

# **MultiDiFlux Evaluation of Selected Multicomponent Couples**

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# MultiDiFlux<sup>©</sup>

## **Analysis of Concentration Profiles of Single-Phase Multi-component Diffusion couples for *Interdiffusion Fluxes and Interdiffusion Coefficients***



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[https://engineering.purdue.edu/MSE/Fac\\_Staff/Faculty/dayananda.wshtml](https://engineering.purdue.edu/MSE/Fac_Staff/Faculty/dayananda.wshtml)

# Selected Multicomponent Systems

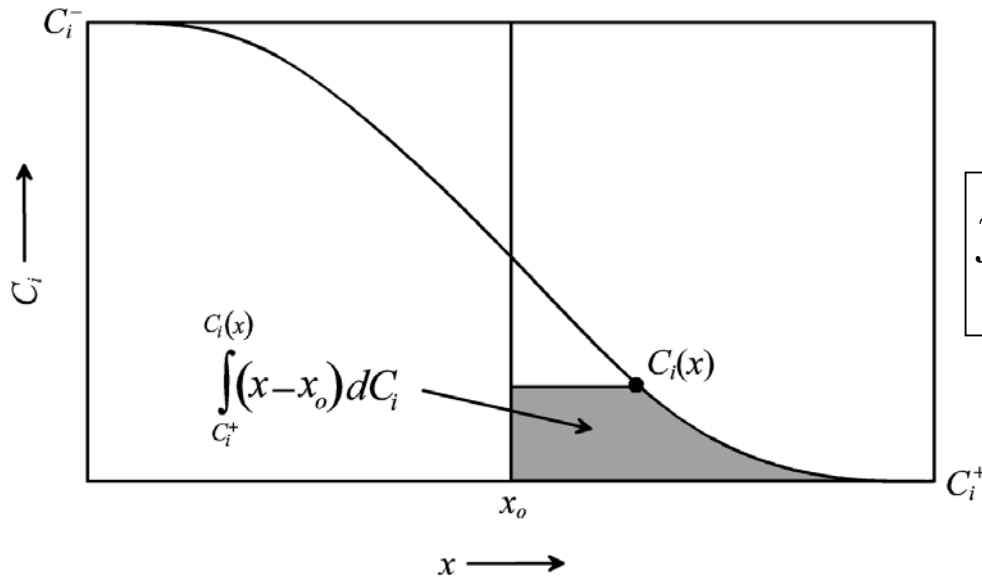
- Cu-Ni-Zn System
- Cu-Ni-Zn-Mn Quaternary System
- Rene 88 (GE Couple)
- Fe-Ni-Al



# Determination of Interdiffusion Fluxes

from Experimental Concentration Profiles<sup>[1,2]</sup>

Generalized Fick's Law<sup>[3,4]</sup>:



$$\tilde{J}_i = -\sum_{j=1}^{n-1} \tilde{D}_{ij}^n \frac{\partial C_j}{\partial x} \quad (i = 1, 2, \dots, n-1)$$

$$\tilde{J}_i(x) = \frac{1}{2t} \int_{C_i^+ \text{ or } C_i^-}^{C_i(x)} (x - x_0) dC_i \quad (i = 1, 2, \dots, n)$$

<sup>1</sup> M.A. Dayananda and C.W. Kim, *Metall. Trans. A*, **10A** 1333-1339 (1979).

