Algorithm for Predicting Diffusion Paths in Ternary Systems

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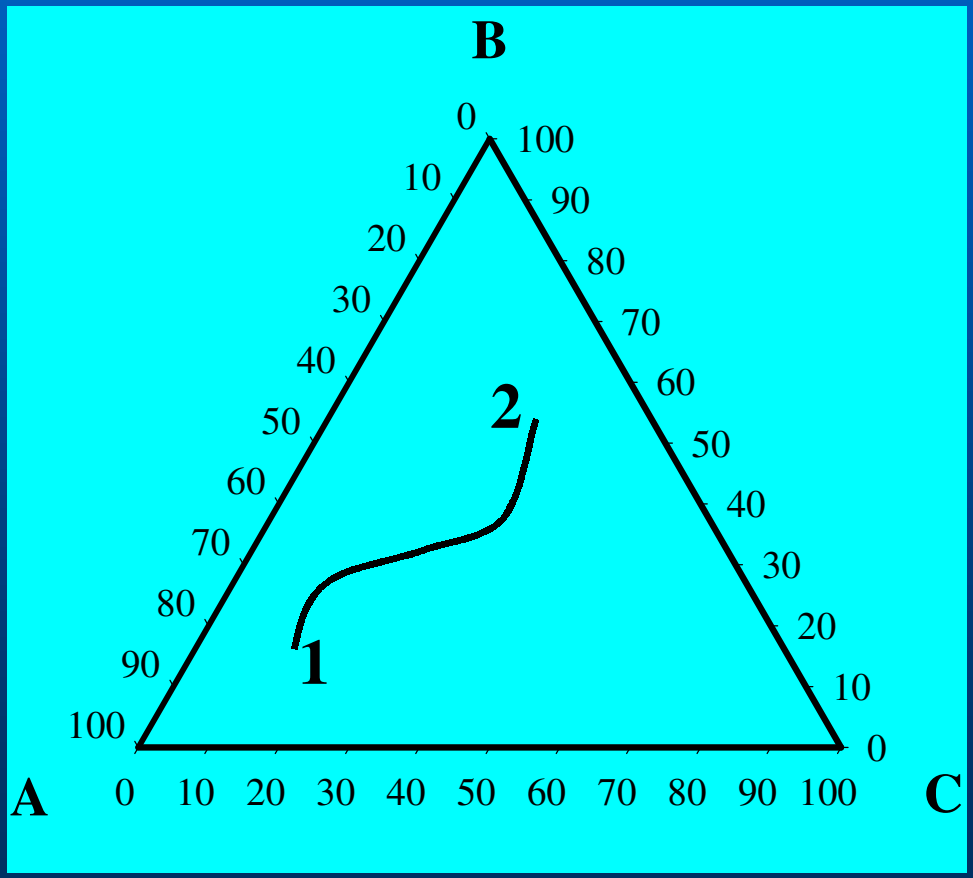
Diffusion Paths

- Result of interdiffusion of the diffusing species at the interface.
- Sequence of phase formation.
- Composition variation in the diffusion zone.
- Represented on the isothermal section of phase diagram as a curve.

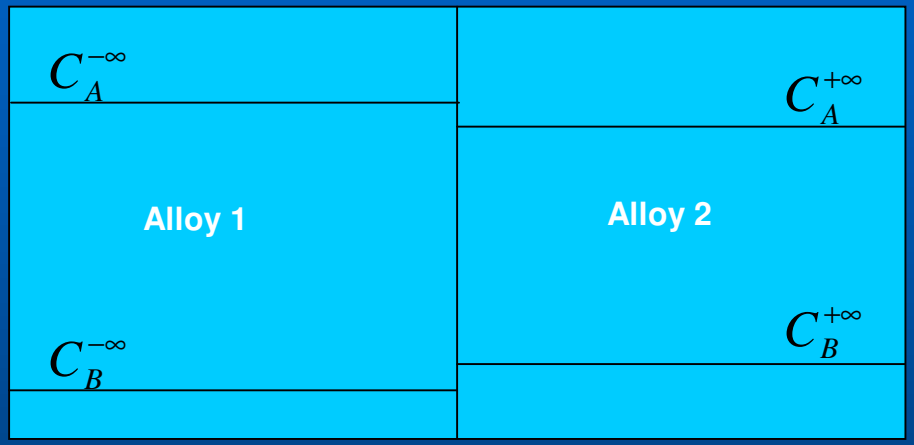
- Binary systems---- relatively easy to predict
- Ternary system is complex

