Call for papers

Phase Stability, Diffusion, Kinetics and Applications

Where: Houston, 2010 MS&T meeting
When: October 18-20, 2010

Included in the symposium will be special sessions honoring
Austin Chang, 2009 ASM J. Willard Gibbs Award recipient
Arthur Pelton, 2010 ASM J. Willard Gibbs Award recipient

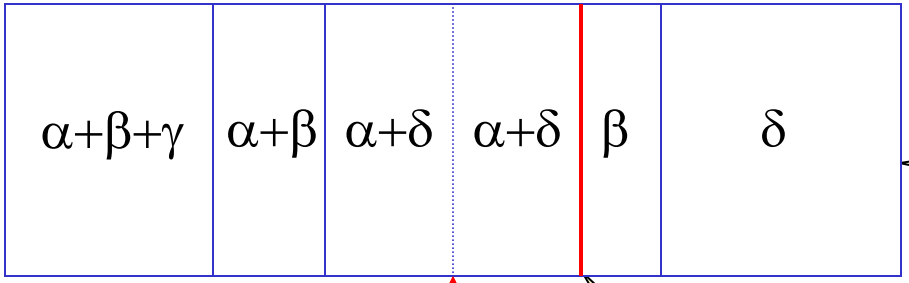
Abstract deadline is Monday March 29, 2010

http://174.120.122.245/program/technical-program/fundamentals-and-characterization/

NIST Diffusion Workshop
May 23-24, 2010, Gaithersburg, MD

Number of phase changes when crossing a boundary

DICTRA Simulations of Type 3 Boundaries Using the Homogenization Model



α+β+γ / δ Diffusion couple

Type 3

Xiaoqin Ke and John Morral
Department of Materials Science and Engineering
The Ohio State University
Columbus, Ohio

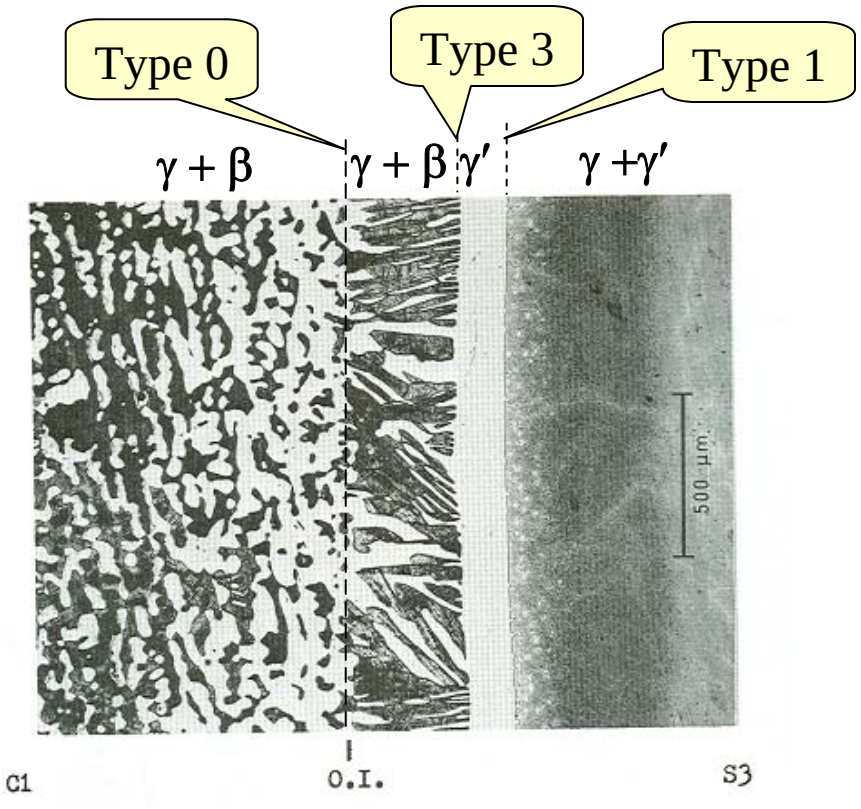
MSE

OUTLINE

- Introduction
  - Boundaries in Microstructures
  - Boundaries in Diffusion paths
  - Dictra simulations of boundaries using the disperse system model
- Dictra simulations of Type 3 boundaries using the homogenization model
- Summary

Introduction - Boundaries in Microstructures

A Type 3 boundary in a $\gamma+\beta/\gamma+\gamma'$ Ni-Cr-Al diffusion couple



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

Introduction - Boundaries in Microstructures

A Type 3 boundary in a β/γ Ni-Cr-Al diffusion couple

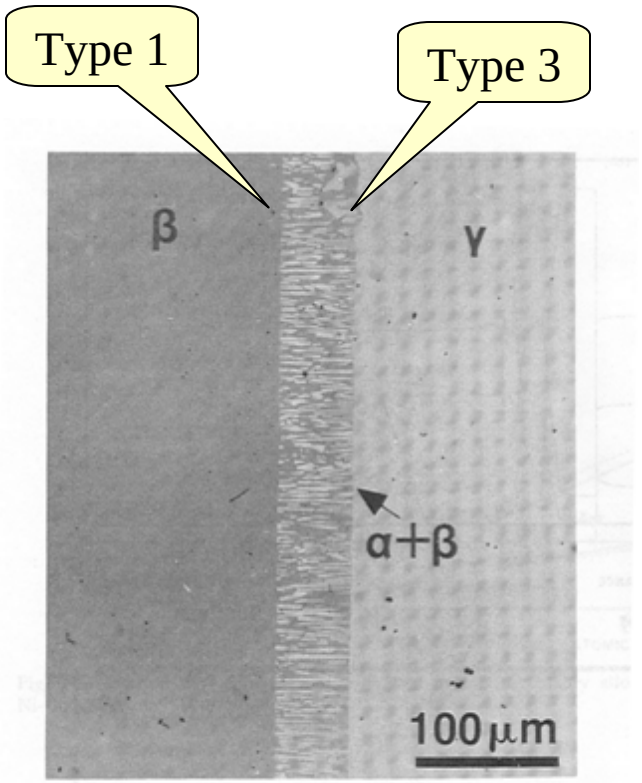
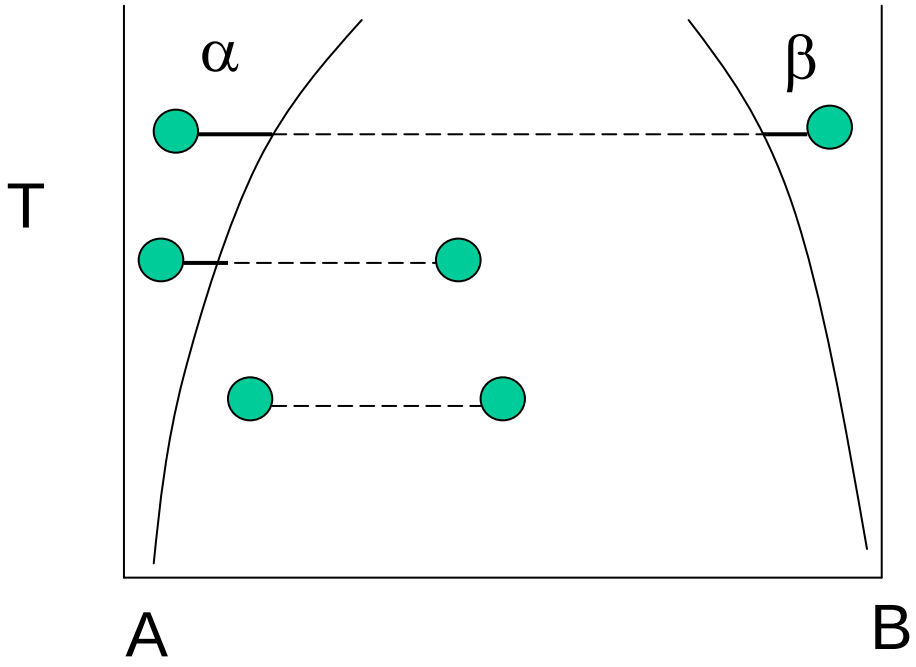
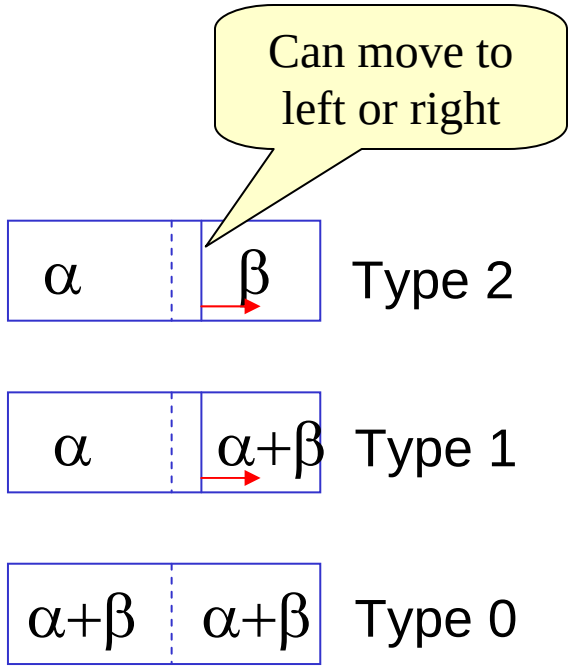


Fig. 10—Typical microstructure of the interdiffusion region of the β-Ni50Al *vs* γ-Ni30.9Cr9.9Al (1150 °C/49 h) diffusion couple.

