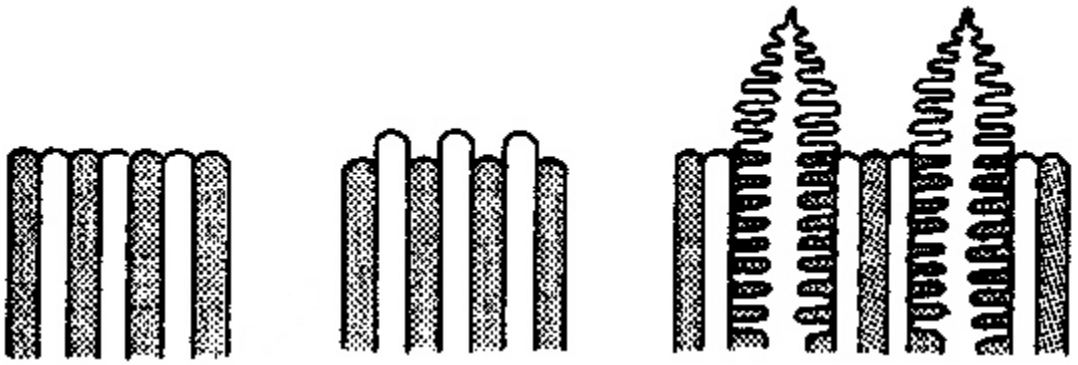
Figure 50. Diffusion paths for couples in Series 2 (C1, C2, C3, C4/S2).

From: Lawrence A. Carol, NASA Contractor Report 174852, 1985.

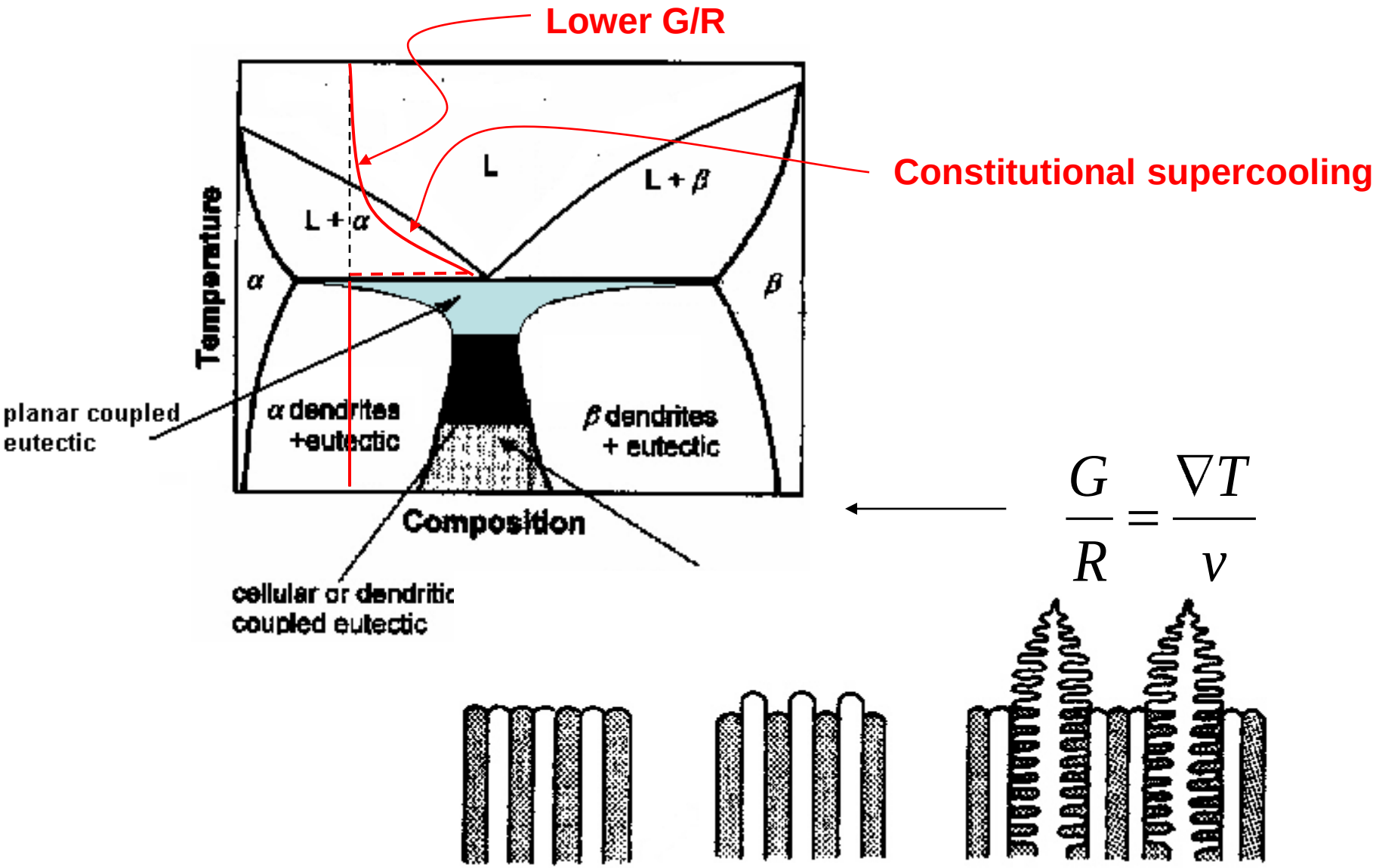
Explanation of Directional Solidification Strange Attractors



