TMS Annual Meeting
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Diffusion Paths and Interdiffusion Microstructures

Applications and Remaining Challenges

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OUTLINE

- Appreciation
- A well defined goal
- Predicting microstructures with the Phase Field Method and DICTRA
- Three questions about interdiffusion microstructures
- Applications
- Remaining Challenges
- Conclusions

My Father

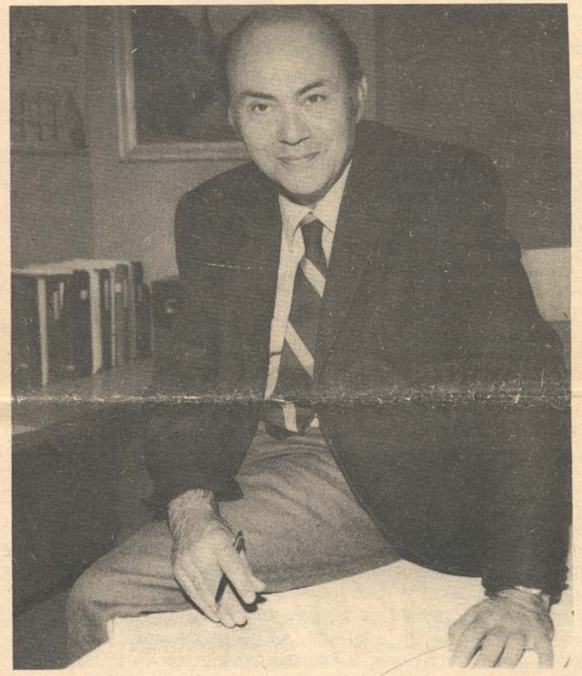
This is "Mr. Cobalt"

Dr. F.R. Morral has been in charge of the Cobalt Information Center Project at Battelle's Columbus Laboratories, Columbus, Ohio, from its beginning in 1956. Since that time he has visited extensively with companies and universities in North America. Occasional visits have also been made to countries in South America and Europe and he has lectured in 18 countries.

Dr. Morral arrived in America from Spain in 1926. He obtained his B.S. in electrochemical engineering at Massachusetts Institute of Technology in 1932. He then hitchhiked cross-country to see the Olympics being held in Los Angeles, Calif. That winter he did graduate work on physical metallurgy and X-ray diffraction crystal analysis in Sweden at the University of Stockholm and the Metallorgrafiska Institutet.

After marrying, he returned to Spain for two years where he was involved in research with the University of Barcelona, managed a textile mill and published a metallurgical monthly. He then returned to the United States and in 1940 obtained his Ph.D. in metallurgy from Purdue University.

He has been involved in research, development, production, and management, and teaching metallurgy as an employe of Purdue University, Continental Steel Corporation, Pennsylvania State University, Mellon Institute for Industrial Research, American Cyanamid Company, Syracuse University, and Kaiser Aluminum and Chemical Corporation.



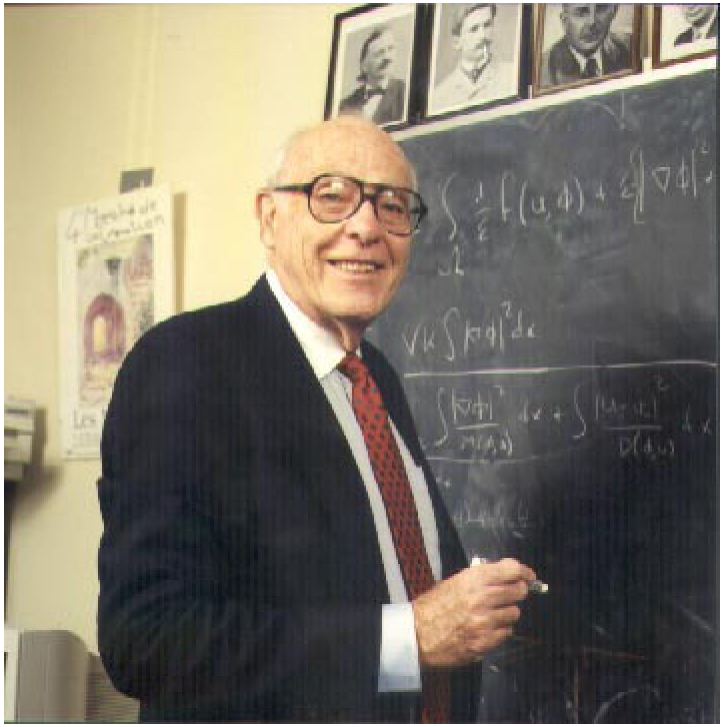
Dr. F. R. Morral

Because of Dr. Morral's interest in education, science, technology, and professionalism, he helped start The Spokane Technical Council (1952-1956), and the Columbus Technical Council (1957-1969), has been an officer of local ASM and AIME Sections, and is a member of 18 national and international scientific and technical societies. He is a Fellow of Sigma Xi, American Association for the Advancement of Science, Ohio Academy of Science, and Institute of Chemists.

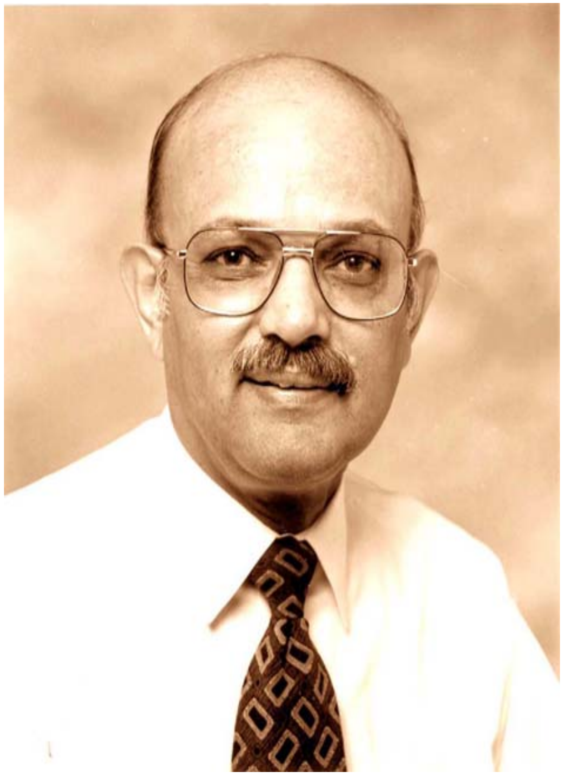
In 1969, the Spanish Royal Academy of Sciences elected him

(Continued on page 8A)

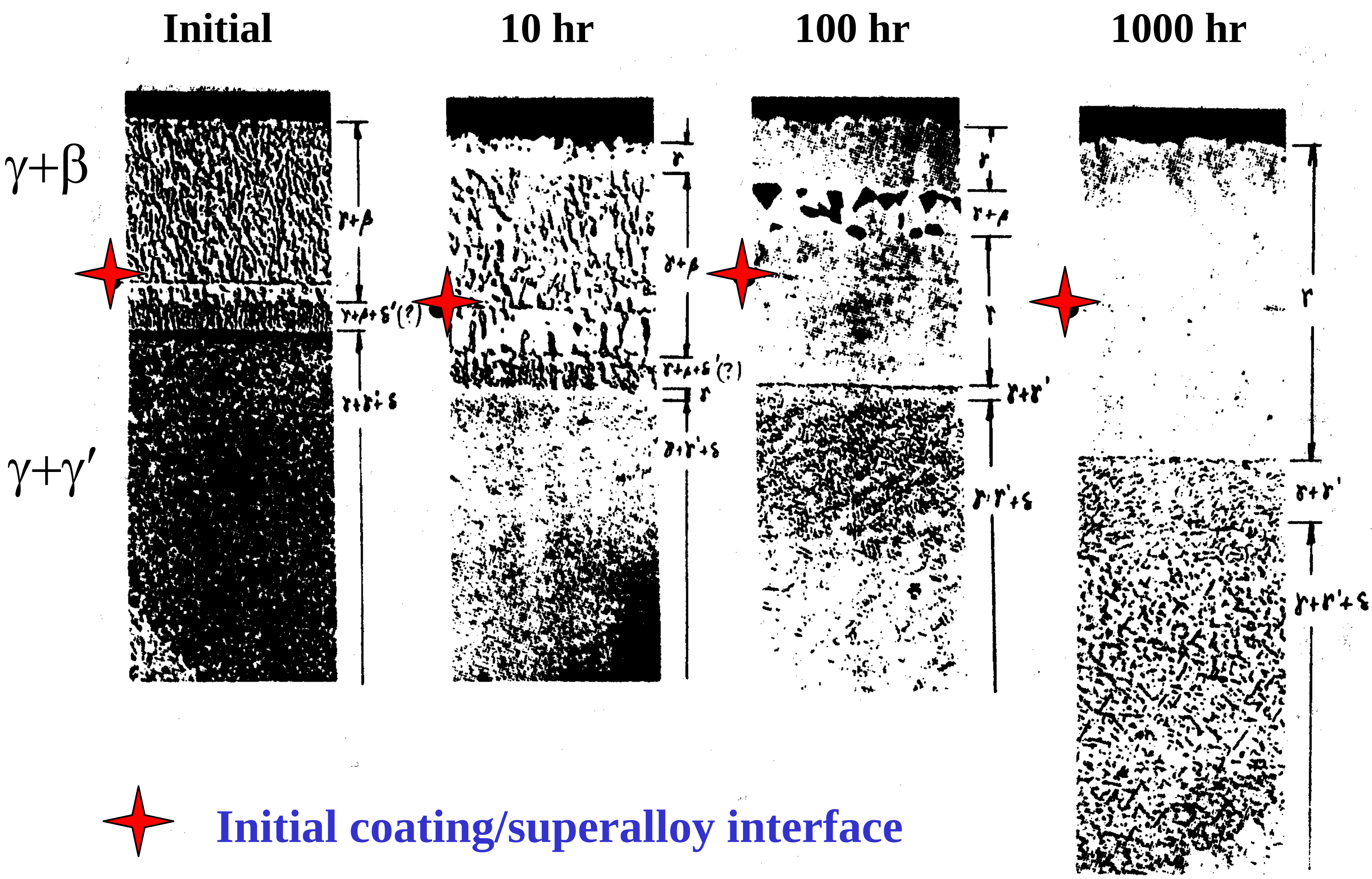
My Teacher and Mentor



My Multicomponent Diffusion Protagonist

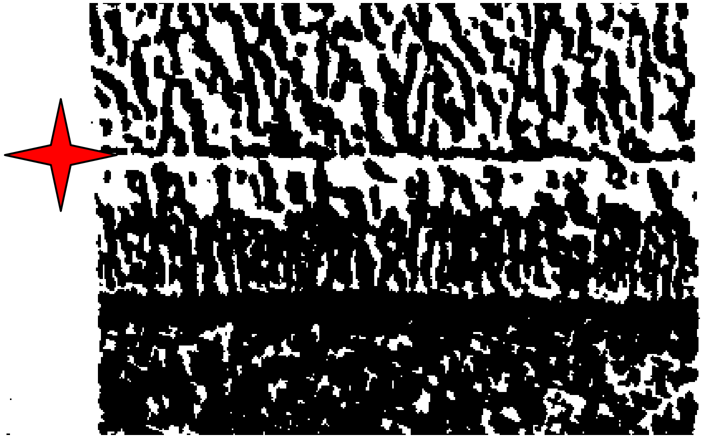


Interdiffusion microstructures seen in coated turbine blades during the summer of 1980.