1. more degrees of freedom
2. out of various possible diffusion paths only one is stable
3. may exhibit zero flux plane
4. flux reversal possible in some species
5. generally serpentine but double serpentine is also reported

Ternary Diffusion Path



Experimental

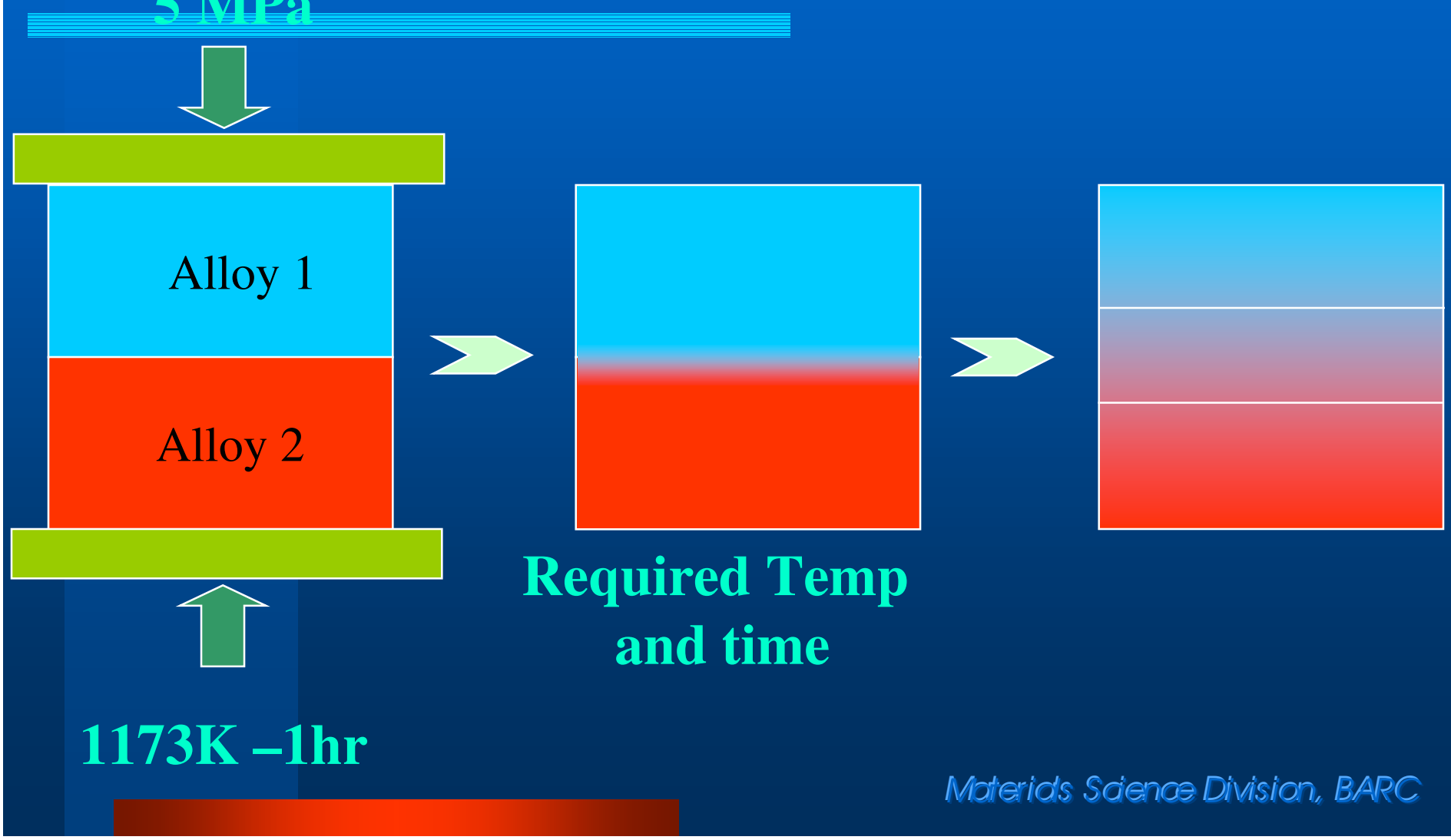


Diffusion couples can be uniquely defined by:

ΔC_A and ΔC_B

$$\Delta C_A = C_A^{-\infty} - C_A^{+\infty}$$
$$\Delta C_B = C_B^{-\infty} - C_B^{+\infty}$$