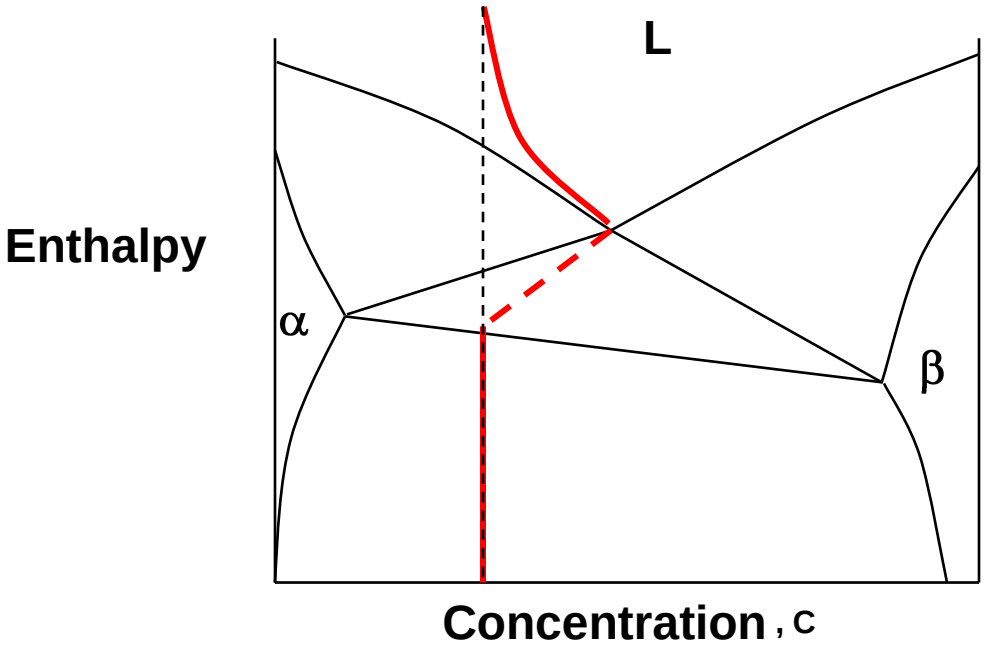
$$\frac{G}{R} = \frac{\nabla T}{v}$$



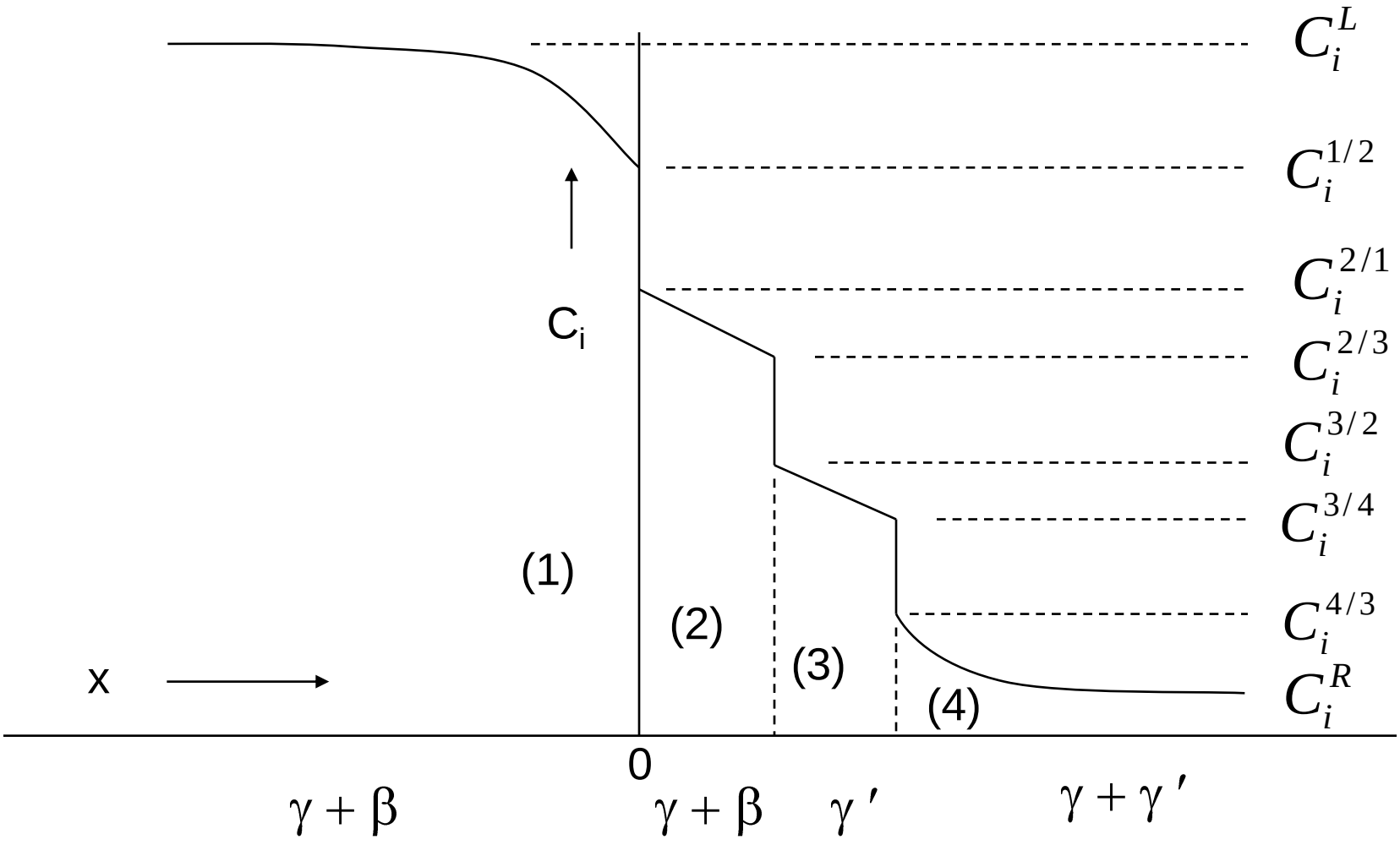
Explanation of Directional Solidification Strange Attractors