Initial coating/superalloy interface

Magnified view of interdiffusion microstructures seen in coated turbine blades



A Simple Well Defined Goal

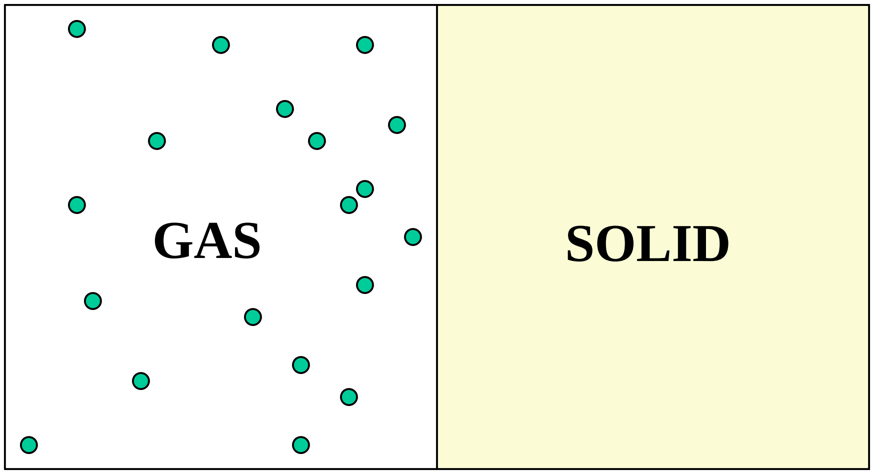
Predict the microstructure that occurs when two materials interdiffuse.

Diffusion Couple model

$$c(x,t) = c^{ave} + \Delta C \, erf\left(\frac{x}{2\sqrt{Dt}}\right)$$

Application to gas-solid reactions

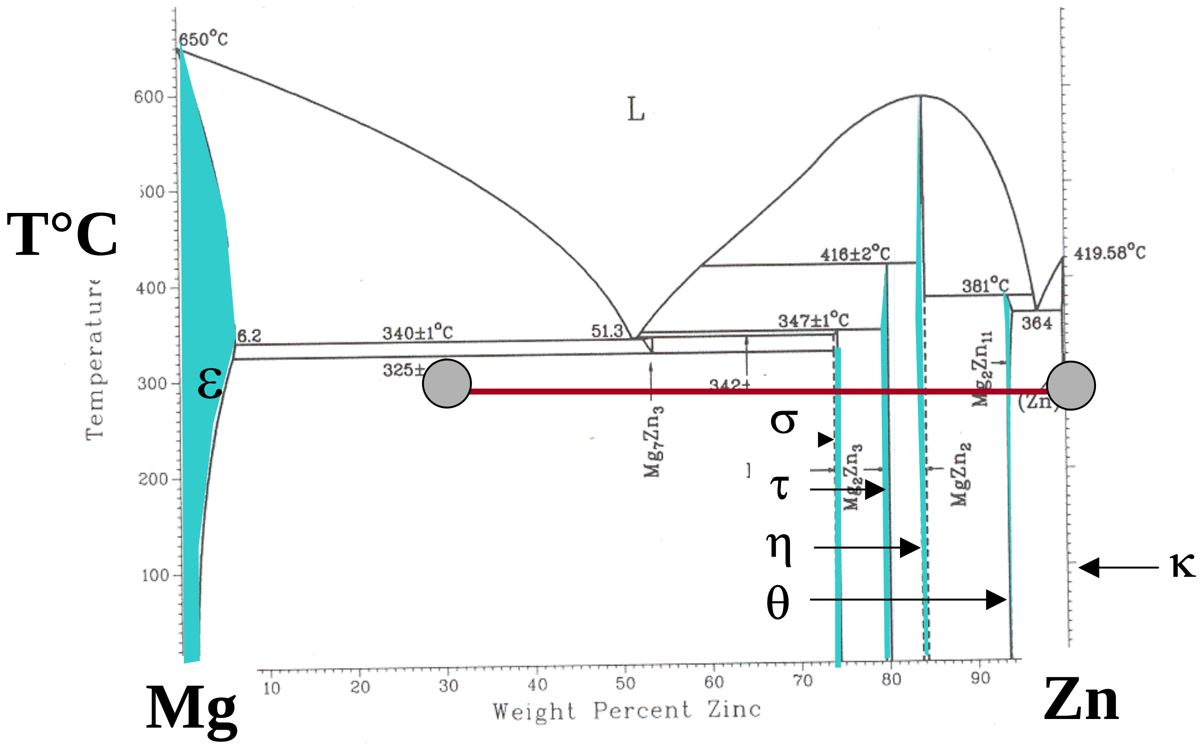
Treat the solid like half a diffusion couple



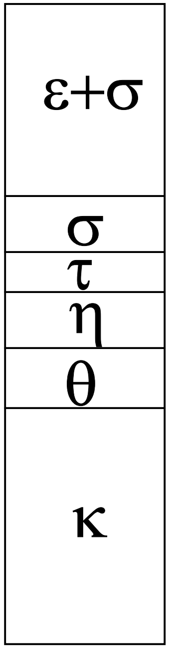
X = 0

Predicting microstructures in binary systems with diffusion paths

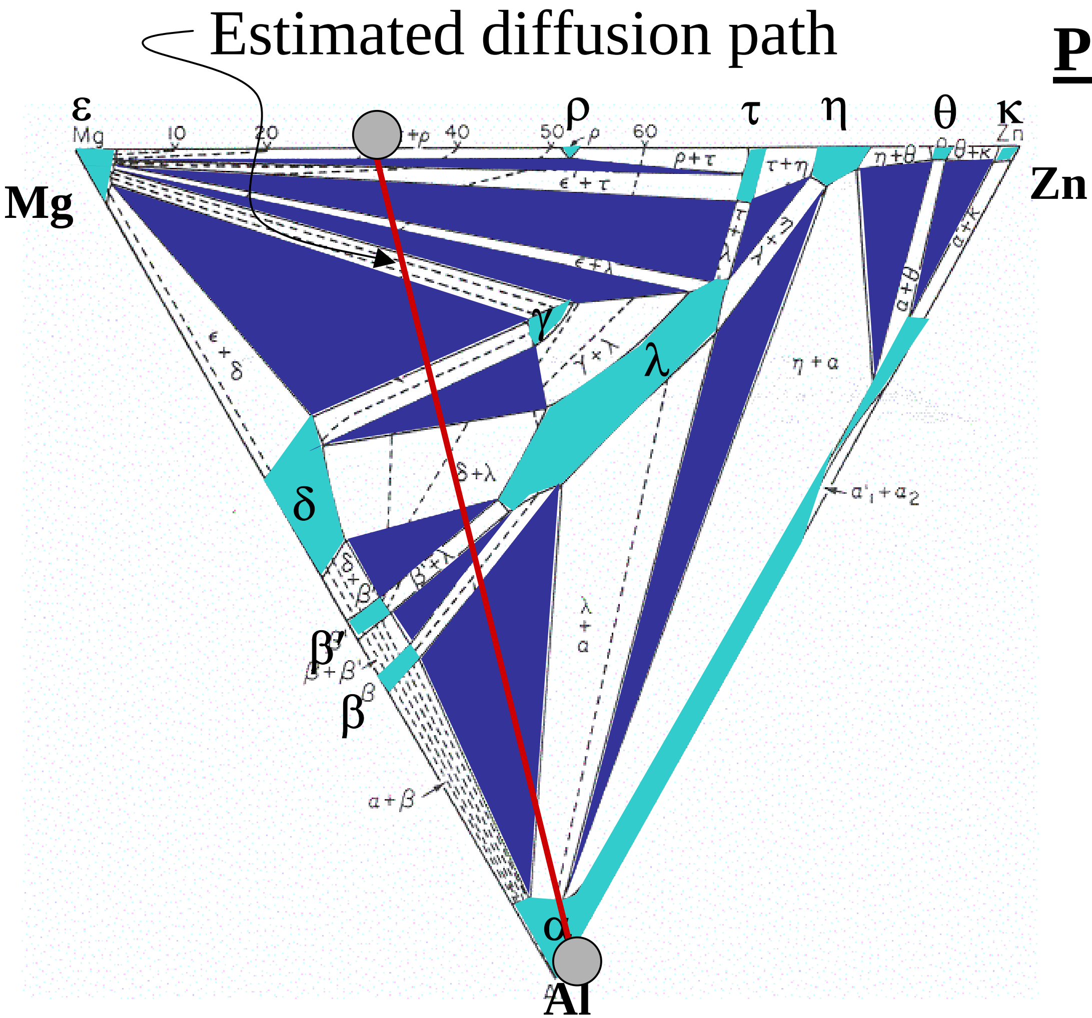
- Draw an isothermal line between initial alloys on the phase diagram.
- Assume all single phase regions yield a layer in the microstructure.



Predicted



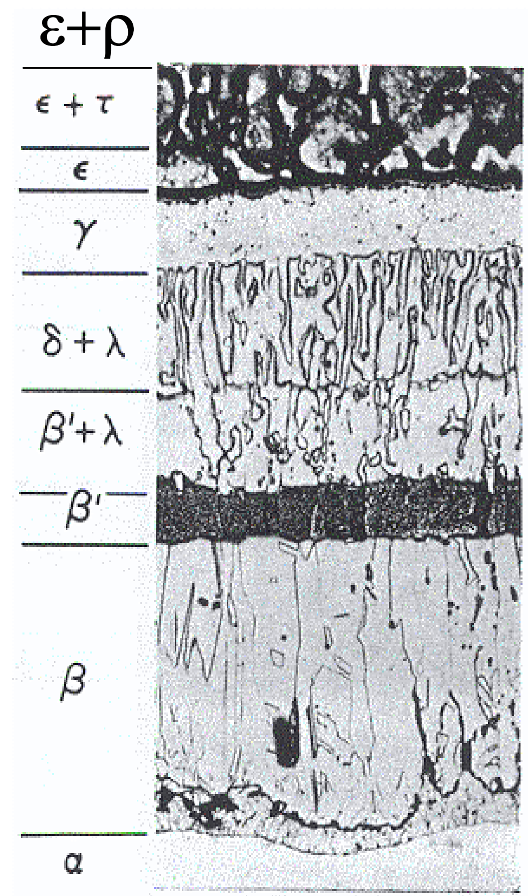
Predicting microstructures in ternary systems