Making Diffusion Couples



Compositions of the alloys

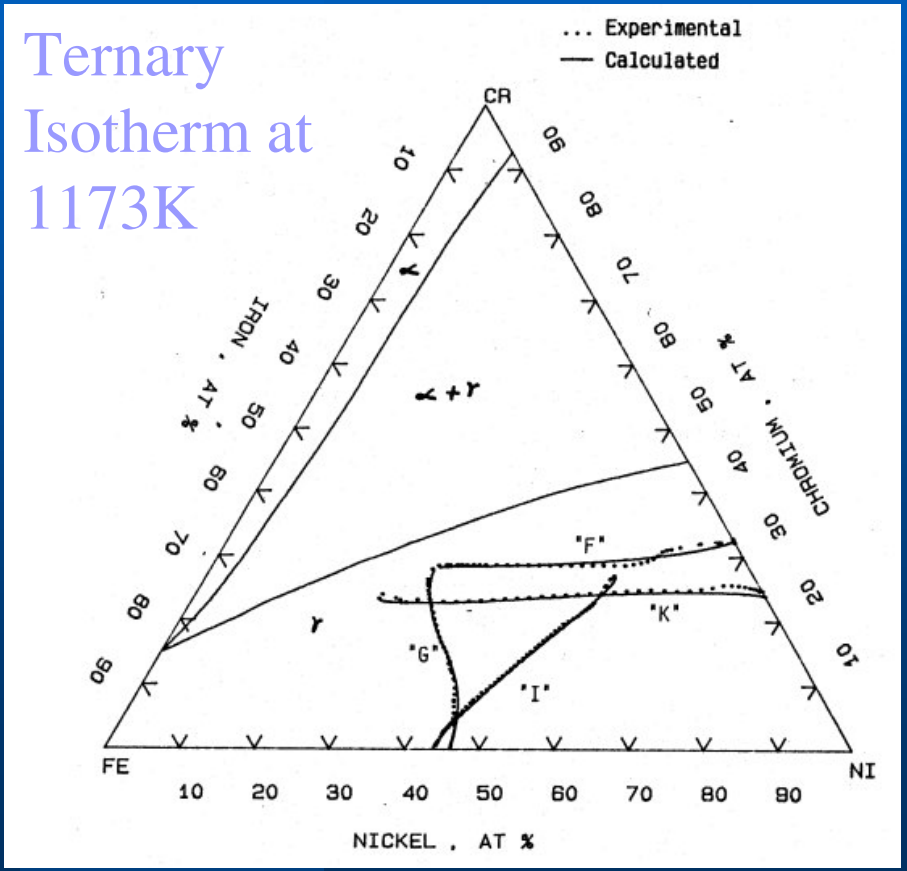
Alloy No.	Fe	Ni	Cr
		(atom%)	
1	41.4	30.3	28.3
2	31.0	37.5	31.5
3	20.3	42.0	37.7
4	18.6	54.7	26.7
5	11.5	57.3	31.2
6	-	67.4	32.6
7	-	76.1	23.9
8	-	100	-
9	6.8	93.2	-
10	43.2	56.8	-
11	53.3	46.7	-
12	63.7	24.6	11.7
13	51.8	25.1	23.1
14	55.9	44.1	-
15	16.9	79.0	4.1
16	4.3	77.1	18.6
17	4.3	82.9	12.8
18	15.4	72.5	12.1
19	31.0	34.5	34.5