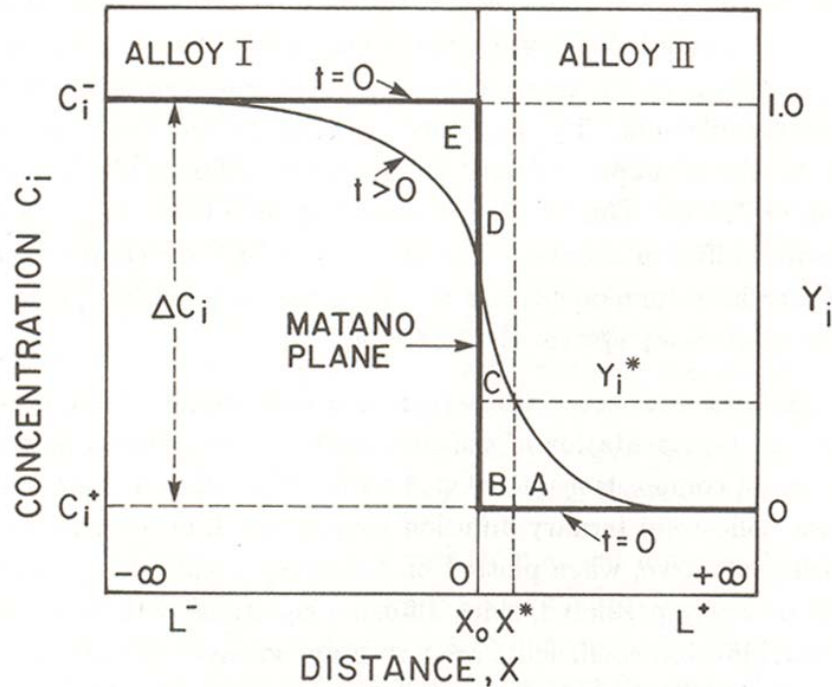
<sup>2</sup> M.A. Dayananda, *Metall. Trans. A*, **14A** 1851-1858 (1983).

<sup>3</sup> L. Onsager, *Phys. Rev.*, **37** 405-426 (1931).

<sup>4</sup> L. Onsager, *Phys. Rev.*, **38** 2265-2279 (1931).



# Flux equations to include molar volume changes



$$Y_i = \frac{C_i - C_i^+}{C_i^- - C_i^+} \quad (i=1,2,3)$$

$$E + D - A = B + C + D$$

$$= (x^* - x_0)$$

$$J_i^M(x^*) = \frac{\Delta C_i}{2t} \left[ Y_i^* \int_{-\infty}^{x^*} \frac{(1-Y_i)}{V_m} dx + (1-Y_i^*) \int_{x^*}^{\infty} \frac{Y_i}{V_m} dx \right] \quad (i=1,2,\dots,n)$$



# Main Steps carried out by the *MultiDiFlux* Program

- Cubic Hermite polynomial fit to the experimental data for concentration profiles
- Determination of the Matano plane from the profile of each component
- Calculation of interdiffusion fluxes
- Calculation of Interdiffusion coefficients
- Generation of concentration profiles

# Basis of *MultiDiFlux* Program

## -Integration of Interdiffusion Fluxes-

On the basis of Onsager's formalism,

$$\tilde{J}_i = \tilde{D}_{i1}^3 \frac{C_1}{x} - \tilde{D}_{i2}^3 \frac{C_2}{x} \quad (i = 1, 2)$$

$$\int_{x_1}^{x_2} \tilde{J}_i dx = \int_{C_1(x_1)}^{C_1(x_2)} \tilde{D}_{i1}^3 dC_1 - \int_{C_2(x_1)}^{C_2(x_2)} \tilde{D}_{i2}^3 dC_2 \quad (i = 1, 2)$$

$$= \bar{\tilde{D}}_{i1}^3 [C_1(x_2) - C_1(x_1)] - \bar{\tilde{D}}_{i2}^3 [C_2(x_2) - C_2(x_1)] \quad (i = 1, 2)$$

$\bar{\tilde{D}}_{i1}^3$  and  $\bar{\tilde{D}}_{i2}^3$  are the average values of main and cross interdiffusion coefficients.

$$\bar{\tilde{D}}_{ij}^3 = \frac{\int_{C_j(x_1)}^{C_j(x_2)} \tilde{D}_{ij}^3 dC_j}{\int_{C_j(x_1)}^{C_j(x_2)} dC_j} \quad (i = 1, 2)$$



$$\tilde{J}_i = -\bar{D}_{i1}^3 \frac{\partial C_1}{\partial x} - \bar{D}_{i2}^3 \frac{\partial C_2}{\partial x} \quad (i = 1,2)$$