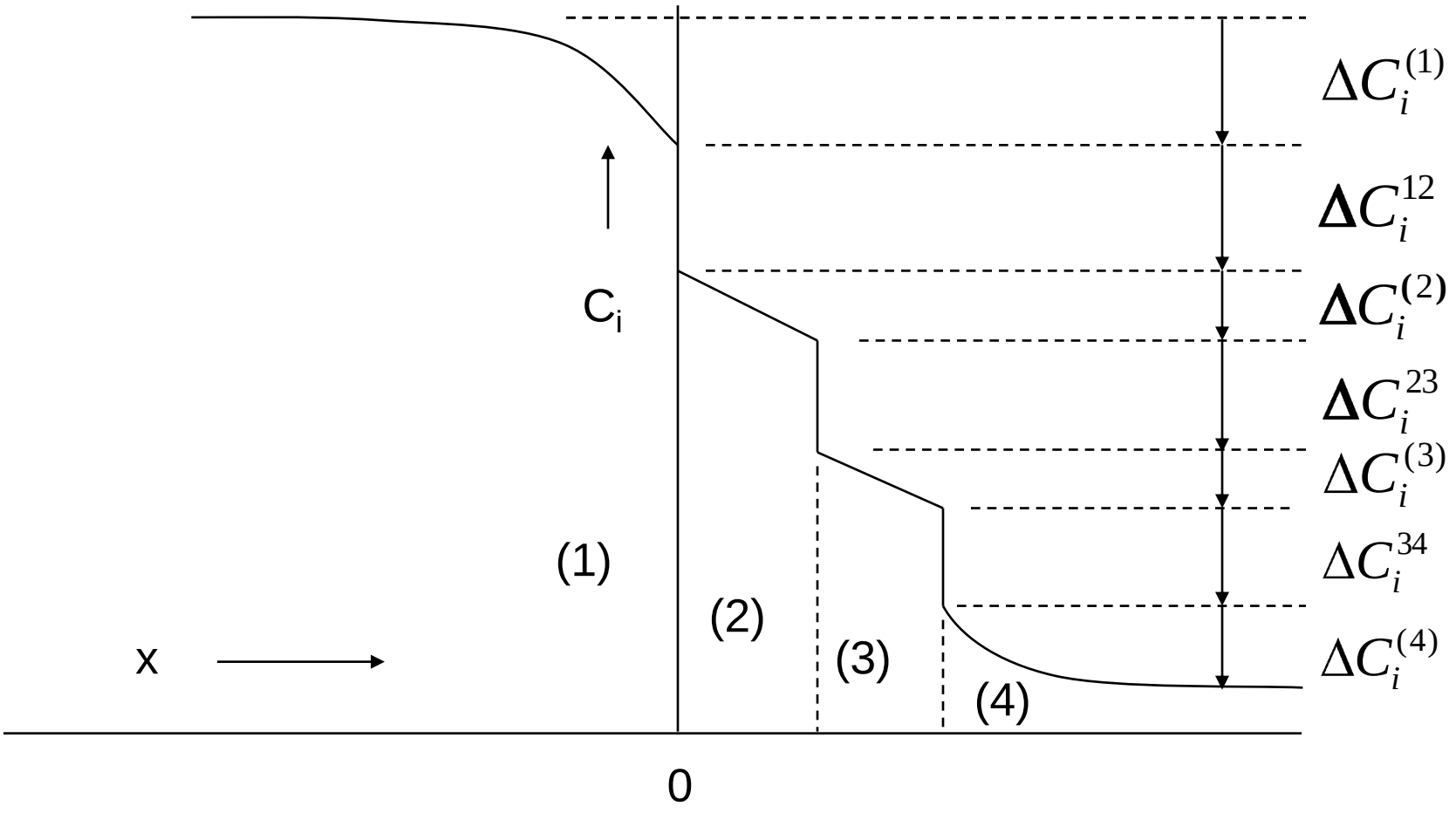
Explanation of Directional Solidification Strange Attractors with non Potential axes



Notation for Solving the Ternary Strange Attractor Problem



Notation Reduction for Solving the Ternary Strange Attractor Problem



Equations Entered in Mathematica to Solve the Ternary Strange Attractor Problem

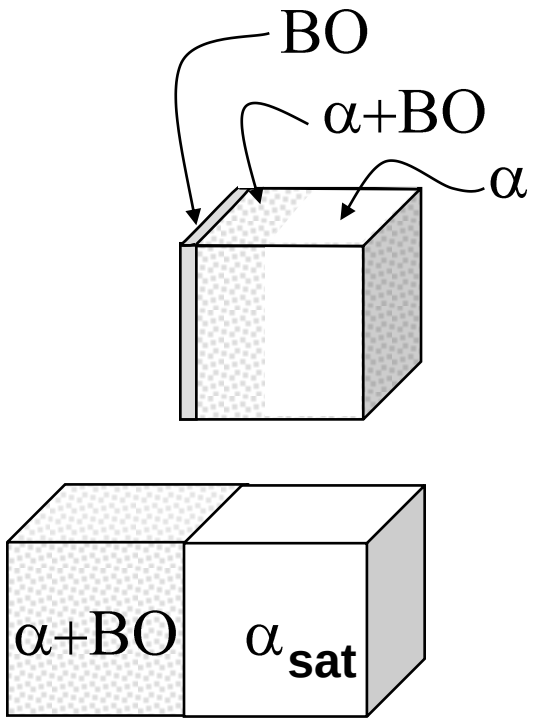
Paul Pavka, 01:2[illegible] 5/1/2007, attractors updates 5-1