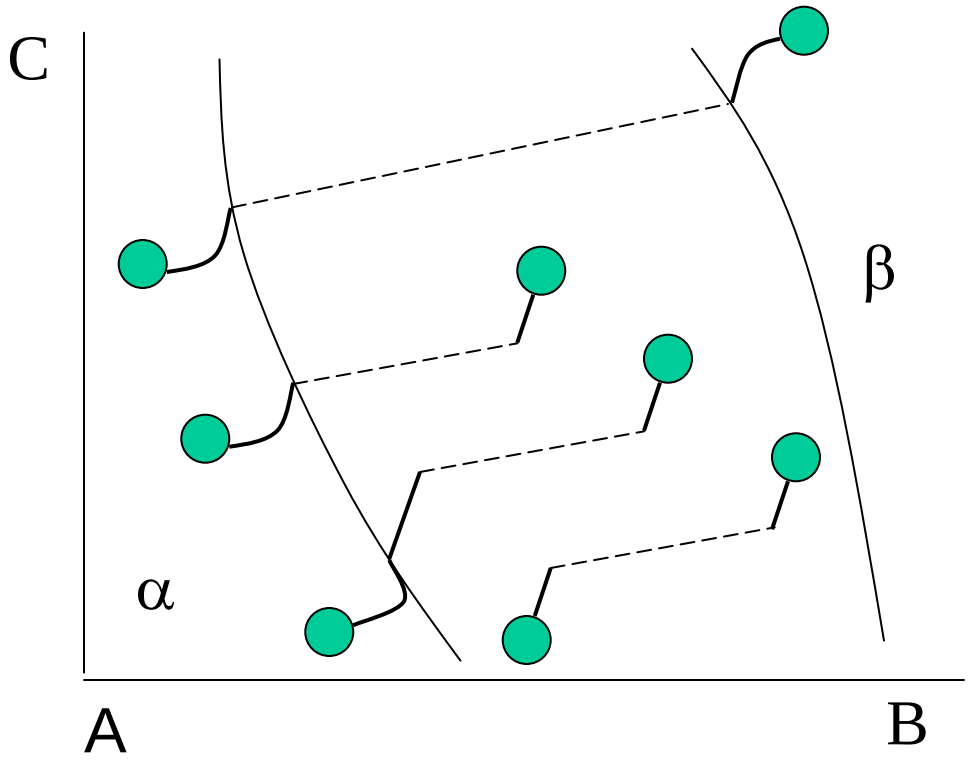
S.M.Merchant, M.R. Notis, J.I.Goldstein, Met.Trans 21A(1990)1901

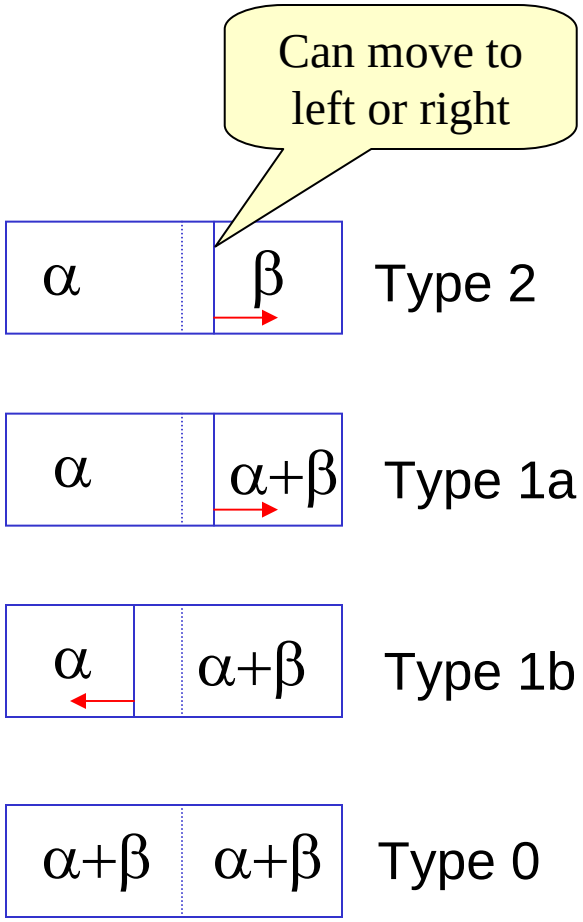
Introduction - Boundaries in Binary Diffusion Paths