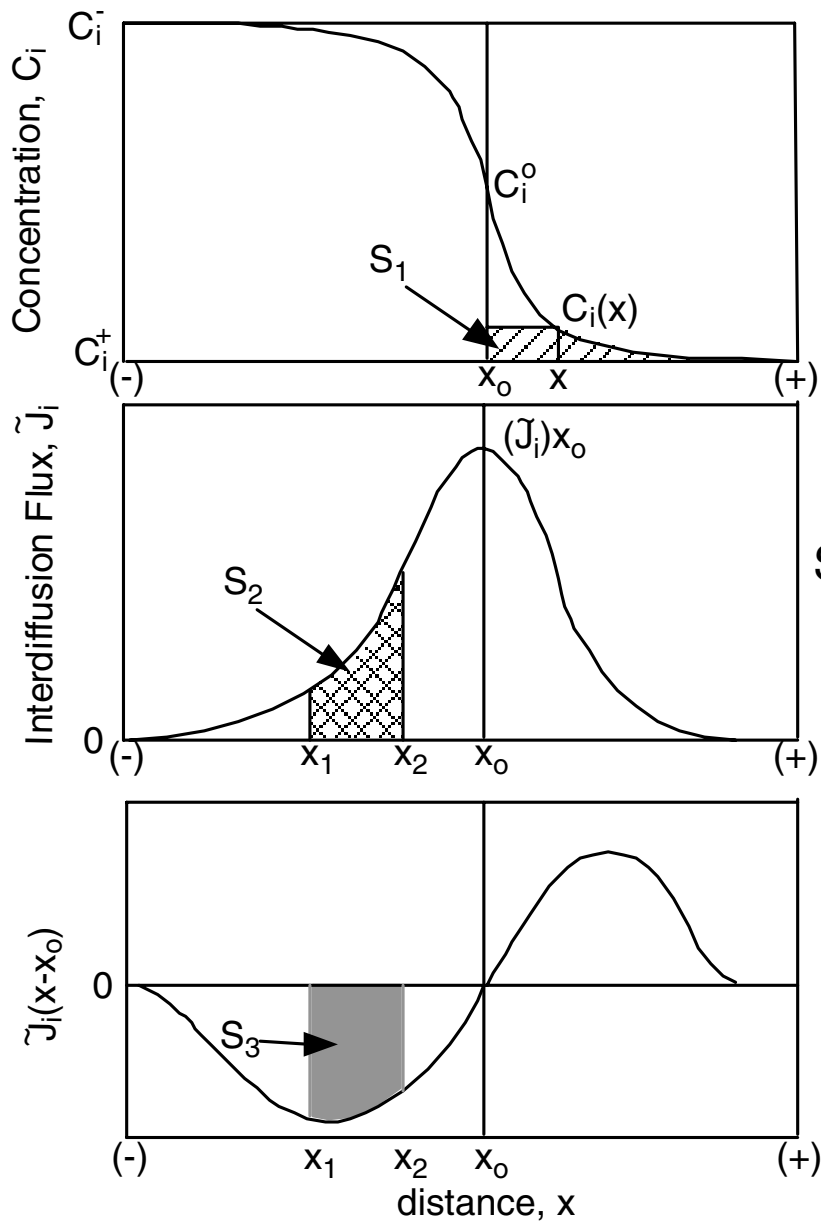
**Multiplying by  $(x-x_0)^n$  and integrating over a range of  $x$**

$$\int_{x_1}^{x_2} \tilde{J}_i (x - x_0)^n dx = -\bar{D}_{i1}^3 \int_{C_1(x_1)}^{C_1(x_2)} (x - x_0)^n dC_1 - \bar{D}_{i2}^3 \int_{C_2(x_1)}^{C_2(x_2)} (x - x_0)^n dC_2 \quad (i = 1,2)$$