Predicted

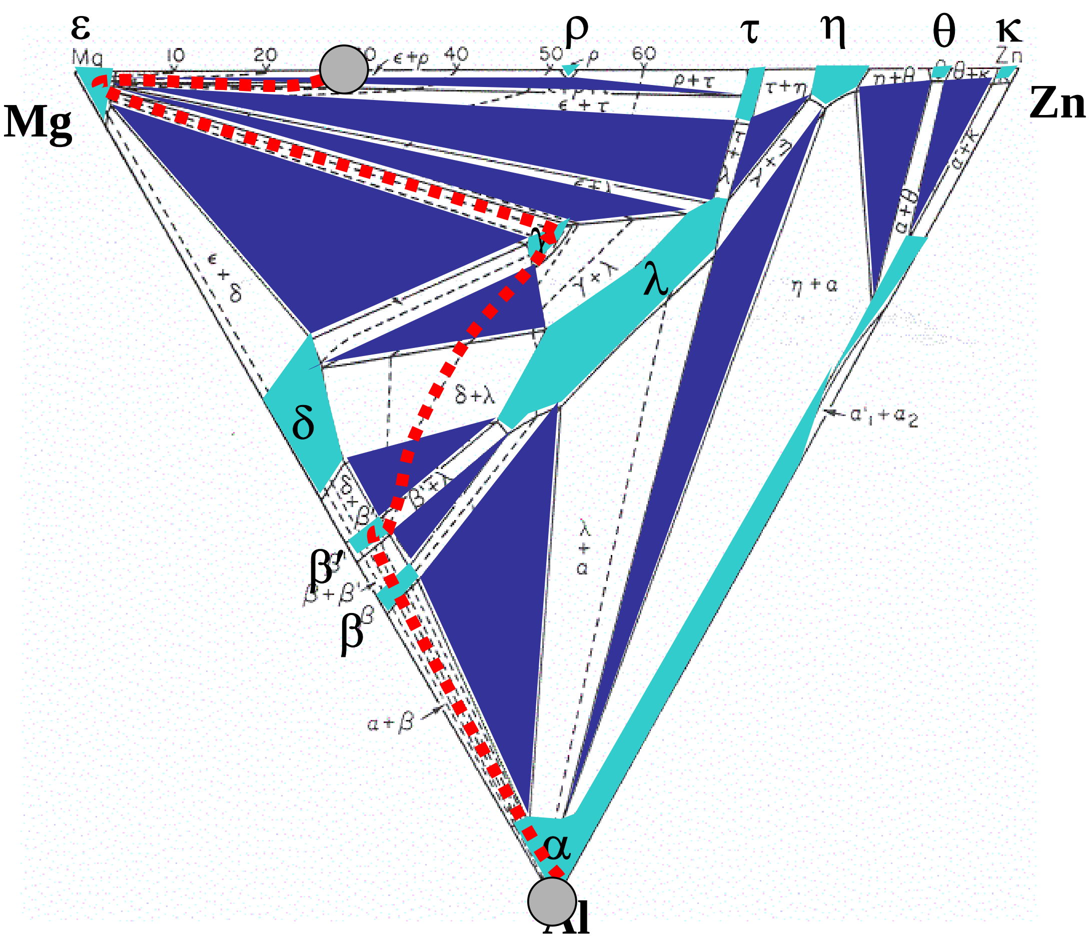
ε+ρ
ε+τ
ε+λ
ε+γ
δ+γ
δ+λ
β′+λ
β+λ
α+λ
α

Actual

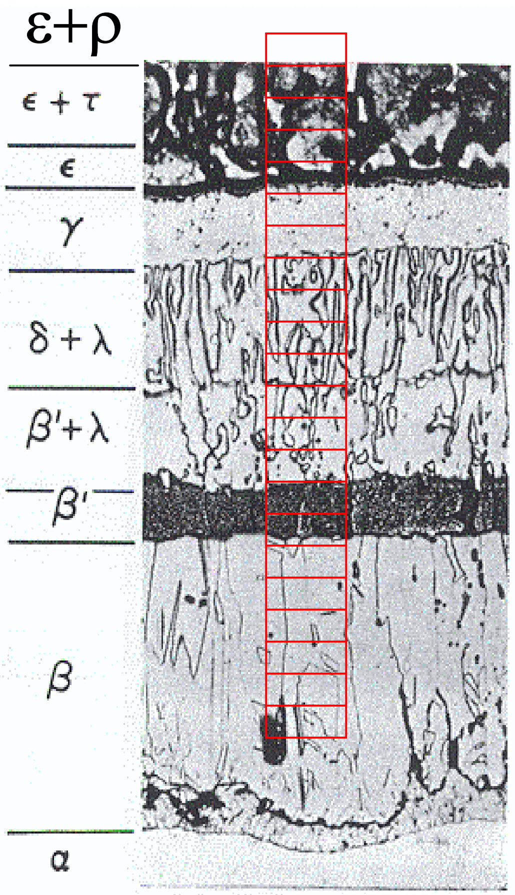


Clark & Rhines.Trans.ASM 51(1959)206

Actual diffusion path

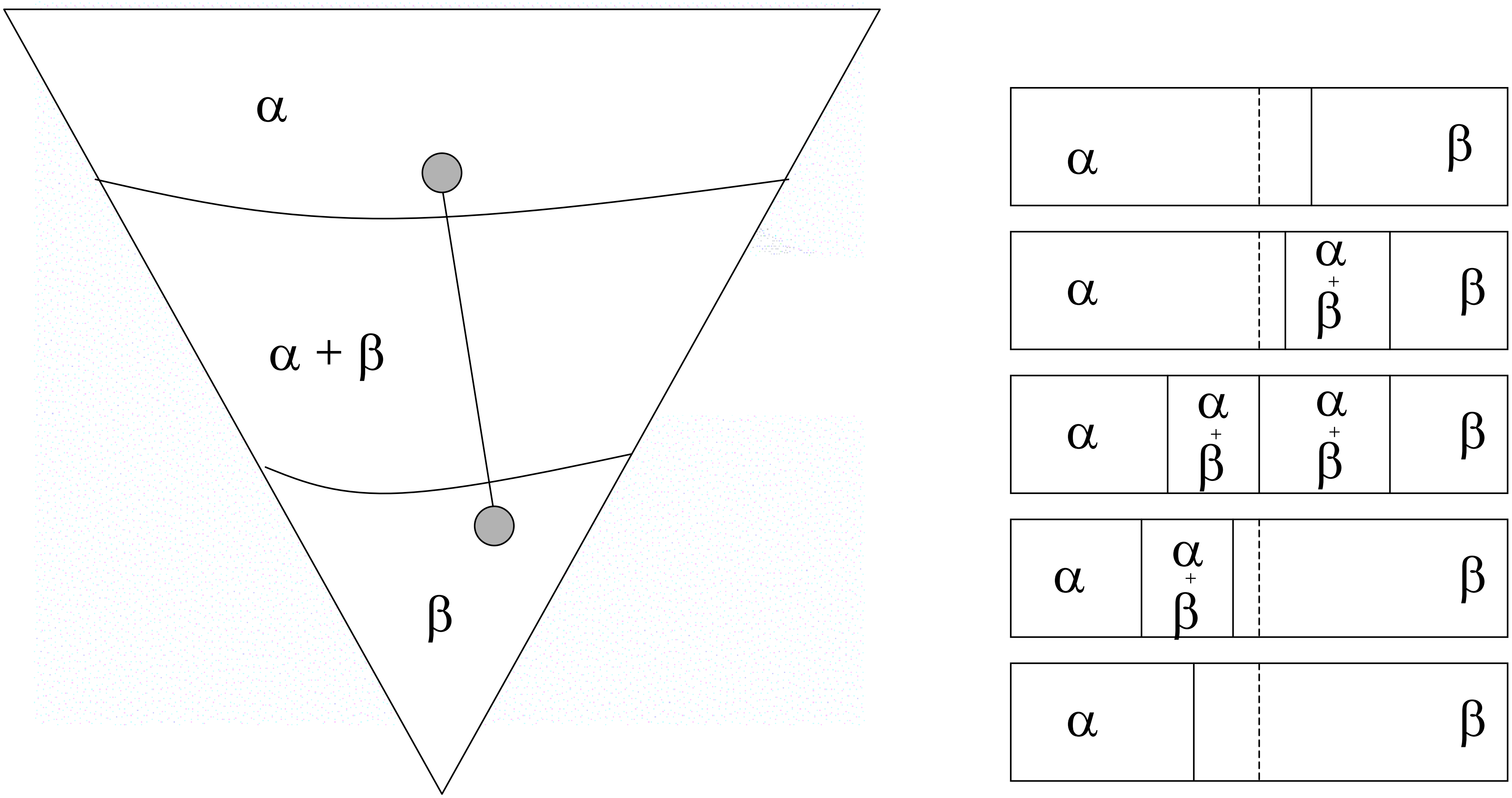


Ave composition measurements



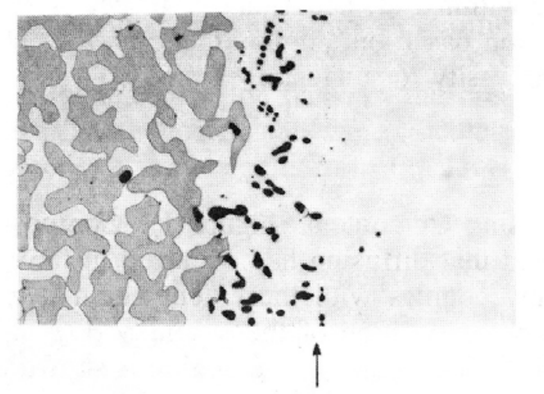
Clark & Rhines.Trans.ASM 51(1959)206

Five possible microstructures when two single phase alloys interdiffuse.

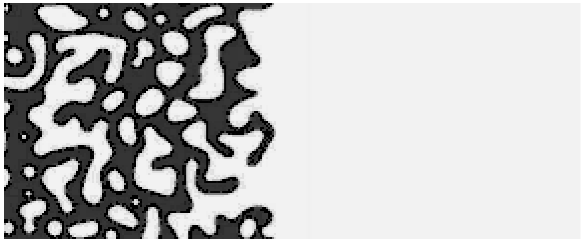


Phase Field Simulation of an interdiffusion microstructure compared with experiment