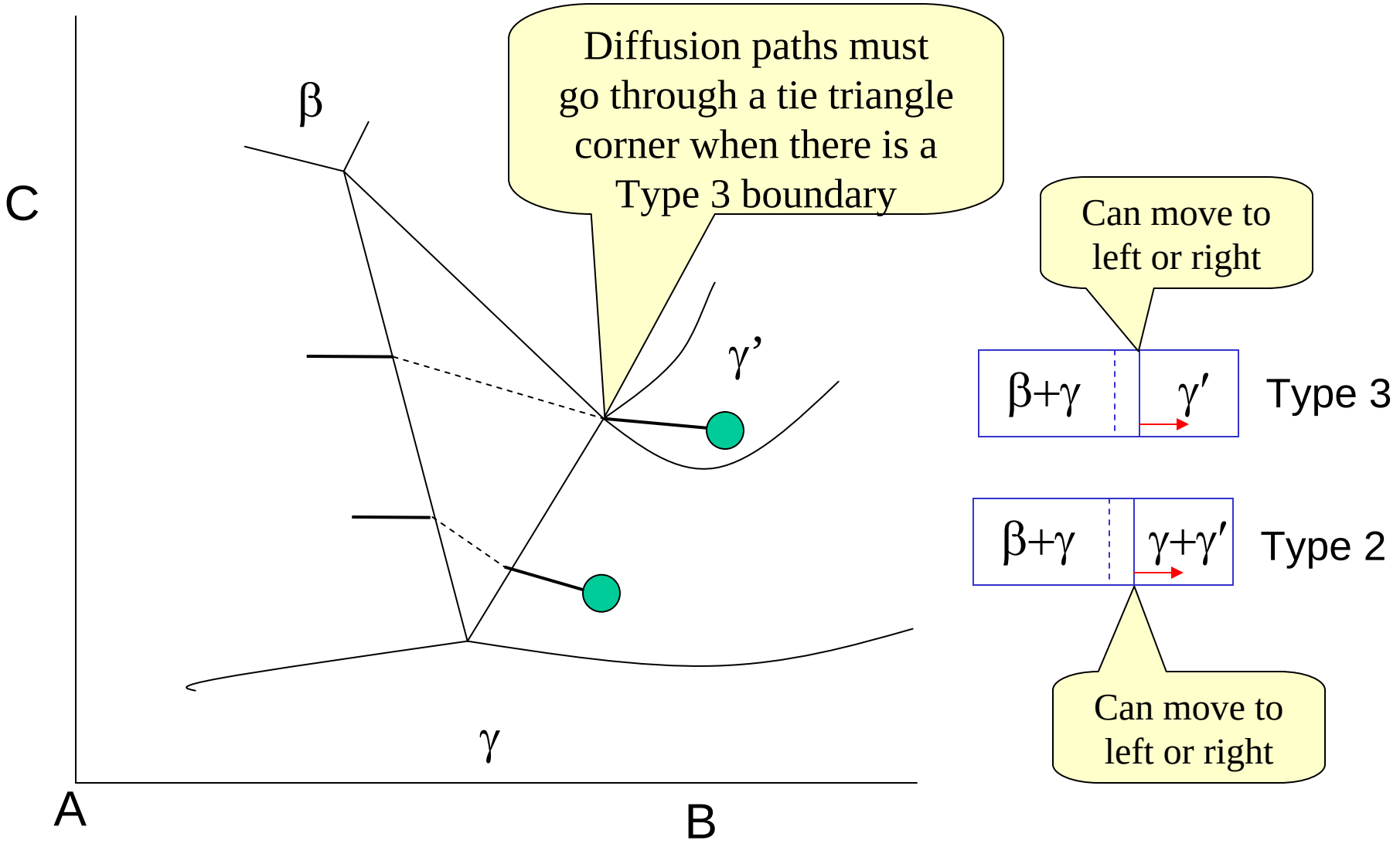


Introduction - Boundaries in Ternary Diffusion Paths



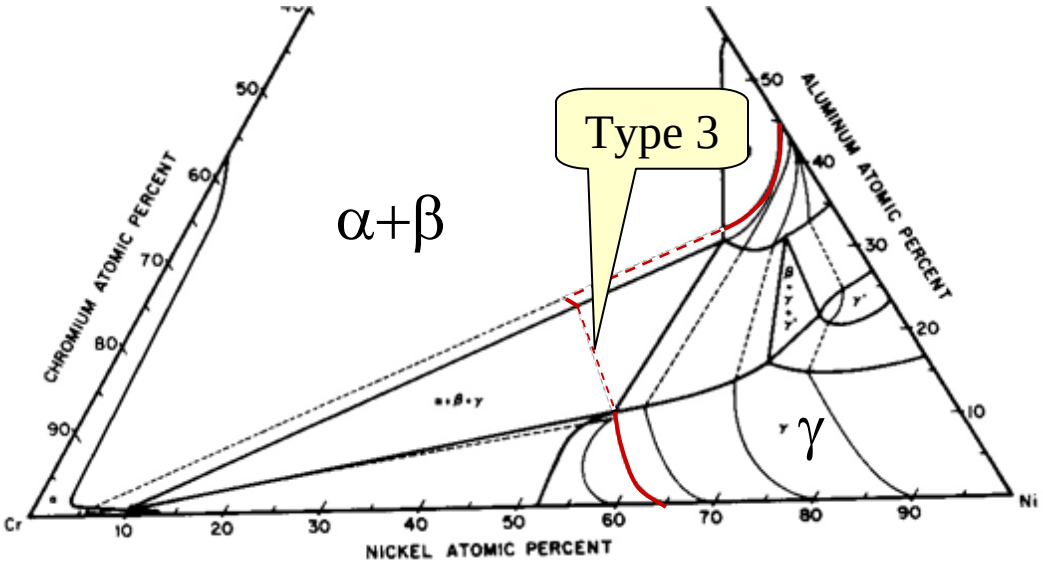


Introduction - Boundaries in Ternary Diffusion Paths



Introduction - Boundaries in Ternary Diffusion Paths

Which directions are the boundaries moving?



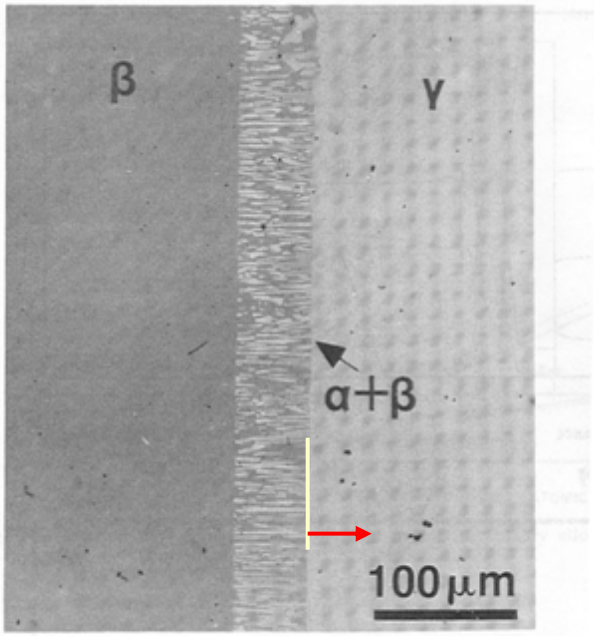
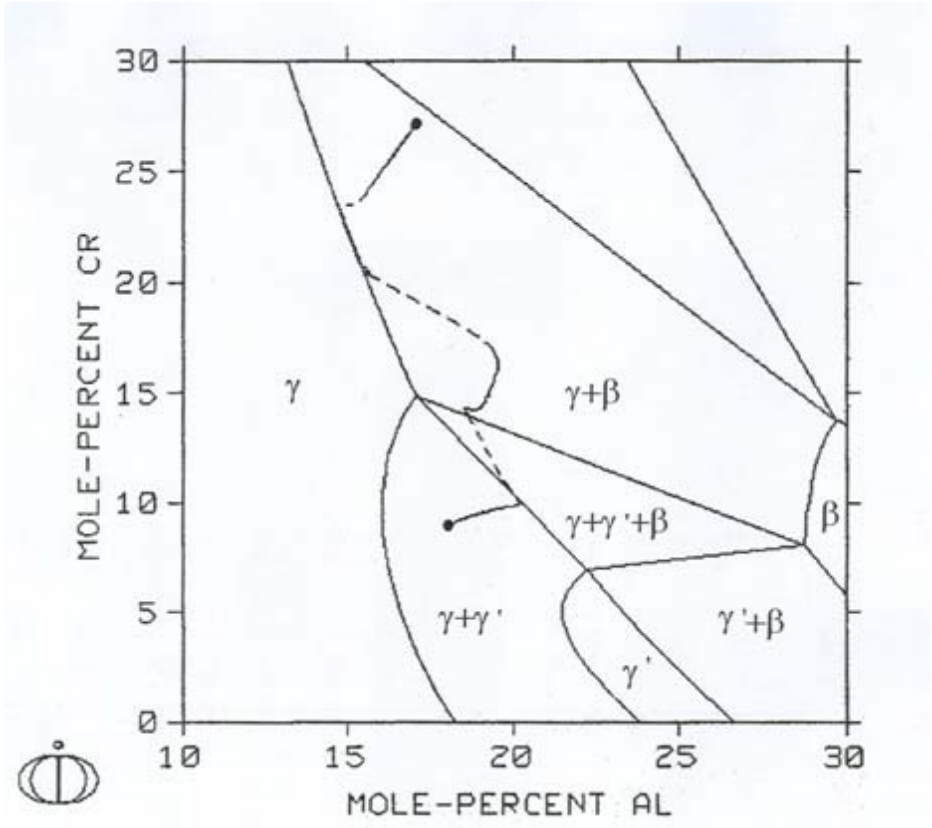


Fig. 10—Typical microstructure of the interdiffusion region of the β-Ni50Al *vs* γ-Ni30.9Cr9.9Al (1150 °C/49 h) diffusion couple.

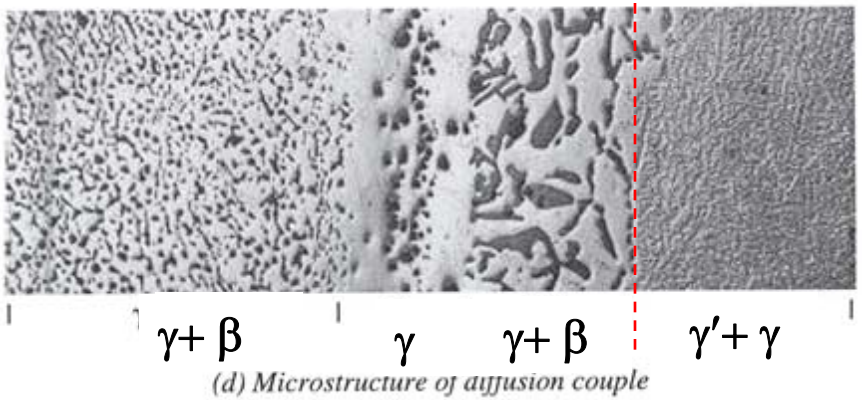
$$\beta > \alpha + \beta > \gamma'$$

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

Dictra simulations of boundaries using the disperse system model



Diffusion Couple microstructure



(d) Microstructure of diffusion couple

$$\gamma + \beta < \gamma > \gamma + \beta > \gamma + \gamma'$$

Xin Qiao, M.S. 1998, Univ. Conn.