Diffusion annealing schedule

COUPLE	ALLOYS	TEMPERATURE (K)	TIME (ks)
A	8/2	1223	432
B	8/3	1223	432
C	8/5	1223	432
D	8/12	1223	432
E	8/13	1223	432
F	1/6	1223	324
G	1/11	1223	324
H	3/11	1223	324
I	4/14	1223	324
J	7/9	1223	324
K	13/7	1223	324
L	12/19	1223	324
M	7/10	1223	324
N	8/4	1173	324
O	8/2	1173	324
P	13/7	1173	324
Q	8/3	1323	180
R	8/19	1323	180
S	13/7	1323	180
T	15/16	1380	259.2
U	17/18	1380	259.2
V	17/18	1403	180
W	15/16	1403	180

Results

Ternary Isotherm at 1173K



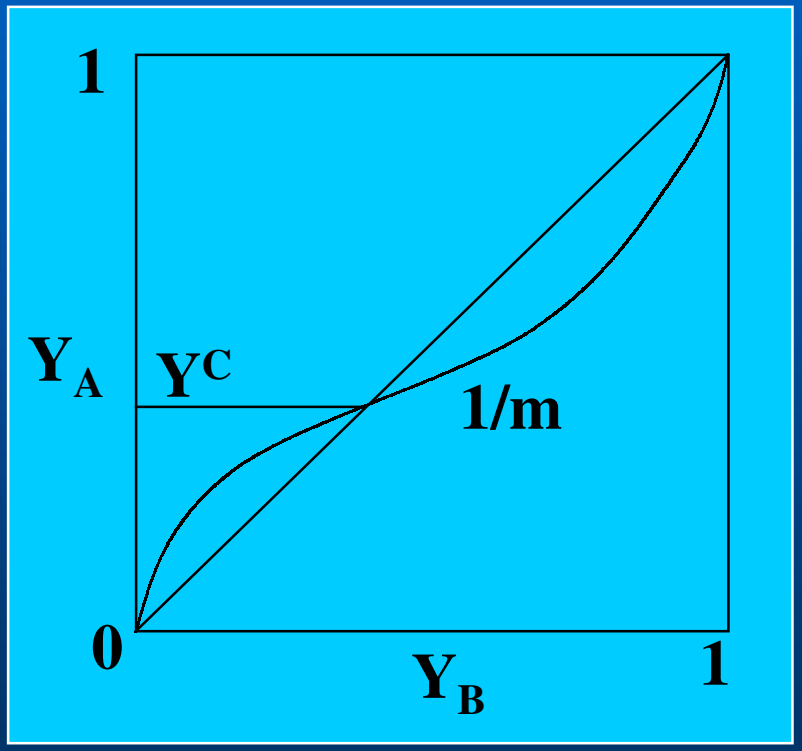
The diffusion paths are mostly S-shaped.