No Viable Solution Yet

```
FindRoot[{
  2*B - (2*C) == A
  Sqrt[Pi]*K == ((B - C)/(22.5 - B))*(                    2*((D - 22.5)/(22.5 - B))*(Exp[(-1)*(K^2)*.25]/(Erf[.5*L] - Erf[.5*K])),
  Sqrt[Pi]*K == ((A - 13)/(7 - A))*(Exp[(-1)*          ]/Erf[K]                    2.5)*(Exp[(-1)*(K^2)*.25]/(Erf[.5*L] - Erf[.5*K])),
  Sqrt[Pi]*L == 2*((D - 22.5)/(.949*D - 23.91))*(Exp[(-1,                          .91 - 1.949*D)/(          - 23.91))*(Exp[(-1)*(L^2)]/(1 - Erf[L])),
  Sqrt[Pi]*L == 2*((5*D - 112.5)/(3.23 - .128*D))*(Exp[(-1)*(L^2)*.2                22.27)/(.8*D))*(Exp[(-1)*L^2]/(1 - Erf[L]))},
 {A, 11}, {B, 23}, {C, 24}, {D, 21.3}, {K, 0.01}, {L, 0.03}]
```

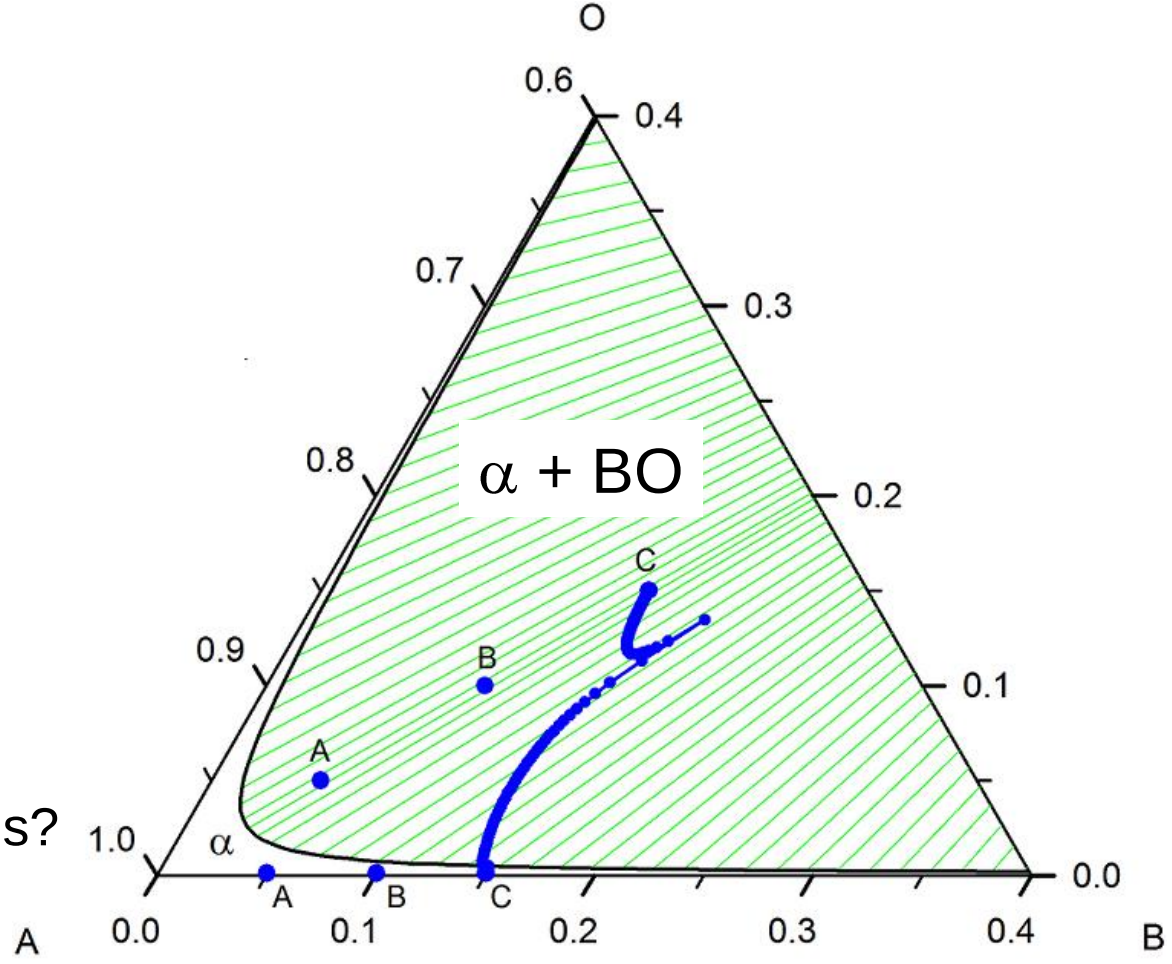
D-value	$C_{21}^{1/2}$ (A)	$C_{11}^{1/2}$ (B)	C_{11}^{0} ©	$C_{12}^{2/3}$ (D)	K_1 (K)	K_2 (L)
D[=1	9.86	25.2	26.8	3.83	0.00957	1.37