Dictra simulations of Type 3 boundaries using the homogenization model

Settings

- Homogenization functions: Hashin Shtrikman lower bounds
  (Wiener bounds, Hashin Shtrikman bounds, Labyrinth factor)
- Degree of implicity when integrating PDEs: 0.5
  (0.0 Euler forwards, 0.5 Trapezoidal rule, 1.0 Euler backwards)
- Ideal flux contribution for fluctuations in composition: 0.05
  (range .01-.05)

Key references on the homogenization model

ELSEVIER

Available online at www.sciencedirect.com
SCIENCE DIRECT®

Acta Materialia 54 (2006) 2431–2439

Acta MATERIALIA
www.actamat-journals.com

A homogenization approach to diffusion simulations applied to $\alpha + \gamma$ Fe–Cr–Ni diffusion couples

Henrik Larsson [a,*], Anders Engström [b]

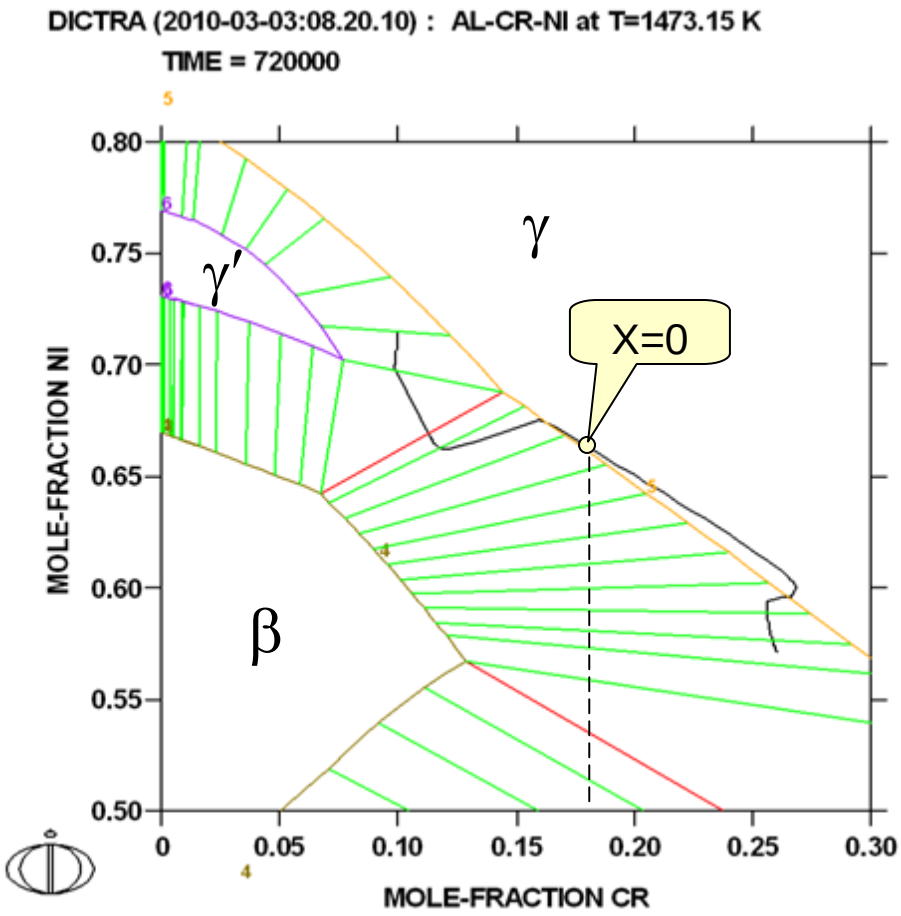
[a] *Division of Physical Metallurgy, Department of Materials Science and Engineering, Brinellv. 23, The Royal Institute of Technology (KTH), SE-100 44 Stockholm, Sweden*
[b] *Thermo-Calc Software, Stockholm Technology Park, SE-113 47 Stockholm, Sweden*

Received 11 November 2005; received in revised form 20 January 2006; accepted 22 January 2006
Available online 13 March 2006

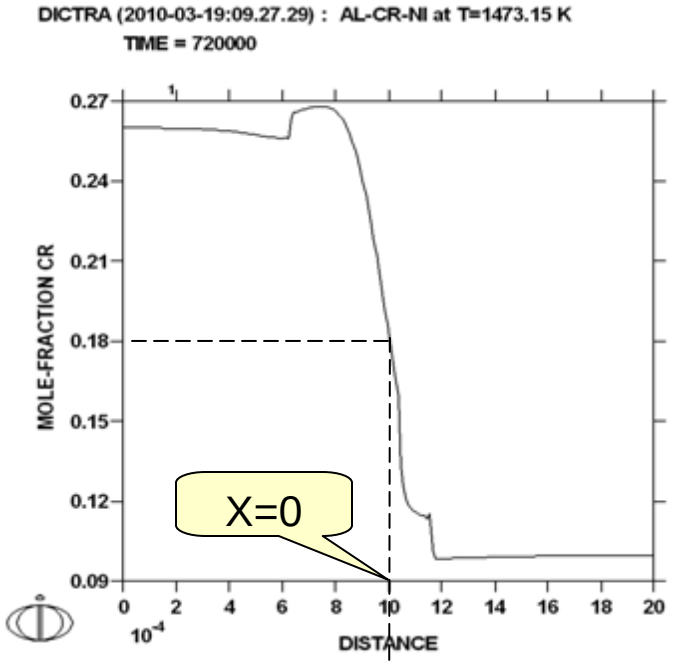
Also

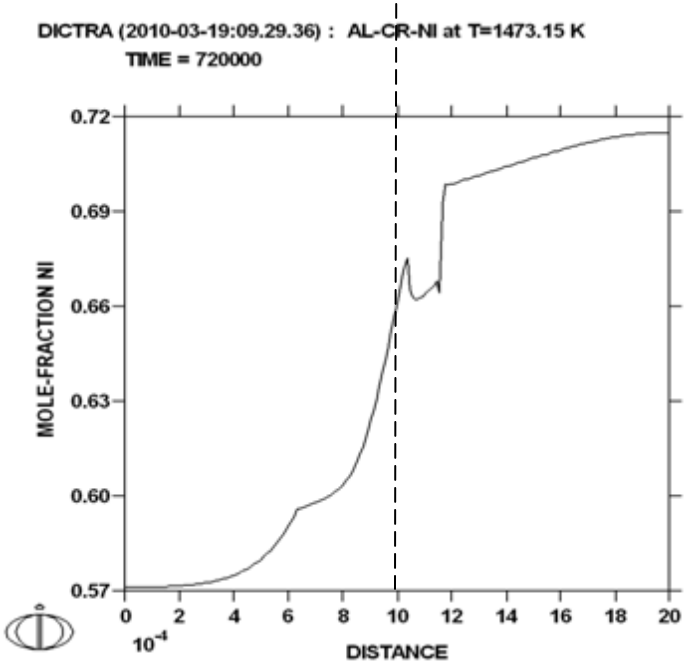
Multiphase diffusion simulations in 1D using the Dictra Homogenization model
Henrik Larsson. Lars Hoglund
CALPHAD, 33(2009) 495-501