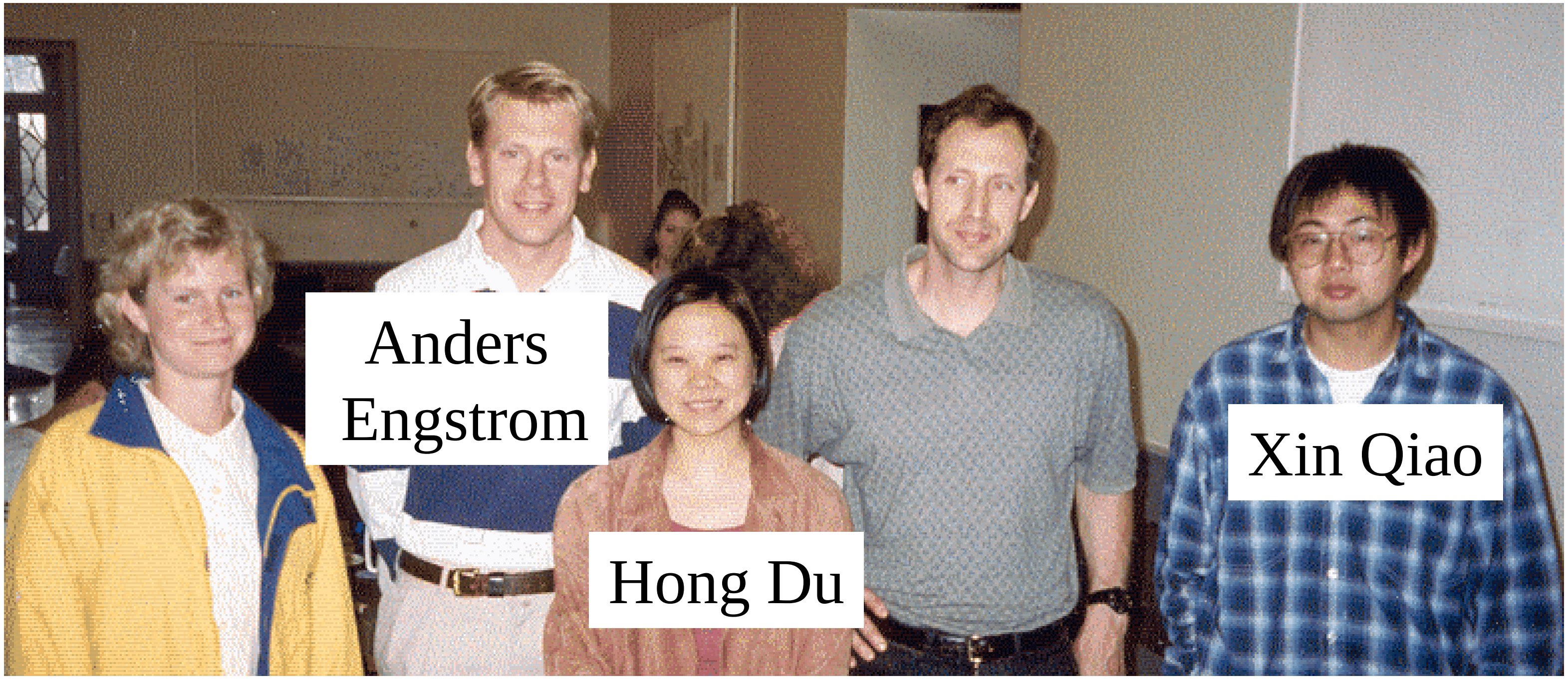
Experimental Ni-Cr-Al Microstructure



Phase Field Ni-Cr-Al Simulation

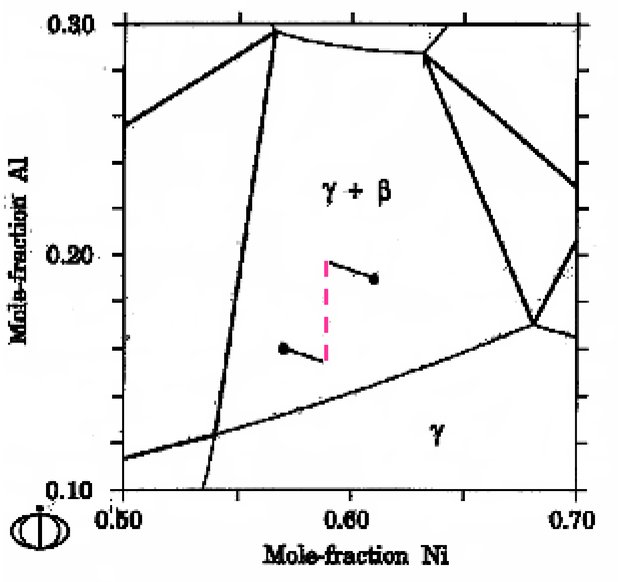


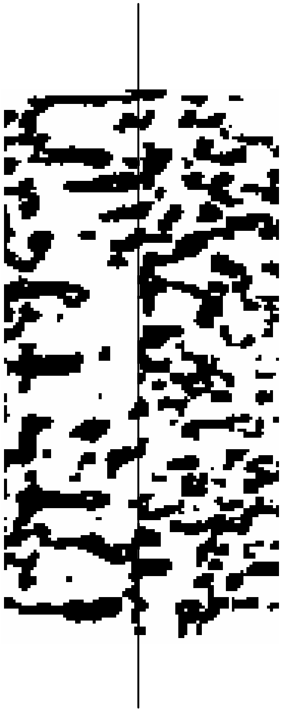
DICTRA and the 1994 Solid-Solid Phase Transformations Meeting in Nemacolin Woodlands, USA



DICTRA simulation of a (γ+β)/(γ+β) diffusion couple and its interpretation

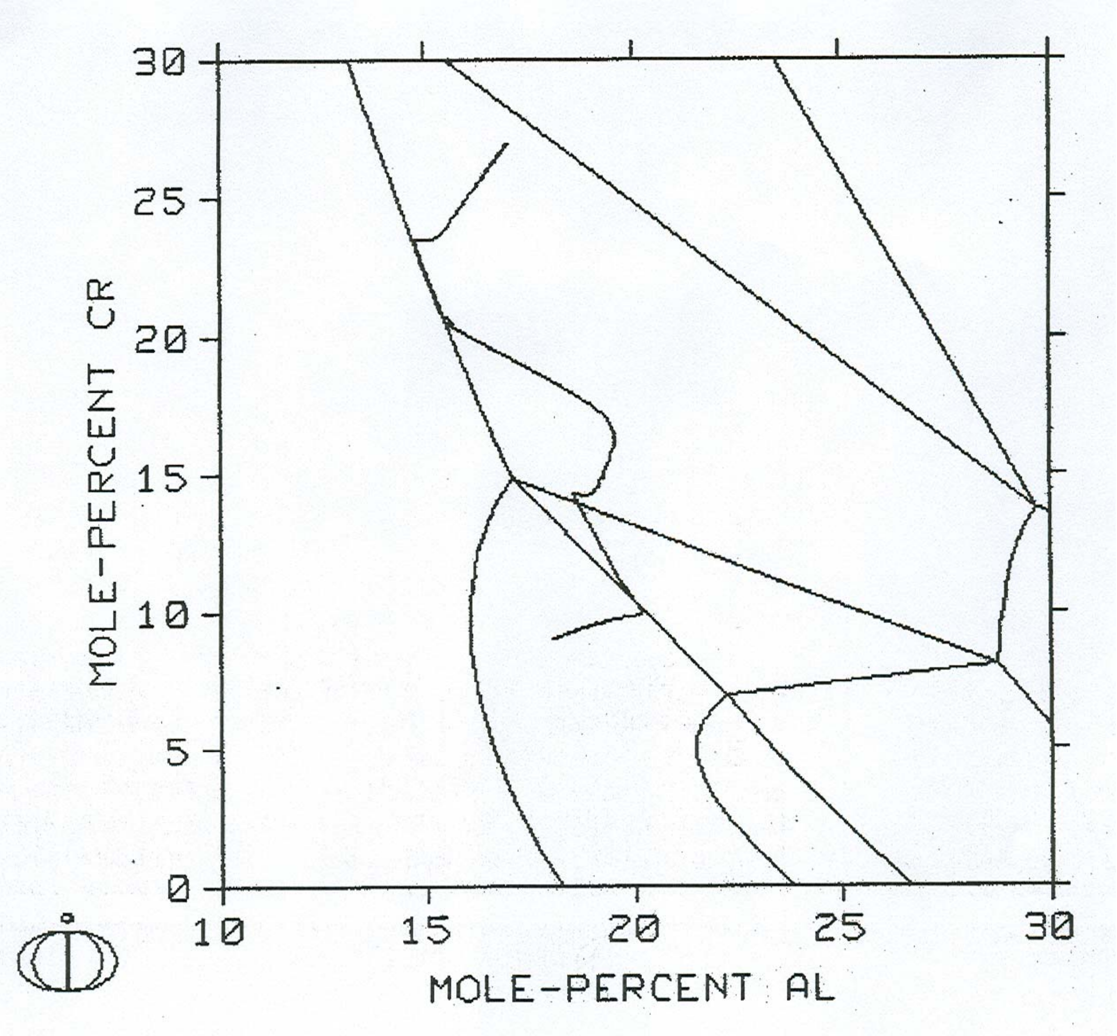
Segmentation of the predicted diffusion path



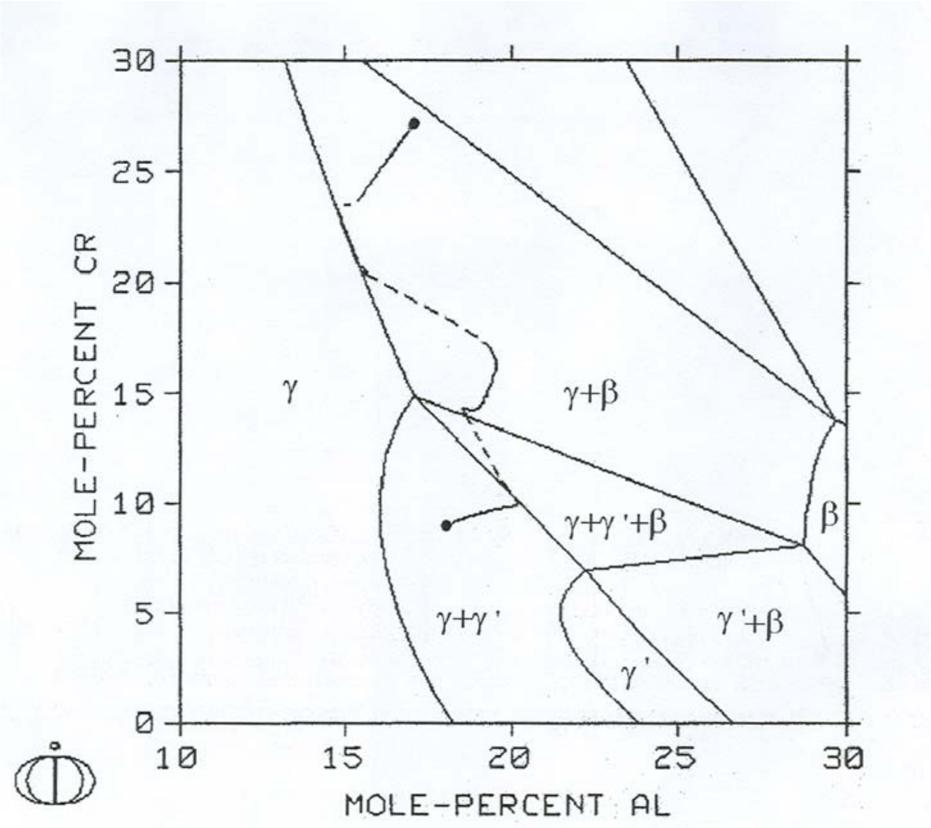


Anders Engstrom, J.E. Morral and John Ågren. Acta Mater. 45 (1997) 1189-1199.

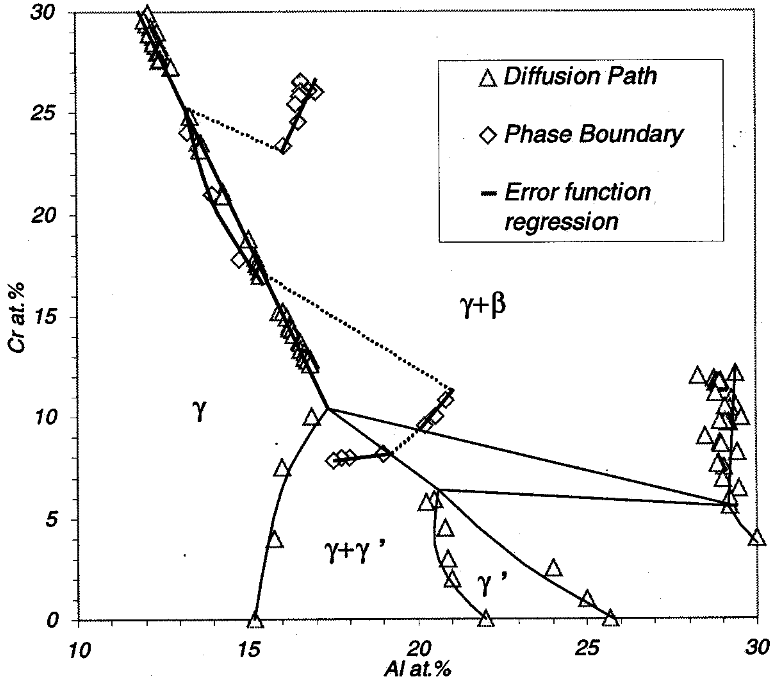
DICTRA simulation of a complex diffusion path



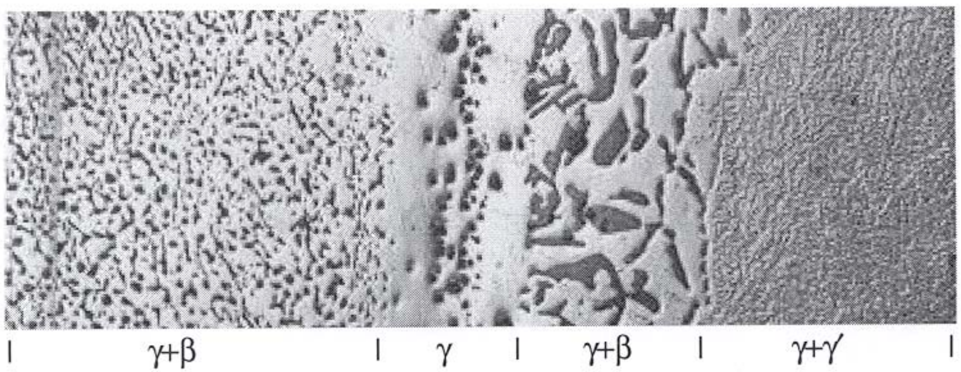
DICTRA simulation after naming the phase diagram regions and segmenting the diffusion path