Single Phase Layer Growth in Gas-Solid Reactions



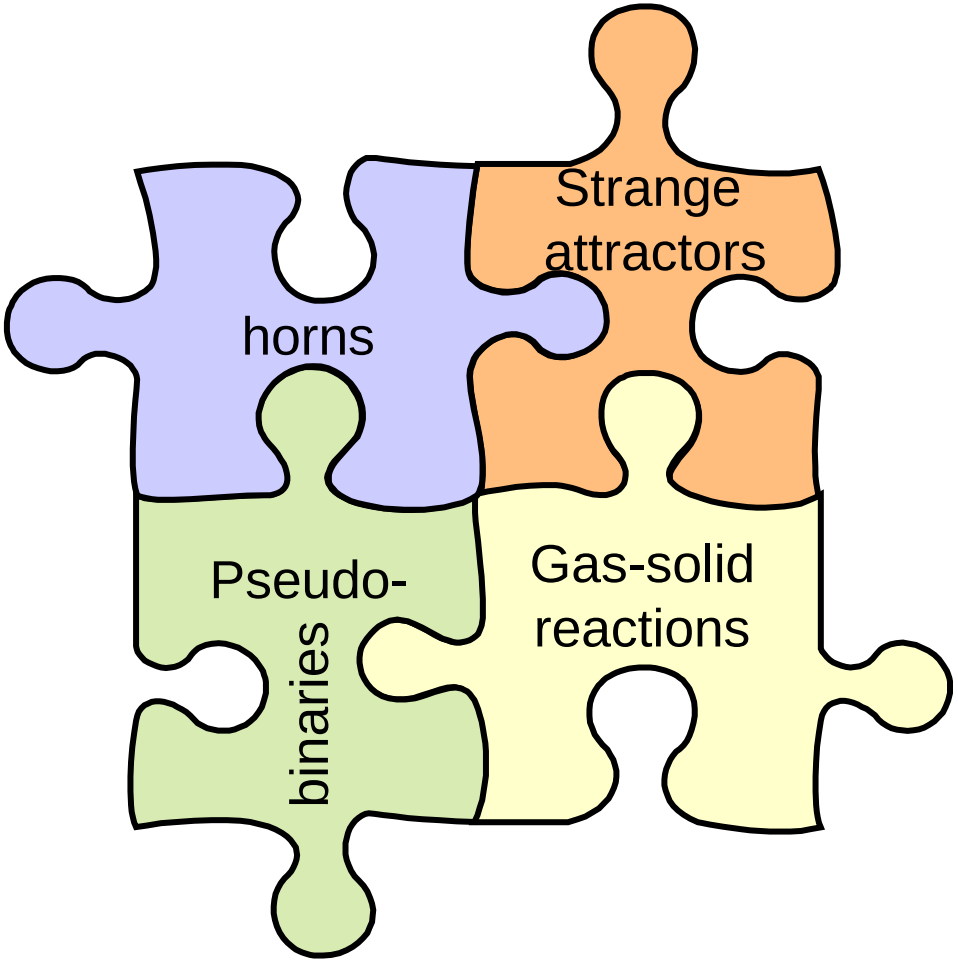
What is the role of
Horns in gas solid reactions?

In-house 1D Finite Difference Model



CONCLUSIONS

Pieces are Still Missing from the
Single Phase Layer Formation Puzzle



Hypothesis violations by “strange attractors”