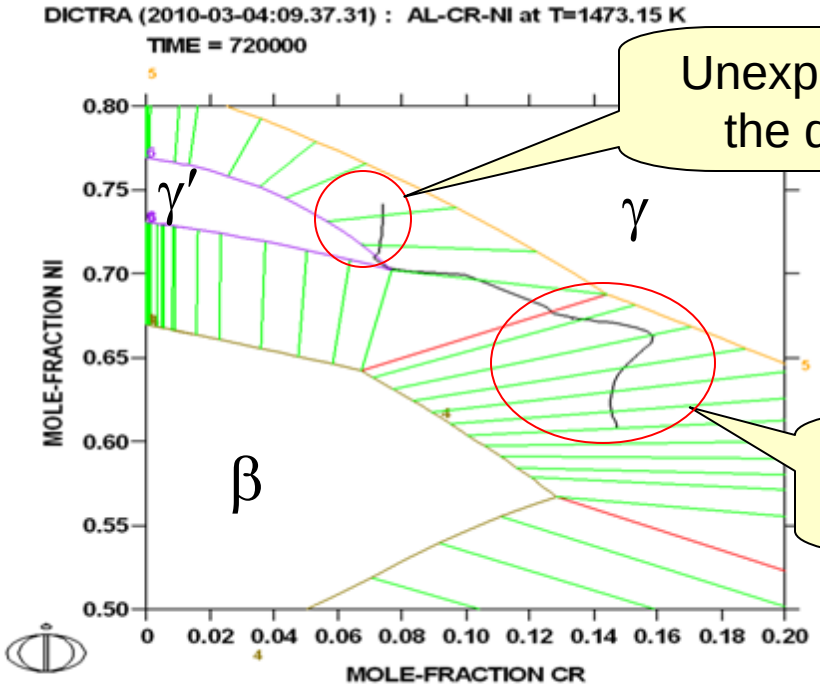
Dictra simulation using the Homogenization model



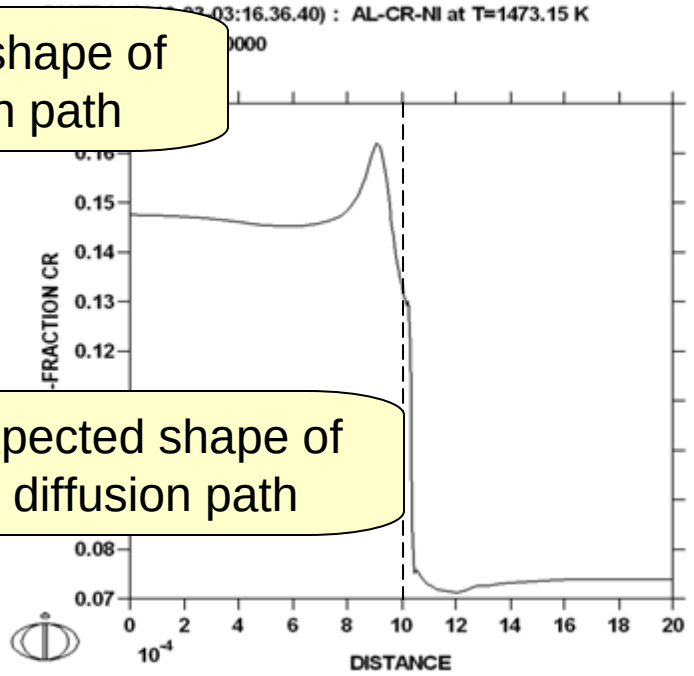
$$\gamma + \gamma' < \gamma + \beta < \gamma > \gamma + \beta$$