Experimental verification of the DICTRA simulation



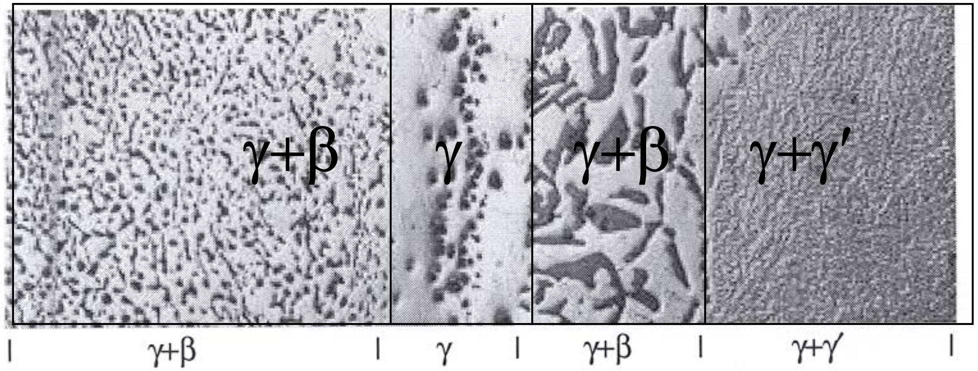
(c) Diffusion path of diffusion couple



(d) Microstructure of diffusion couple

Xin Qiao. M.S. Thesis. University of Connecticut. 1998

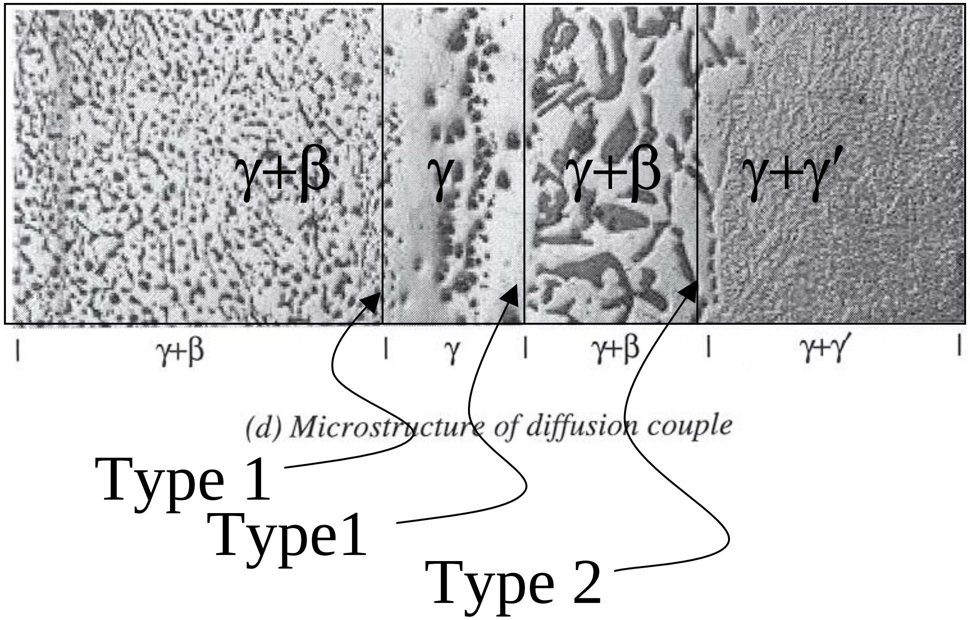
Three questions about interdiffusion microstructures



(d) Microstructure of diffusion couple

1. How can one classify the boundaries between regions?
2. Which way do the boundaries move?
3. How can represent an interdiffusion microstructure with an efficient notation

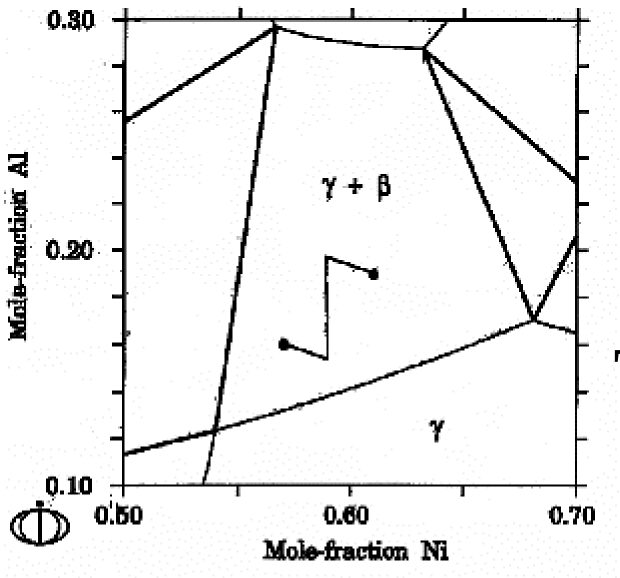
How can one classify the boundaries between regions?

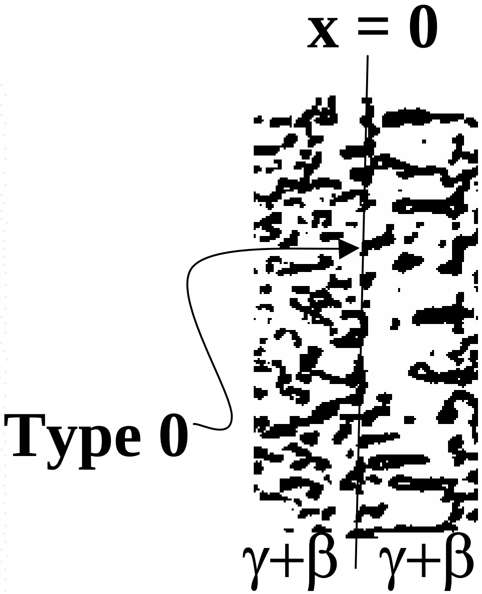


By the number of phases that change on crossing the boundary

J.E.Morral,, Cheng Jin, Anders Engström and John Ågren, Scripta Mater. 34 (1996) 1661-1666.

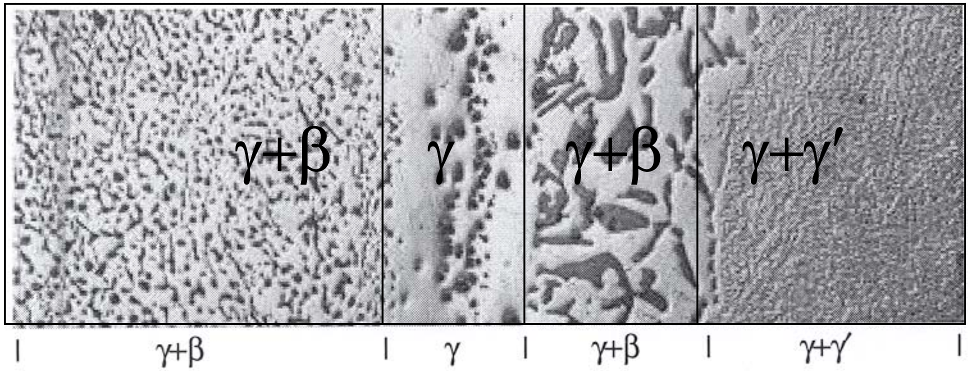
How can one classify the boundaries between regions?





Three Types of Boundaries: Type 0, 1, and 2.

Which way do the boundaries move?

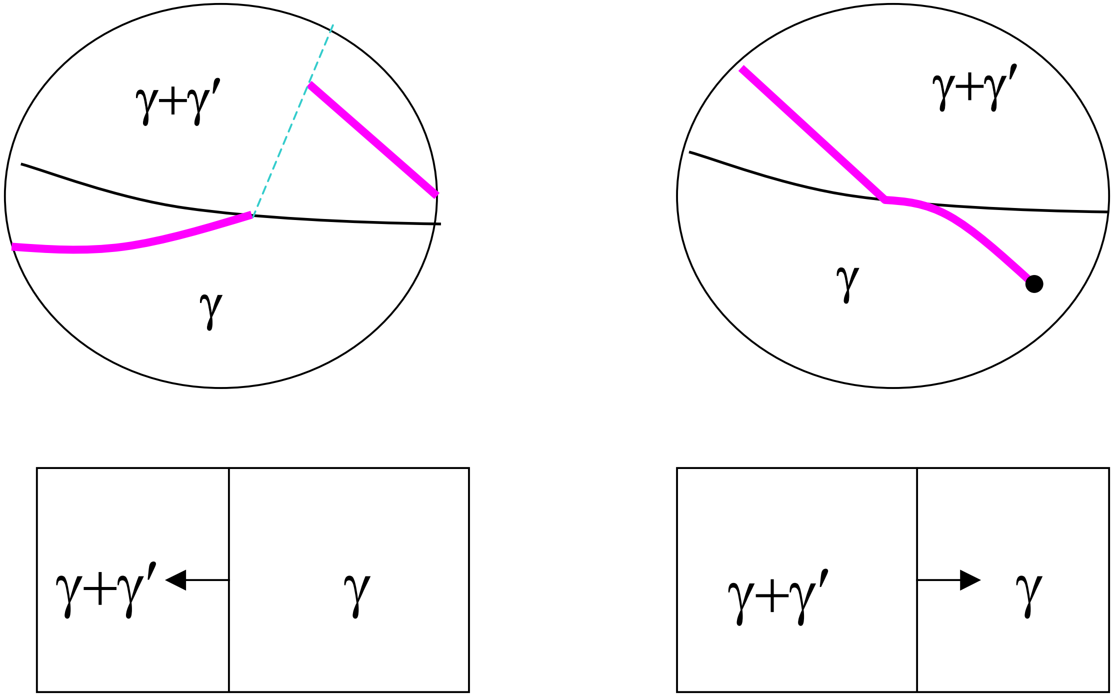


Boundaries move away from the initial interface

But where is the initial interface?