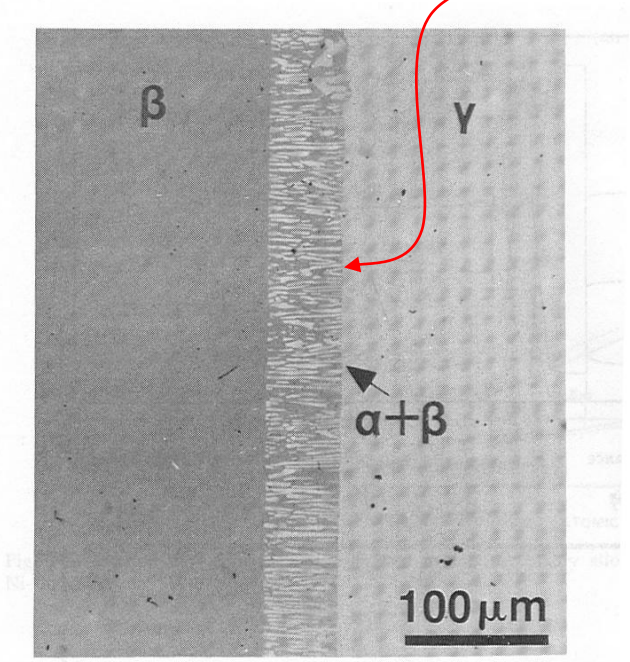
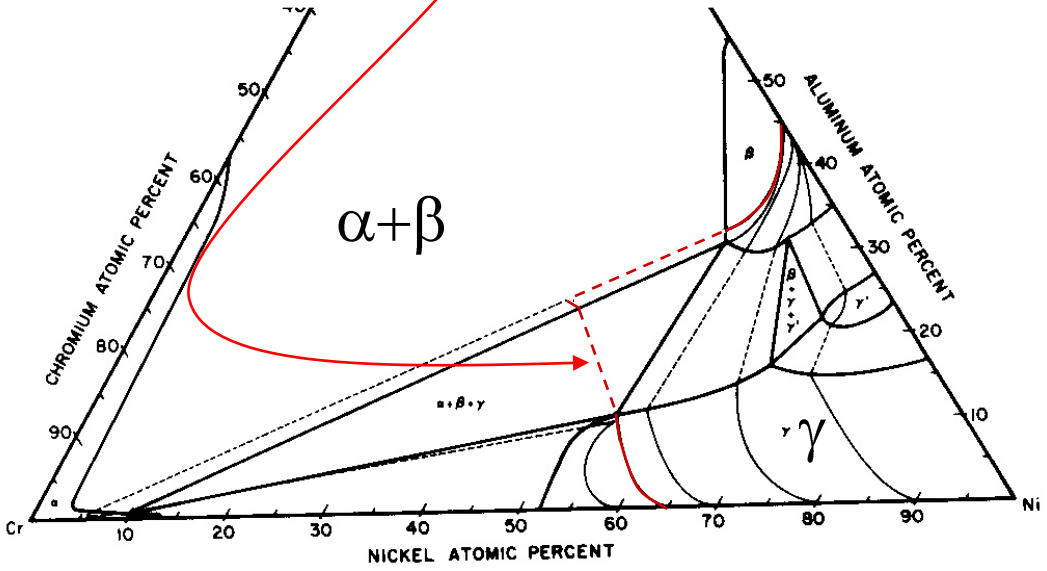


Fig. 10—Typical microstructure of the interdiffusion region of the β-Ni50Al *vs* γ-Ni30.9Cr9.9Al (1150 °C/49 h) diffusion couple.

Type 3



S.M.Merchant, M.R. Notis, J.I.Goldstein, Met.Trans 21A(1990)1901

Hypothesis violation: Four types of Boundary and a “strange attractor”

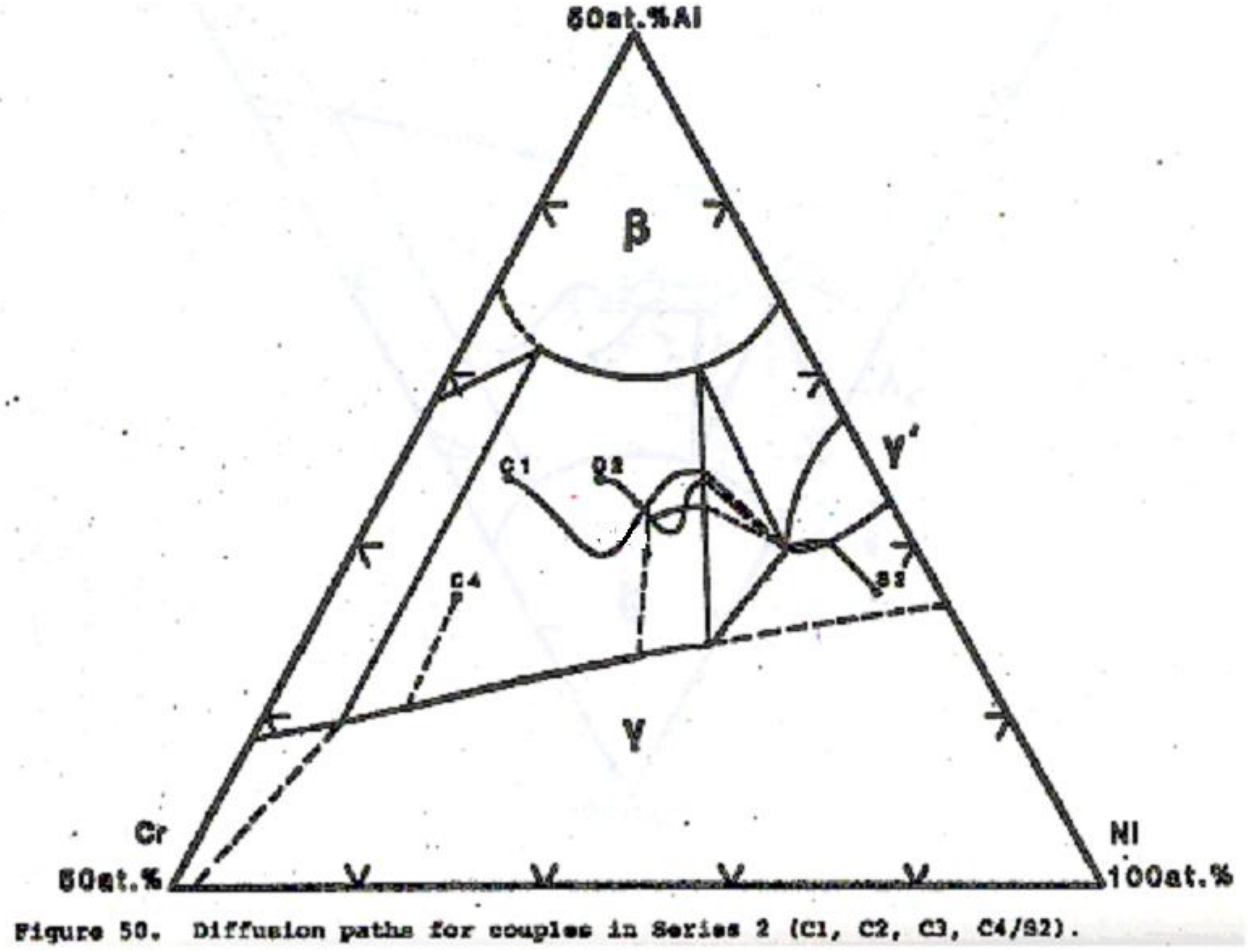


Figure 50. Diffusion paths for couples in Series 2 (C1, C2, C3, C4/S2).