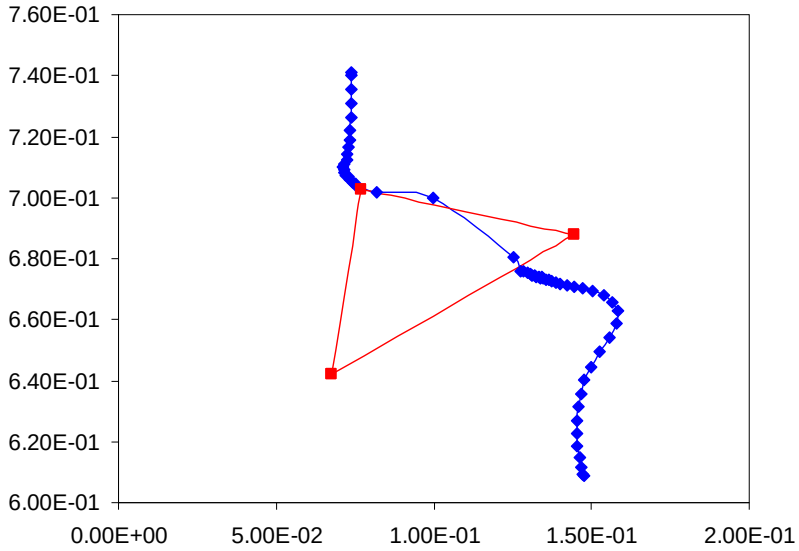


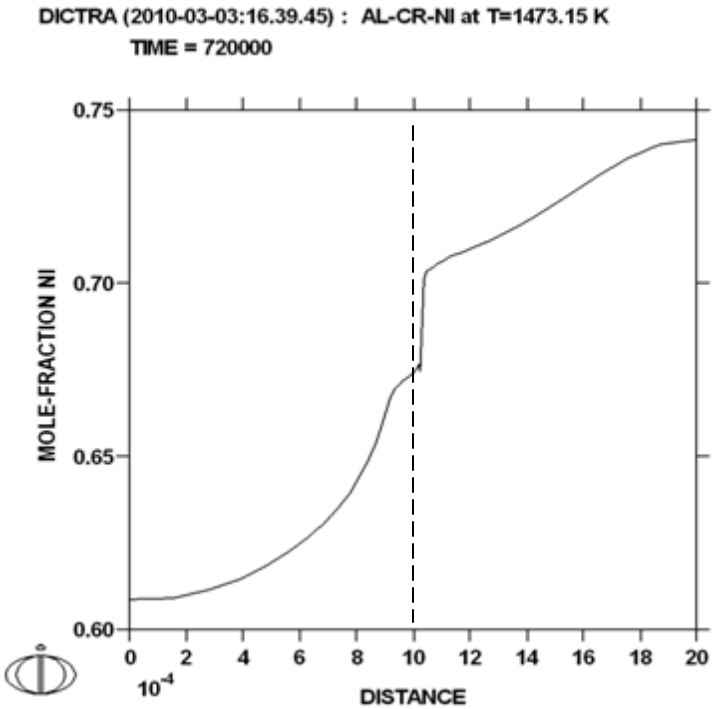


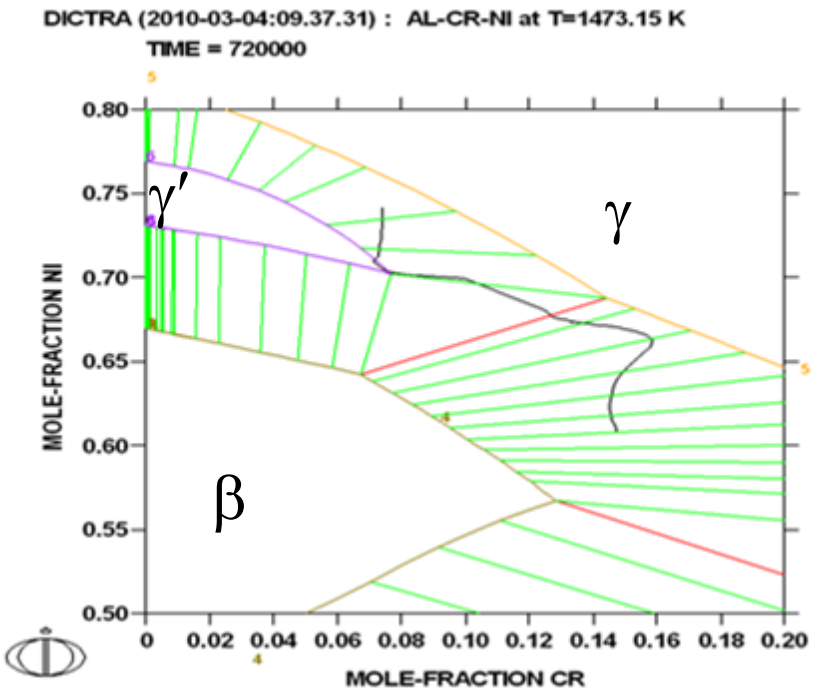
Unexpected shape of the diffusion path

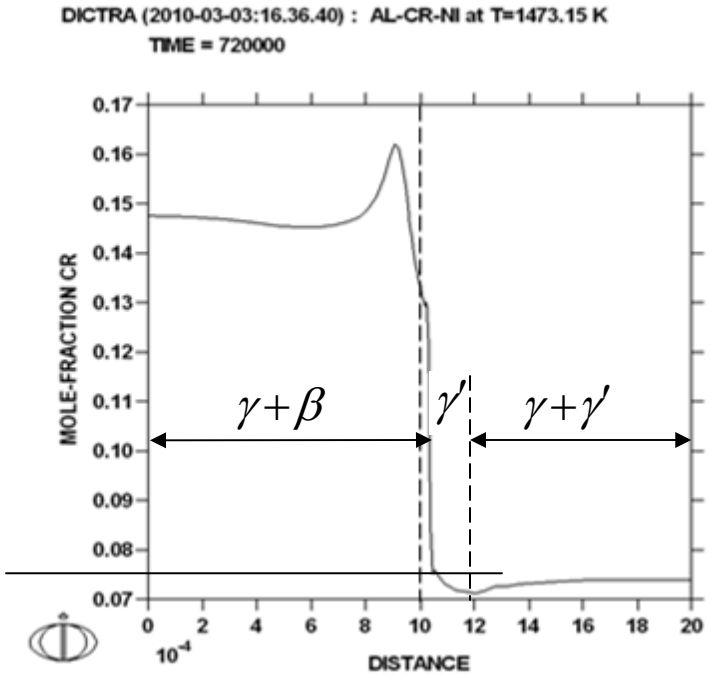


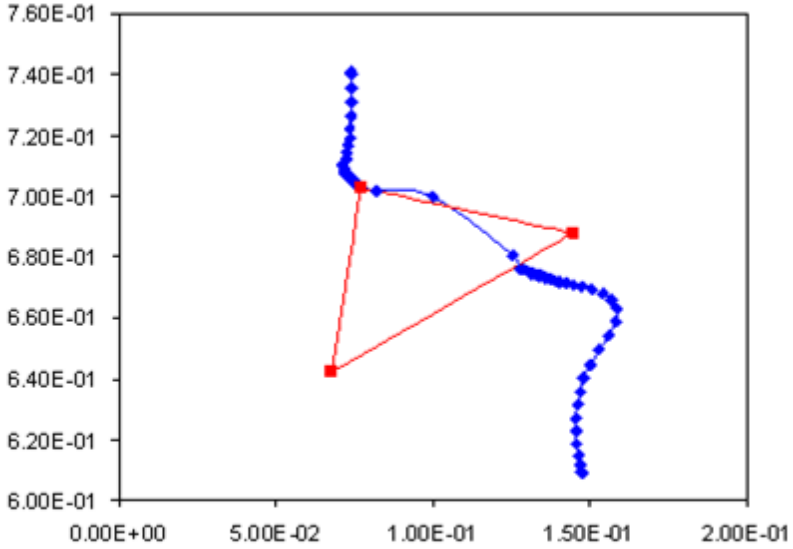
Unexpected shape of the diffusion path

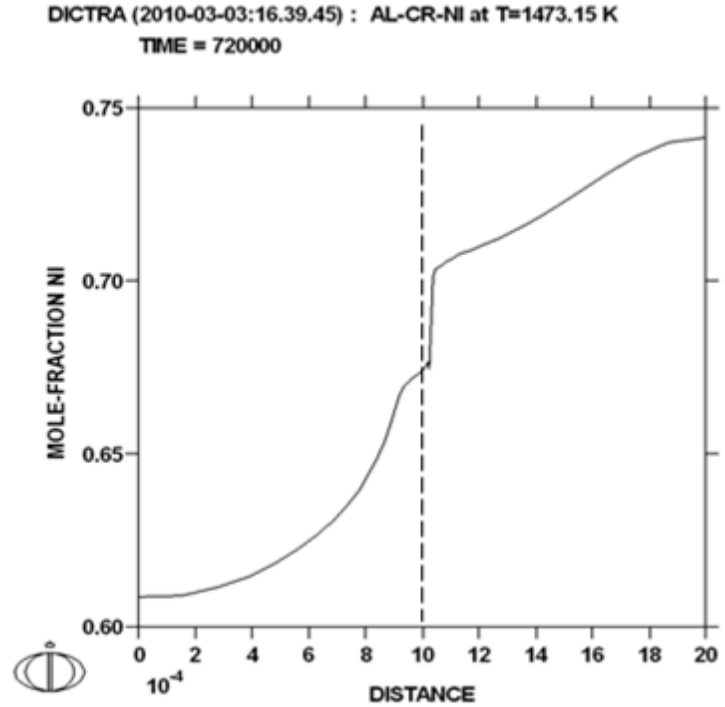




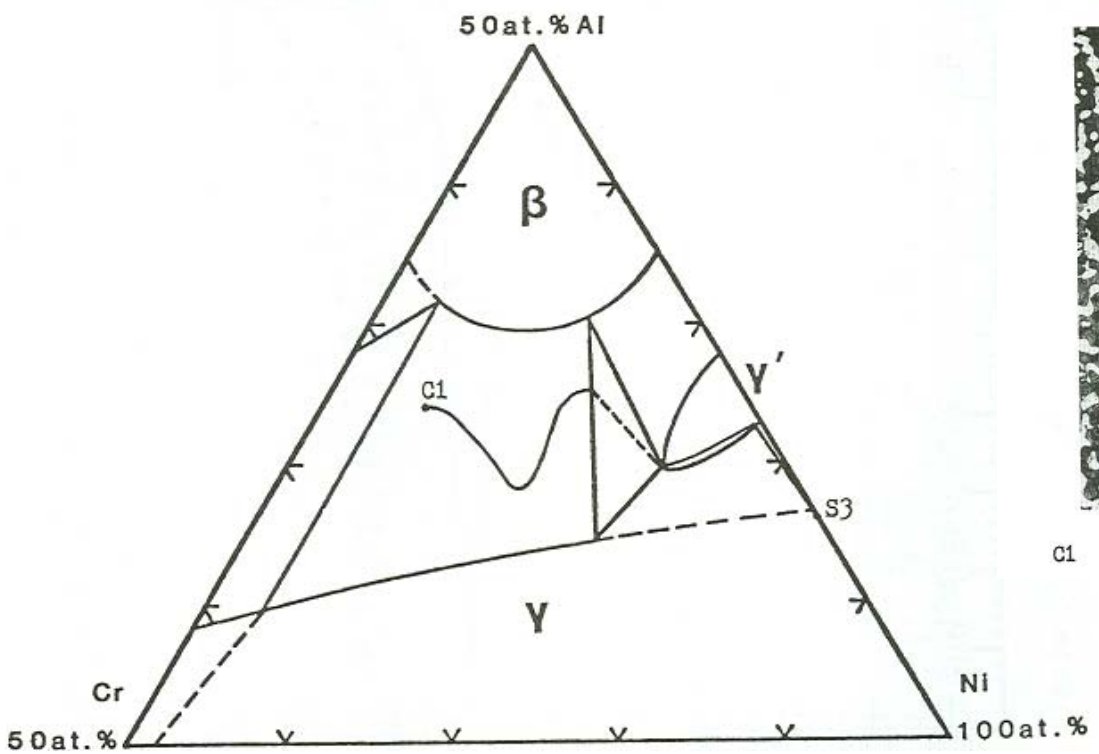

DICTRA (2010-03-04:09.37.31) : AL-CR-NI at T=1473.15 K
TIME = 720000
γ′
γ
β
MOLE-FRACTION NI
MOLE-FRACTION CR
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
0.18
0.20

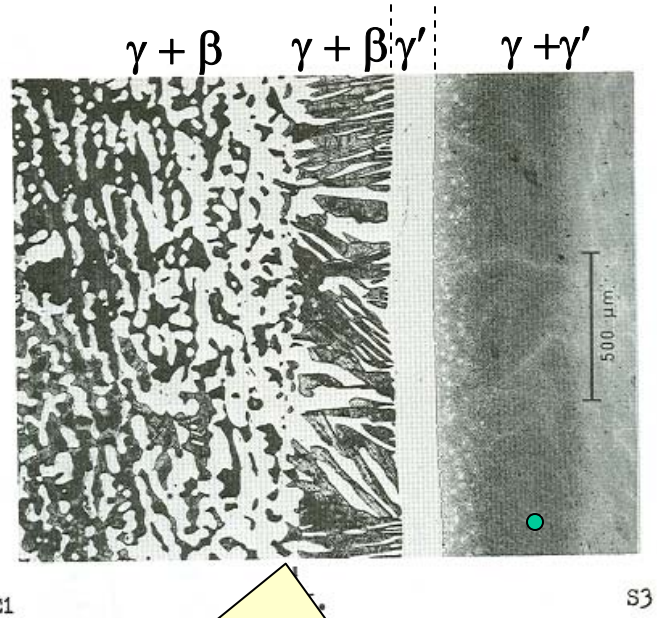

DICTRA (2010-03-03:16.36.40) : AL-CR-NI at T=1473.15 K
TIME = 720000
γ+β
γ′
γ+γ′
MOLE-FRACTION CR
DISTANCE
10⁻⁴
0.17
0.16
0.15
0.14
0.13
0.12
0.11
0.10
0.09
0.08
0.07
0
2
4
6
8
10
12
14
16
18
20