1. **Matano plane**
2. **Initial alloy edge**
3. **~Kirkendall markers**
4. **Type zero boundary**
5. **Diffusion path shape**

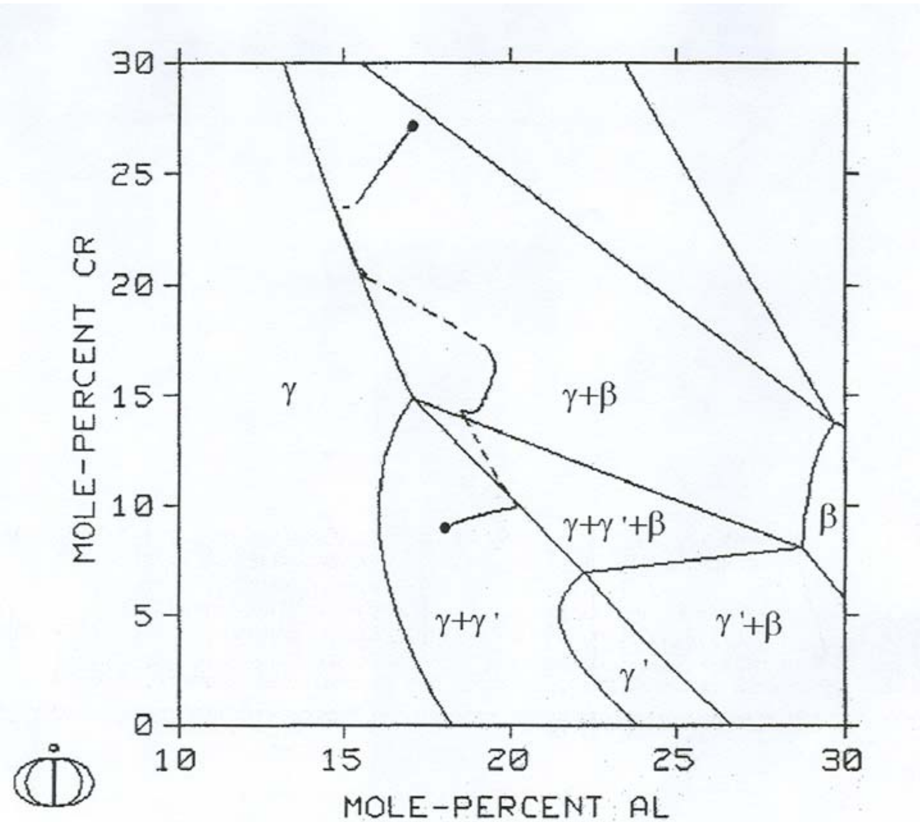
Type 1 boundary direction as a function of diffusion path shape

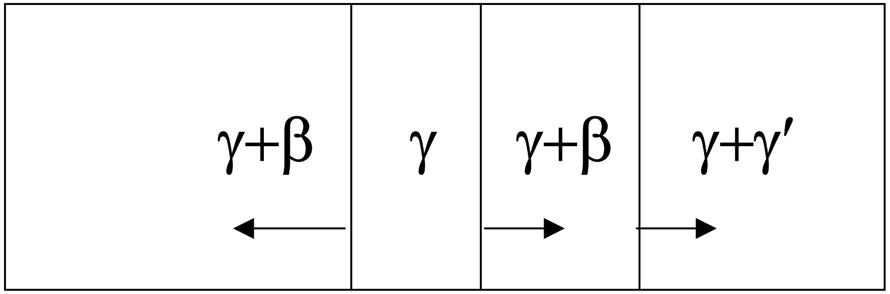


W.J. Boettinger, S.R. Coriell, C.E. Campbell and G.B. McFadden, Acta Metall.Mater. 48 (2000) 481-492. (3 component)

J. E. Morral and H. Chen, Scripta Mater. 43 (2000) 699-703. (n component)

Boundary motion deduced from the diffusion path

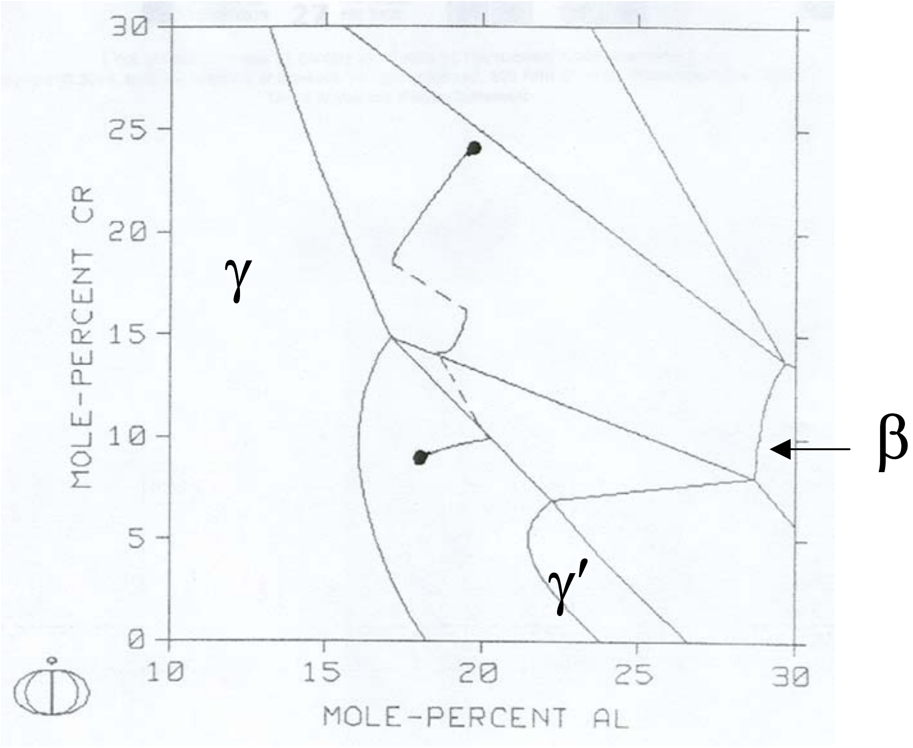




Shorthand notation for interdiffusion microstructures

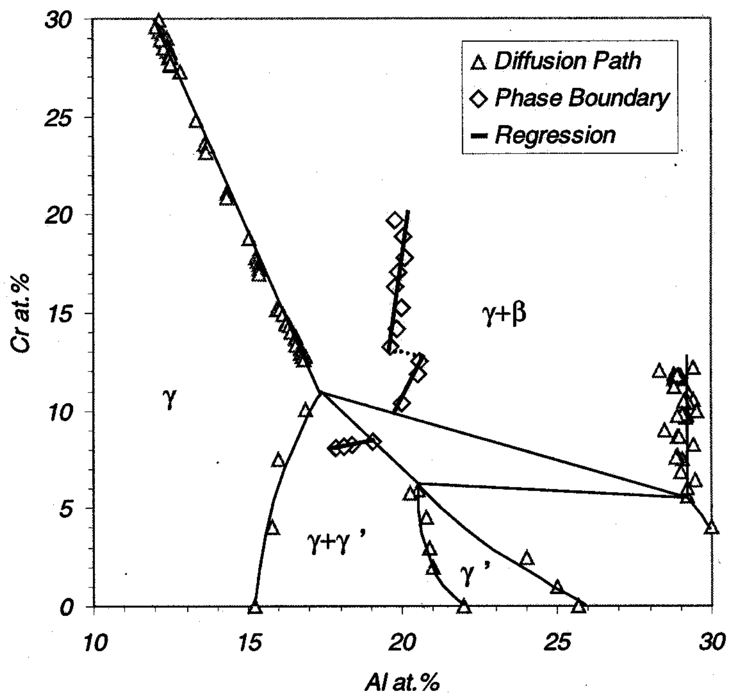
$\gamma+\beta \quad < \gamma > \gamma+\beta > \gamma+\gamma'$