Orthogonal Transformation

$$Y_i = \frac{C_i - C_i^{+\infty}}{C_i^{-\infty} - C_i^{+\infty}}$$

Eqn. 1

$$0 \le Y_i \le 1$$



Two variables: *Yc* and *m*

The Model

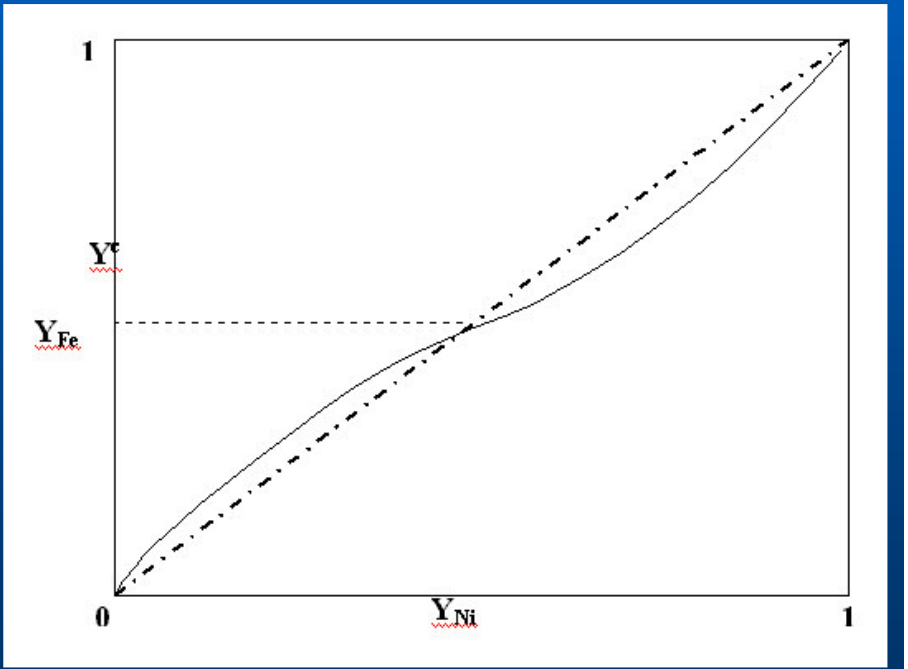
$$Y_A^m = (Y^c)^{m-1} Y_B$$

for $(0 \le Y_A \le Y^C)$

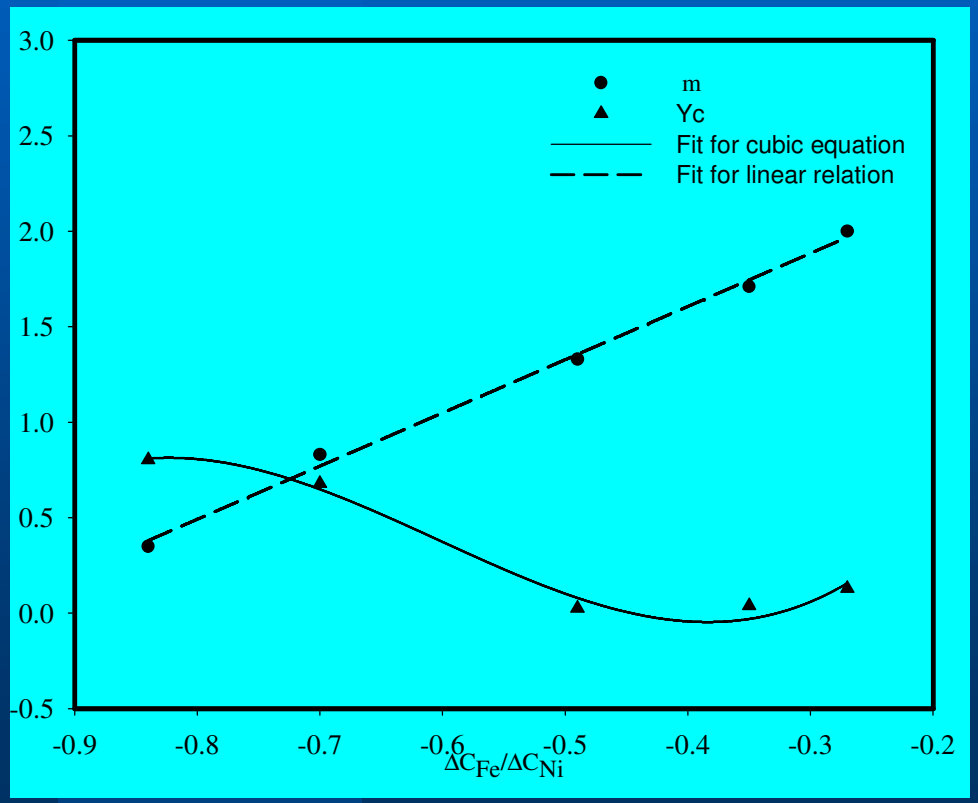
$$(1-Y_A)^m = (1-Y^c)^{m-1}(1-Y_B)$$

for $(Y^C \le Y_A \le 1)$

Eqn. 2



Curve Fitting