From: Lawrence A. Carol, NASA Contractor Report 174852, 1985.

Carol Diffusion Paths Containing Three Types of Boundary

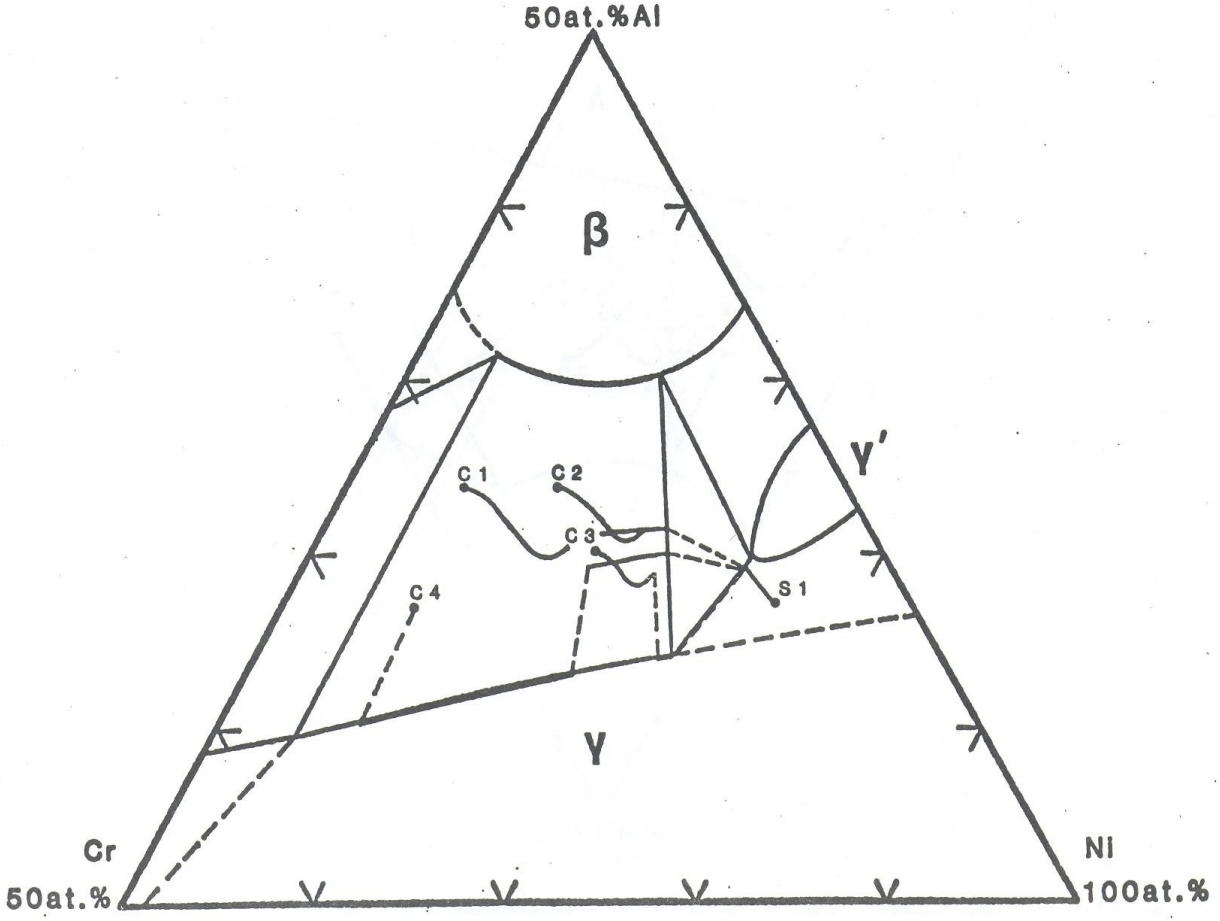


Figure 49. Diffusion paths for couples in Series 1 (C1, C2, C3, C4/S1).

From: Lawrence A. Carol, NASA Contractor Report 174852, 1985.

Another hypothesis violation: Four types of boundary and a “strange attractor”