Another DICTRA simulation for a Ni-Cr-Al diffusion couple

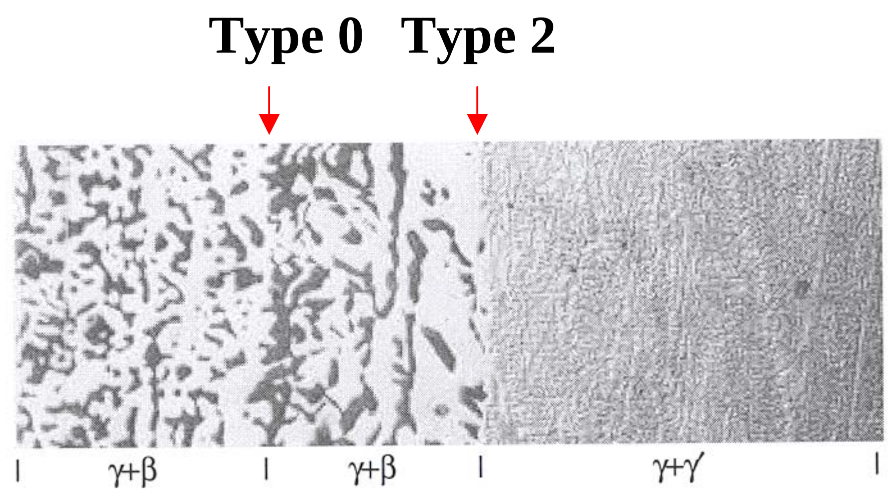


Shorthand notation: γ+β | γ+β > γ+γ′

Experimental measurements of MCrAlY/Superalloy interdiffusion



(c) Diffusion path of diffusion couple

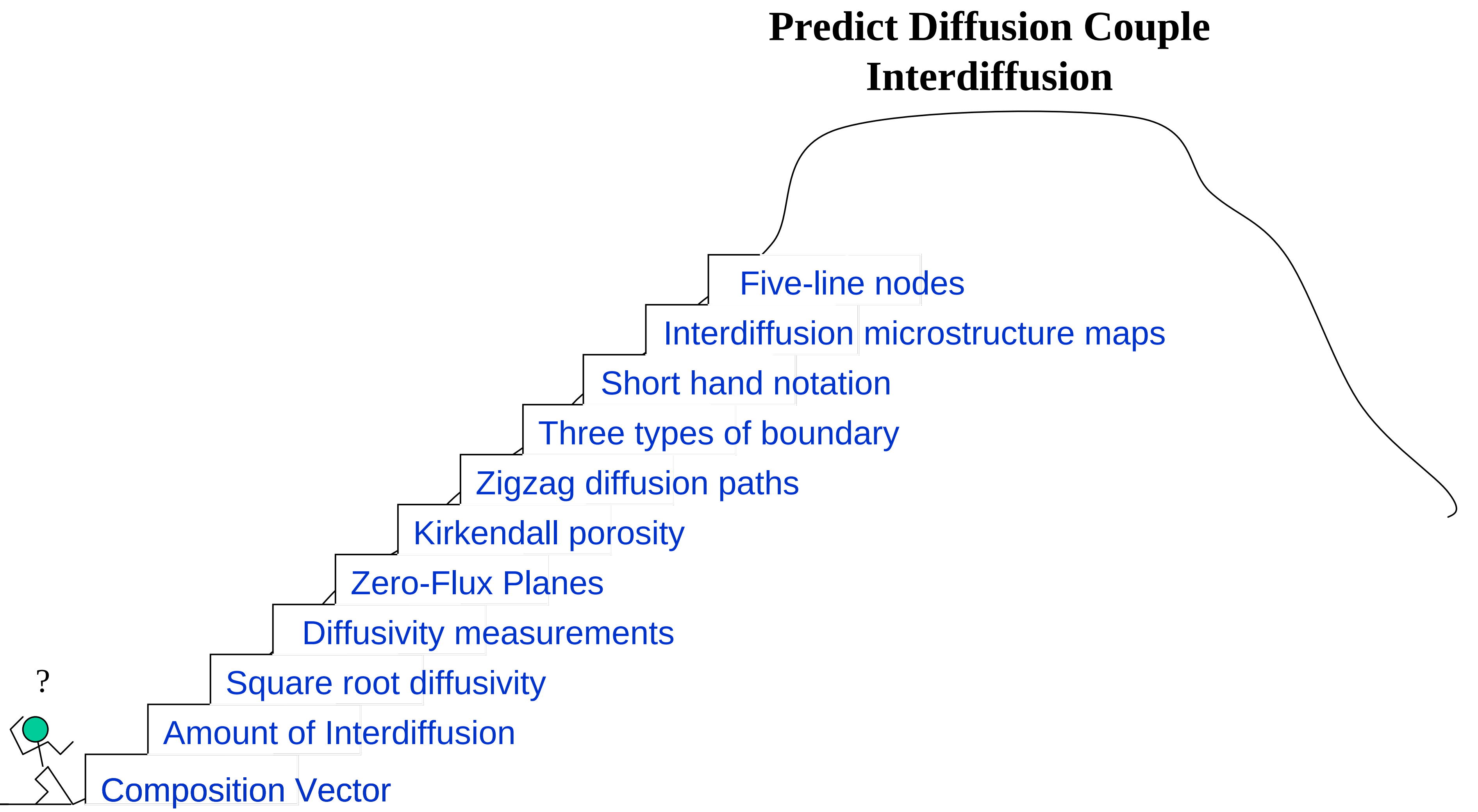


(d) Microstructure of diffusion couple

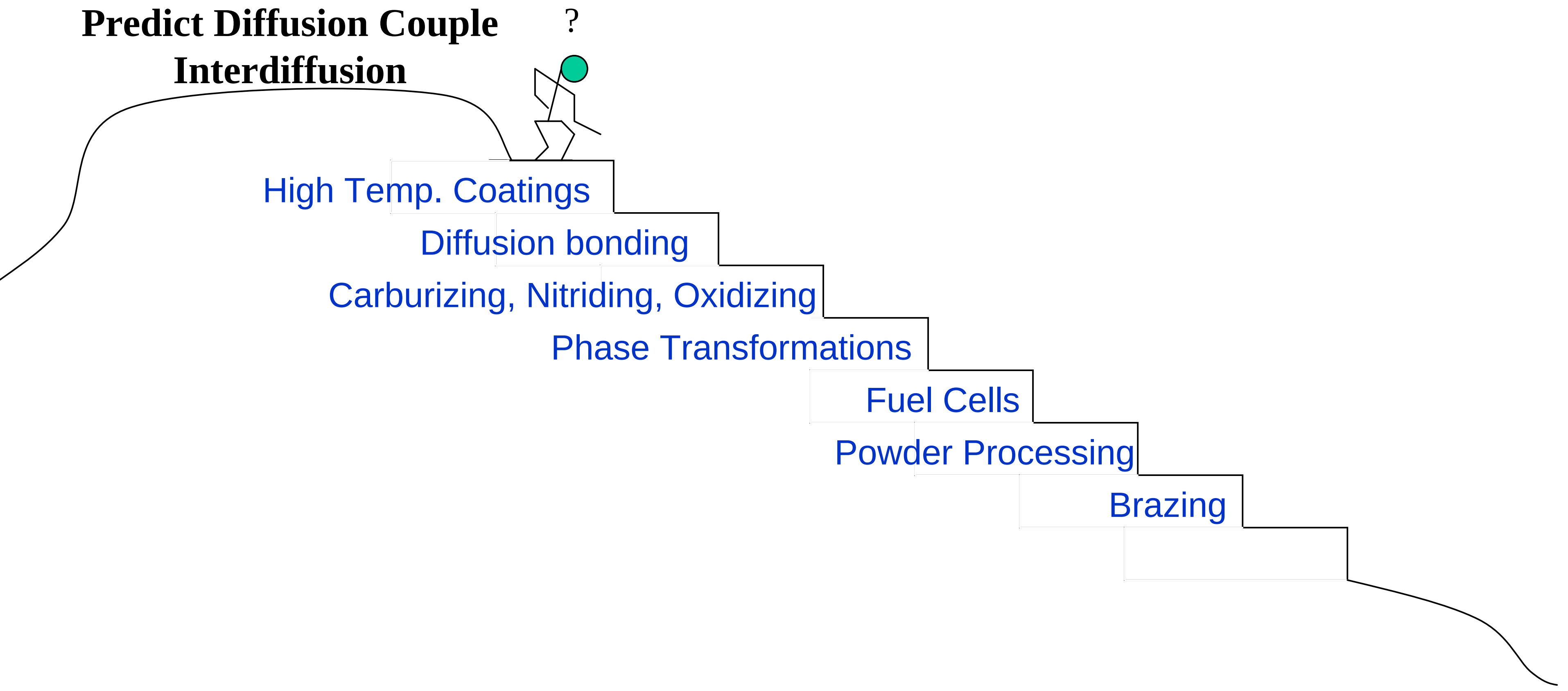
γ+β|γ +β>γ+γ′

Xin Qiao. M.S. Thesis. University of Connecticut. 1998

The Multicomponent Mountain

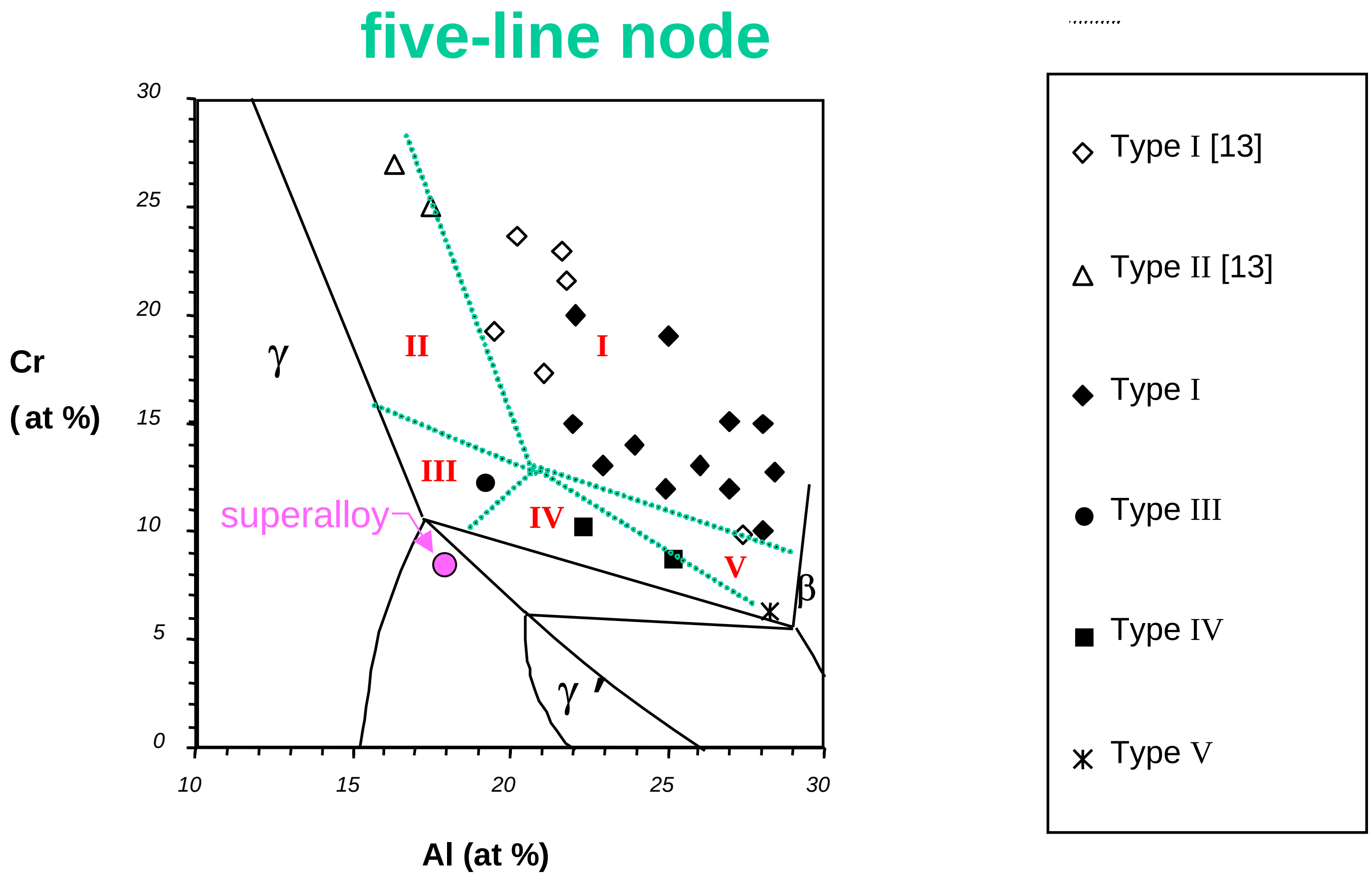


The Other Side of the Multicomponent Mountain - Applications



Application to MCrAlY coatings on turbine blades

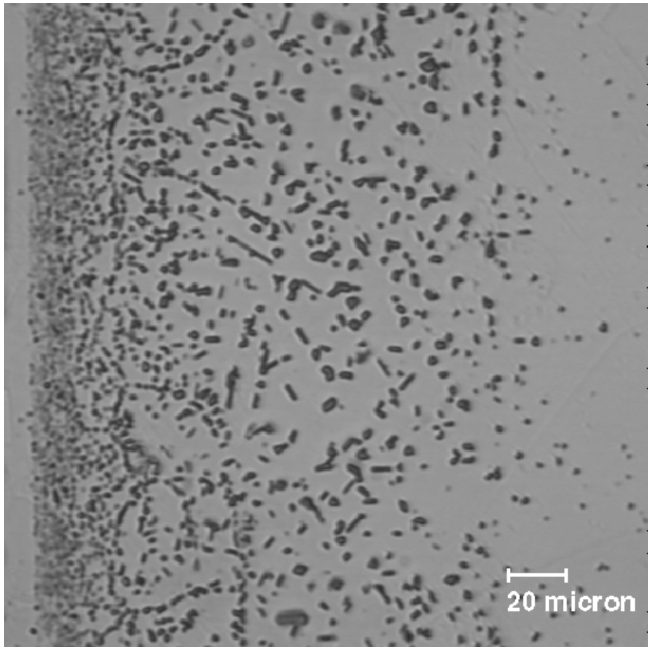
Interdiffusion Microstructure Map



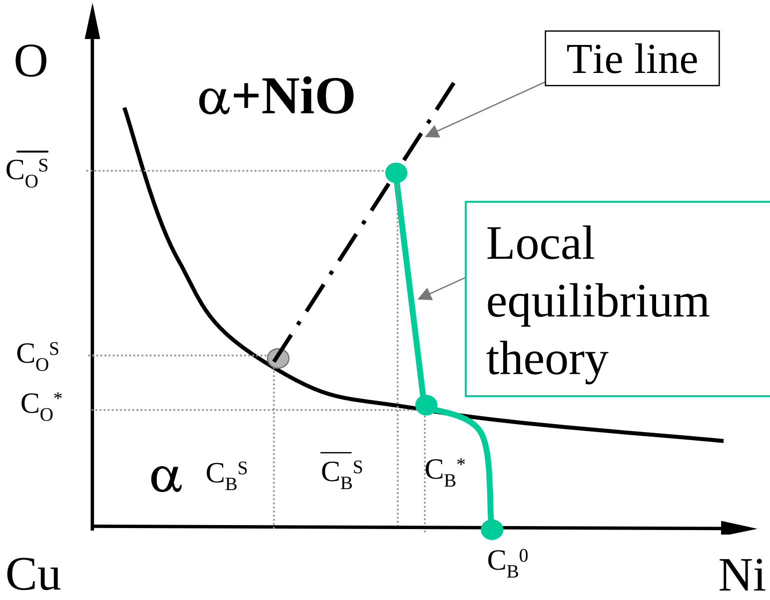
Frederick Meisenkothen. M.S. Thesis. University of Connecticut. 1998