$$Y^C = 3.073 + 19.22\left(\Delta C_{Fe}/\Delta C_{Ni}\right) + 36.71\left(\Delta C_{Fe}/\Delta C_{Ni}\right)^2 + 20.27\left(\Delta C_{Fe}/\Delta C_{Ni}\right)^3$$

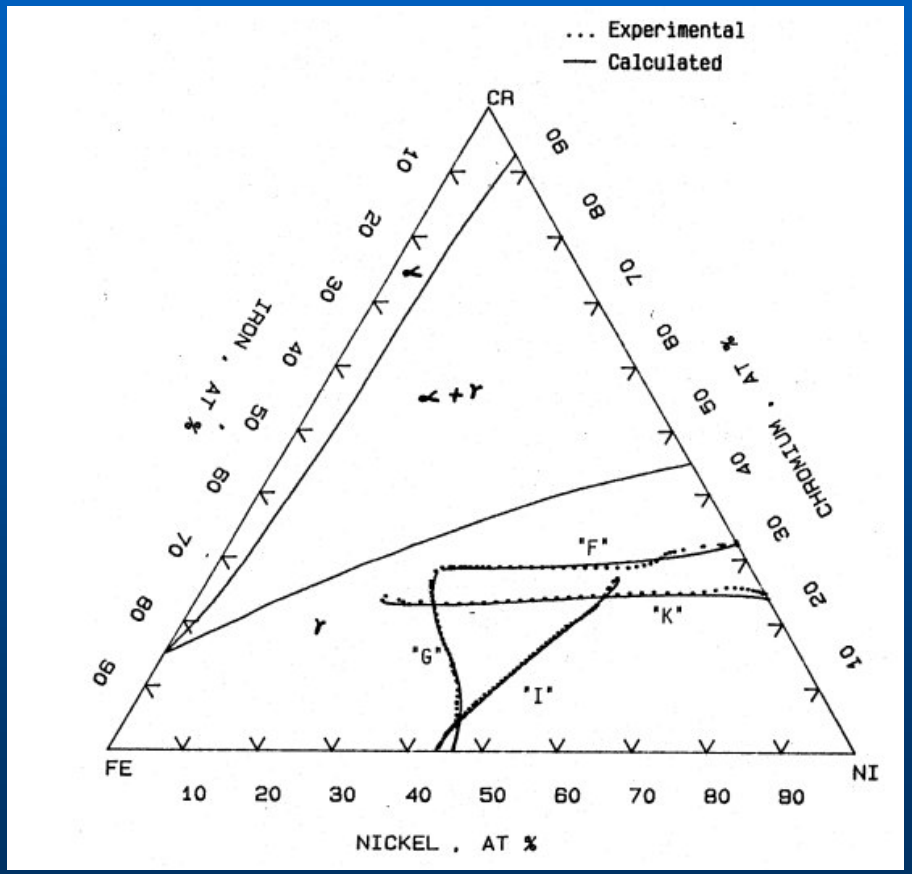
Eqn. 3

$$m = 2.72 + 2.786\left(\Delta C_{Fe}/\Delta C_{Ni}\right)$$

Eqn. 4

Validation

Good match between experimental and predicted diffusion paths



Algorithm

Plots the diffusion path for couples of Fe-Ni-Cr system