7.60E-01
7.40E-01
7.20E-01
7.00E-01
6.80E-01
6.60E-01
6.40E-01
6.20E-01
6.00E-01
0.00E+00
5.00E-02
1.00E-01
1.50E-01
2.00E-01


DICTRA (2010-03-03:16.39.45) : AL-CR-NI at T=1473.15 K
TIME = 720000
MOLE-FRACTION NI
DISTANCE
10⁻⁴
0.75
0.70
0.65
0.60
0
2
4
6
8
10
12
14
16
18
20

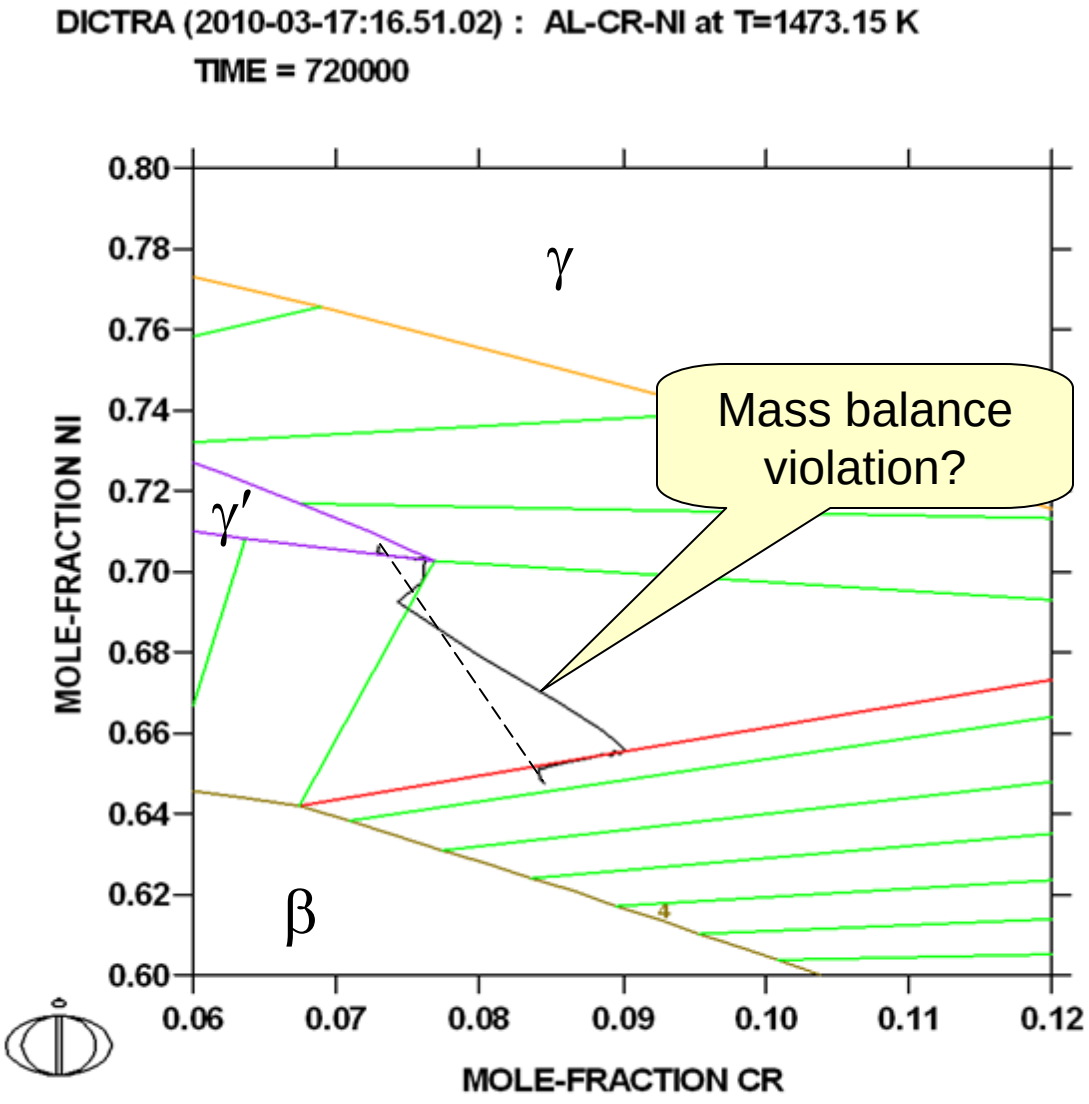
Similar diffusion path in the γ+β region given in the NASA Report