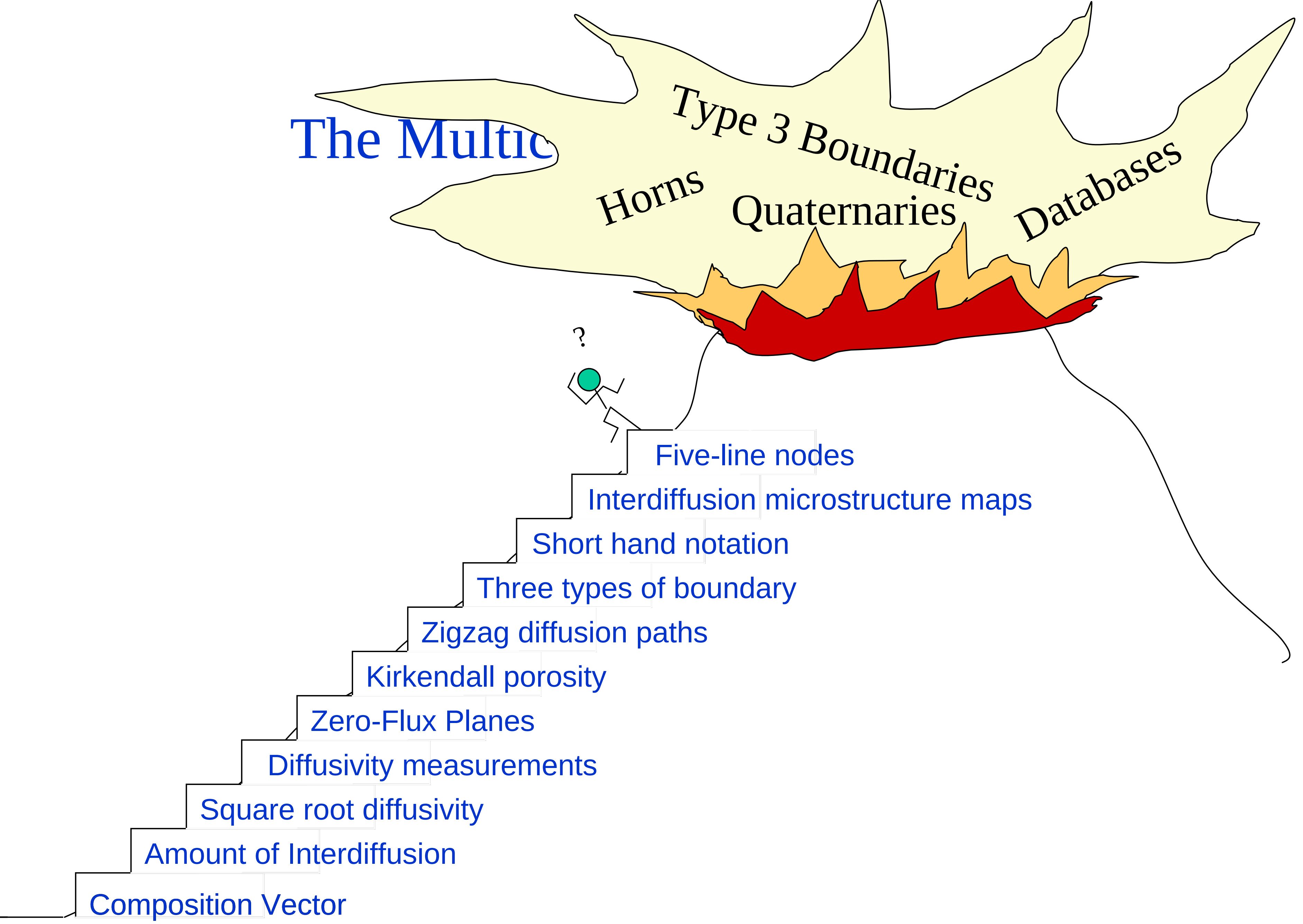
Application to internal oxidation of Cu-Ni

Experimental Microstructure

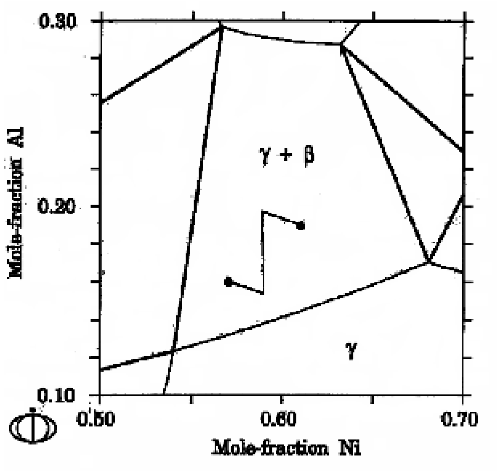


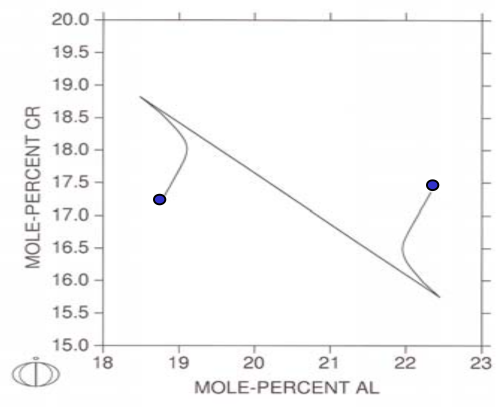
Diffusion Paths



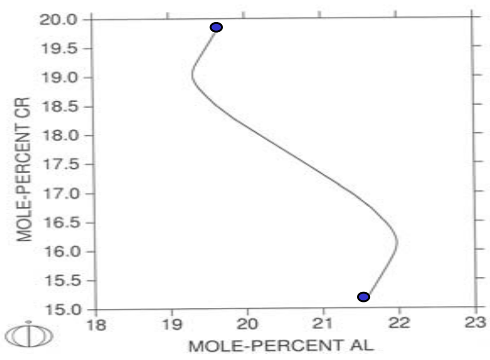

The Multic
Type 3 Boundaries
Horns
Quaternaries
Databases
?
Five-line nodes
Interdiffusion microstructure maps
Short hand notation
Three types of boundary
Zigzag diffusion paths
Kirkendall porosity
Zero-Flux Planes
Diffusivity measurements
Square root diffusivity
Amount of Interdiffusion
Composition Vector

Challenge 1: Understanding when and why horns form and how to predict them



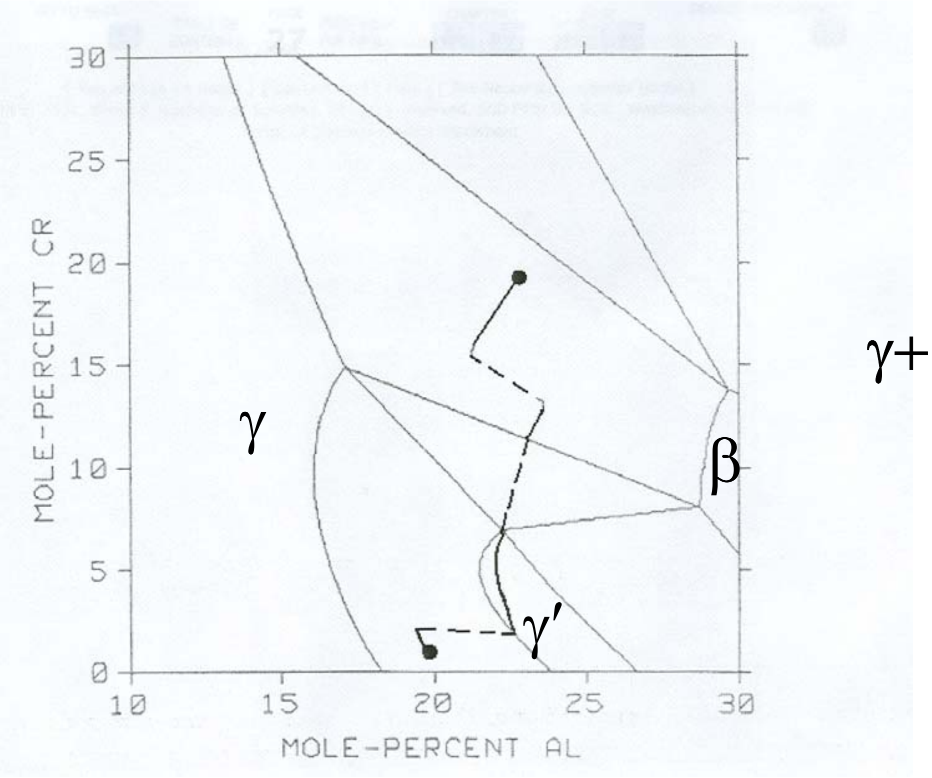


Horns point outward



Horns point inward

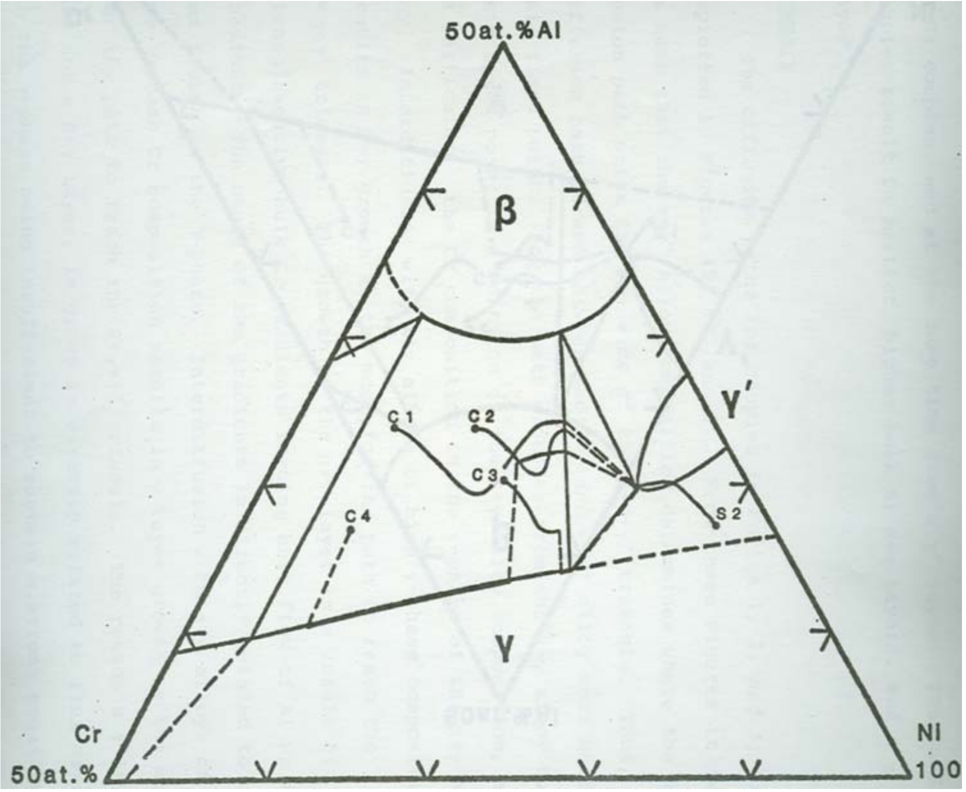
Challenge 2: To understand when and why Type 3 boundaries form



$\gamma+\beta \mid \gamma+\beta > \gamma' > \gamma'+\gamma$

Example
Type 3 boundary

Experimental evidence of Type 3 boundaries



Carol, L.A. A study of Interdiffusion in b+g/g+g ′ Ni-Cr-Al Alloys at 1200°C, NASA Contractor Report 174852 (1985).

Challenge 3: To represent diffusion paths in quaternary and higher order systems.

Challenge 4: To develop thermodynamic and kinetic databases that will enable the discovery of new or improved materials and processes.

CONCLUSIONS

- Diffusion paths obtained using DICTRA can be a valuable tool for predicting interdiffusion behavior.
- There are still phenomena associated with diffusion paths that need explaining.
- Developing thermodynamic and kinetic databases needs to become an international priority before computational materials science’s potential can be fully realized.