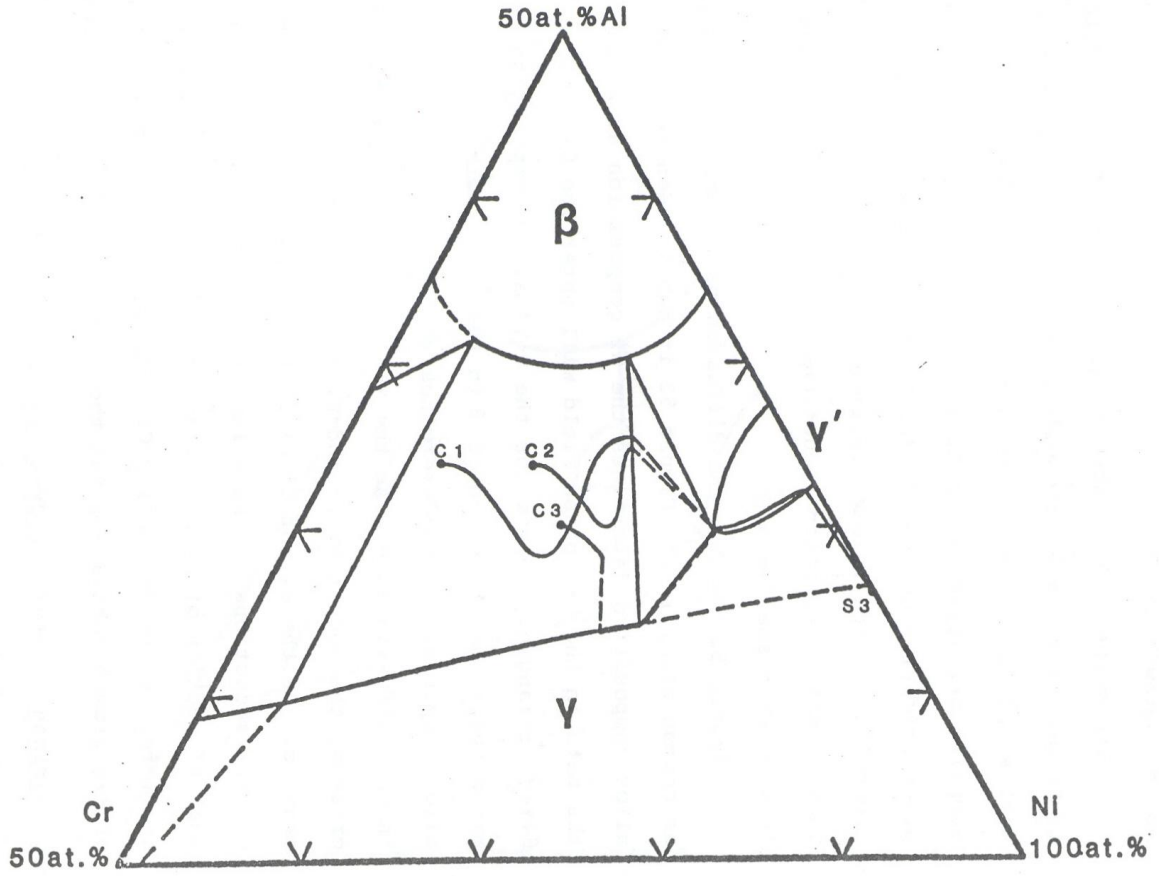


Figure 51. Diffusion paths for couples in Series 3 (C1, C2, C3/S3).

From: Lawrence A. Carol, NASA Contractor Report 174852, 1985.

Hypothesis violations by “strange attractors”

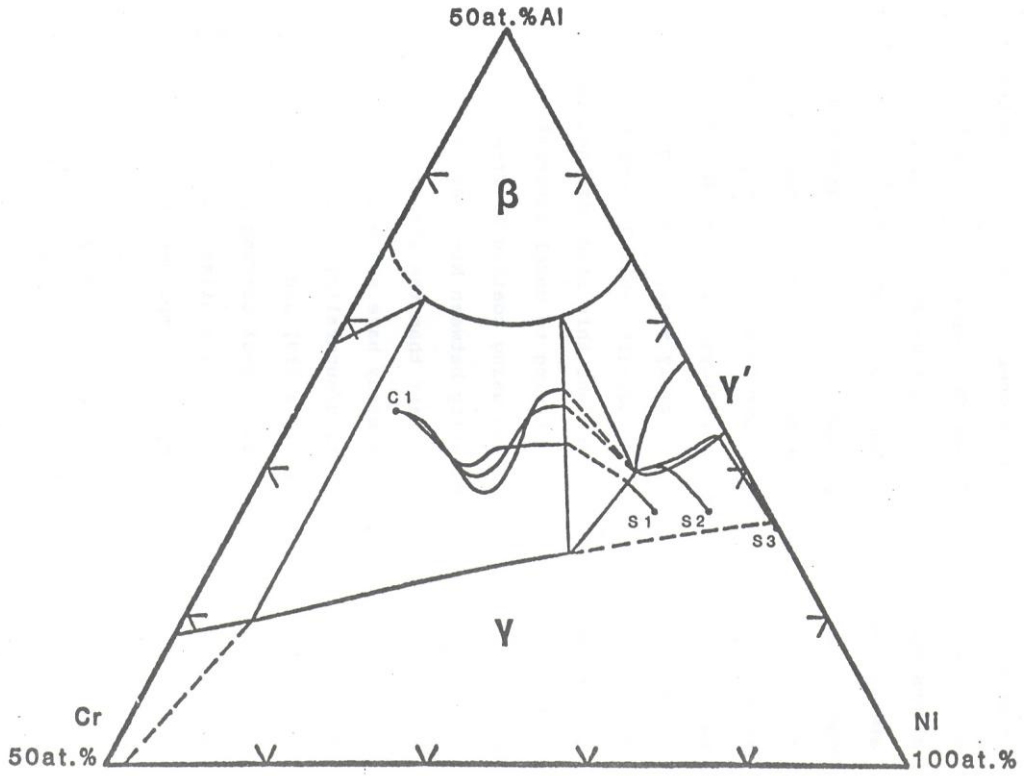


Figure 52. Diffusion paths for couples with C1 as the common alloy (C1/S1, S2, S3).

From: Lawrence A. Carol, NASA Contractor Report 174852, 1985.