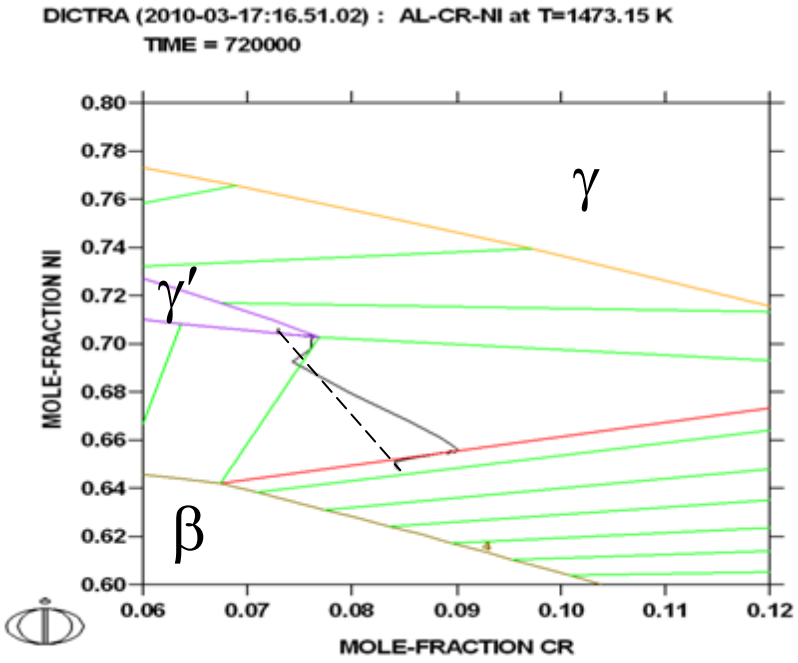


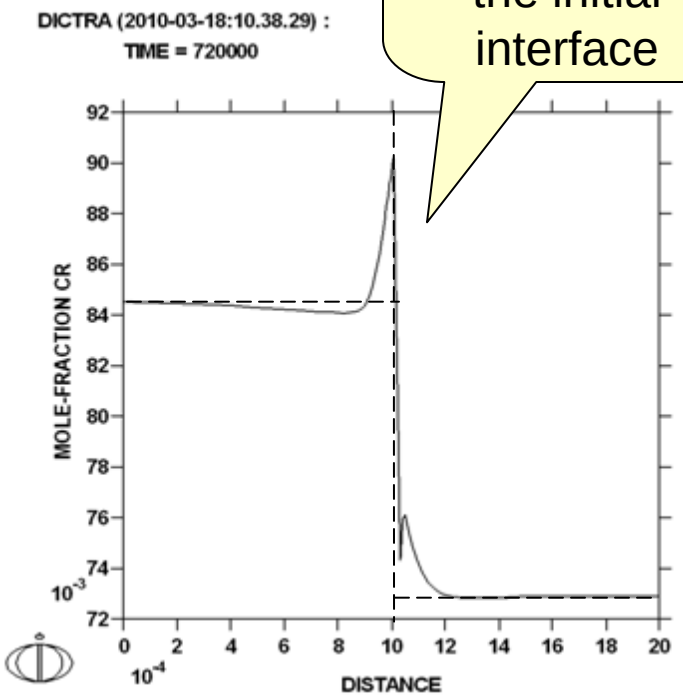


But the microstructure shows a sharp Type 0 boundary

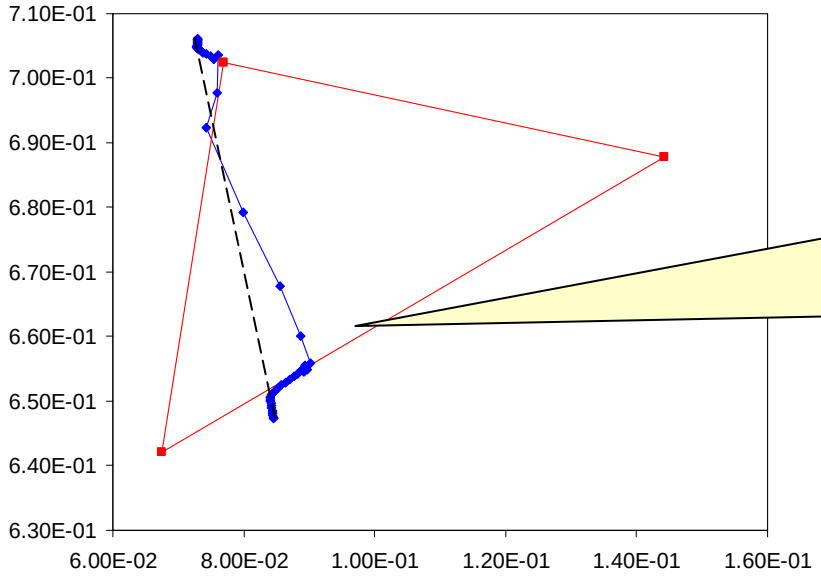
From: Lawrence A. Carol, NASA Contractor Report 174852, 1985.


DICTRA (2010-03-17:16.51.02) : AL-CR-NI at T=1473.15 K
TIME = 720000
0.80
0.78
0.76
0.74
0.72
0.70
0.68
0.66
0.64
0.62
0.60
MOLE-FRACTION NI
0.06
0.07
0.08
0.09
0.10
0.11
0.12
MOLE-FRACTION CR
γ
γ′
β
Mass balance violation?



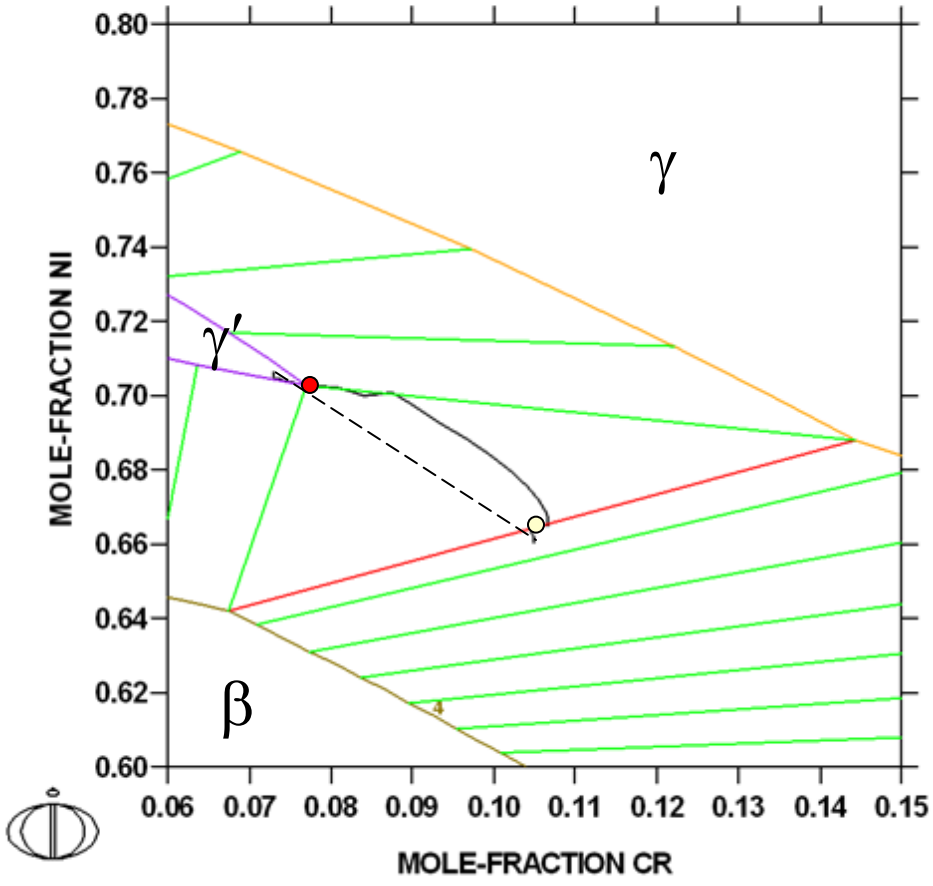


Extra Cr on both sides of the initial interface

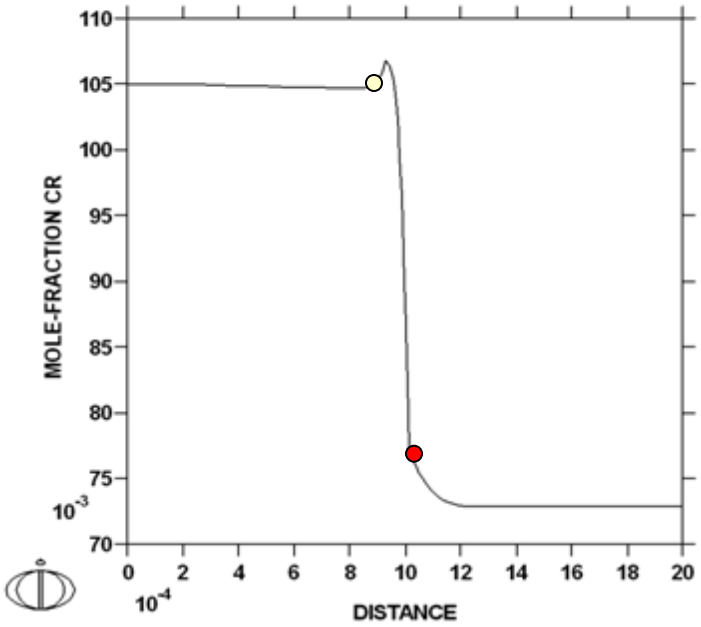


Diffusion path doesn't cross the line between the initial alloys

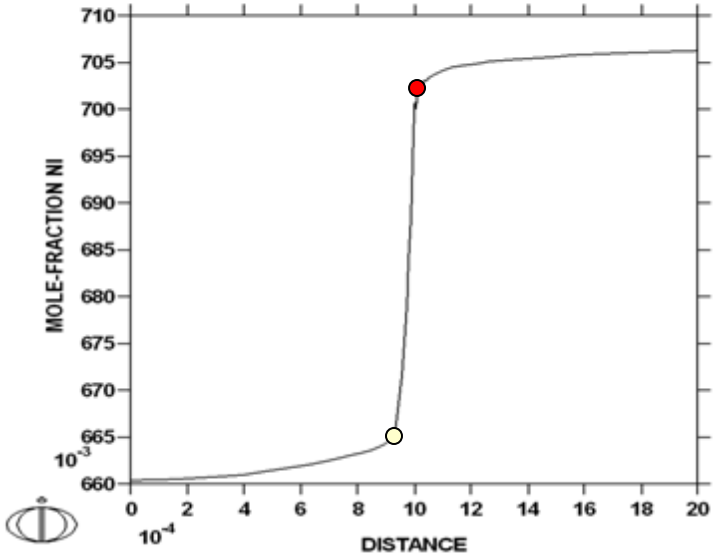
DICTRA (2010-03-19:08.20.11) : AL-CR-NI at T=1473.15 K
TIME = 720000



DICTRA (2010-03-19:09.33.01) : AL-CR-NI at T=1473.15 K
TIME = 720000



DICTRA (2010-03-19:09.34.23) : AL-CR-NI at T=1473.15 K
TIME = 720000



Summary

- Homogenization model successfully predicted a Type 3 boundary

- Questionable observations in homogenization model simulations
  - diffusion path at a Type 1a boundary
  - large deviations from a linear diffusion path in a two phase region
  - apparent mass balance violation