**For  $n=1$**

$$\begin{aligned} \int_{x_1}^{x_2} \tilde{J}_i (x - x_0) dx &= -\bar{D}_{i1}^3 \int_{C_1(x_1)}^{C_1(x_2)} (x - x_0) dC_1 - \bar{D}_{i2}^3 \int_{C_2(x_1)}^{C_2(x_2)} (x - x_0) dC_2 \\ &= 2t \left\{ \bar{D}_{i1}^3 [\tilde{J}_1(x_1) - \tilde{J}_1(x_2)] + \bar{D}_{i2}^3 [\tilde{J}_2(x_1) - \tilde{J}_2(x_2)] \right\} \quad (i = 1,2) \end{aligned}$$





## Determination of $\bar{D}_{ij}^3$ ( $i, j = 1, 2$ ) Coefficients

$$S_1 = \int_{C_i^+}^{C_i^-} x - x_0 dC_i; \quad S_2 = \int_{x_1}^{x_2} \tilde{J}_i dx; \quad S_3 = \int_{x_1}^{x_2} \tilde{J}_i x - x_0 dx$$

$$\bar{D}_{ij}^3 = \frac{\int_{C_j, x_1}^{C_j, x_2} \tilde{D}_{ij}^3 dC_j}{\int_{C_j, x_1}^{C_j, x_2} dC_j} \quad (i = 1, 2)$$



# Regeneration of Concentration Profiles

$$C_1 = K_1 \left[ \frac{\operatorname{erf}\left(\frac{x-x_0}{2\sqrt{u^*t}}\right) - \operatorname{erf}\left(\frac{x_I-x_0}{2\sqrt{u^*t}}\right)}{\operatorname{erf}\left(\frac{x_{II}-x_0}{2\sqrt{u^*t}}\right) - \operatorname{erf}\left(\frac{x_I-x_0}{2\sqrt{u^*t}}\right)} \right] + K_2 \left[ \frac{\operatorname{erf}\left(\frac{x-x_0}{2\sqrt{v^*t}}\right) - \operatorname{erf}\left(\frac{x_I-x_0}{2\sqrt{v^*t}}\right)}{\operatorname{erf}\left(\frac{x_{II}-x_0}{2\sqrt{v^*t}}\right) - \operatorname{erf}\left(\frac{x_I-x_0}{2\sqrt{v^*t}}\right)} \right] + C_{II}$$

$$C_2 = K_3 \left[ \frac{\operatorname{erf}\left(\frac{x-x_0}{2\sqrt{u^*t}}\right) - \operatorname{erf}\left(\frac{x_I-x_0}{2\sqrt{u^*t}}\right)}{\operatorname{erf}\left(\frac{x_{II}-x_0}{2\sqrt{u^*t}}\right) - \operatorname{erf}\left(\frac{x_I-x_0}{2\sqrt{u^*t}}\right)} \right] + K_4 \left[ \frac{\operatorname{erf}\left(\frac{x-x_0}{2\sqrt{v^*t}}\right) - \operatorname{erf}\left(\frac{x_I-x_0}{2\sqrt{v^*t}}\right)}{\operatorname{erf}\left(\frac{x_{II}-x_0}{2\sqrt{v^*t}}\right) - \operatorname{erf}\left(\frac{x_I-x_0}{2\sqrt{v^*t}}\right)} \right] + C_{2I}$$

$$K_1 = \frac{1}{\tilde{D}} \left[ \left[ \tilde{D}_{12}^3 (C_{2II} - C_{2I}) \right] - \left( \tilde{D}_{22}^3 - \tilde{D}_{11}^3 - \tilde{D} \right) \left[ \frac{C_{III} - C_{II}}{2} \right] \right] \quad K_2 = \frac{1}{\tilde{D}} \left[ \left[ \tilde{D}_{12}^3 (C_{2I} - C_{2II}) \right] - \left( \tilde{D}_{22}^3 - \tilde{D}_{11}^3 + \tilde{D} \right) \left[ \frac{C_{II} - C_{III}}{2} \right] \right]$$

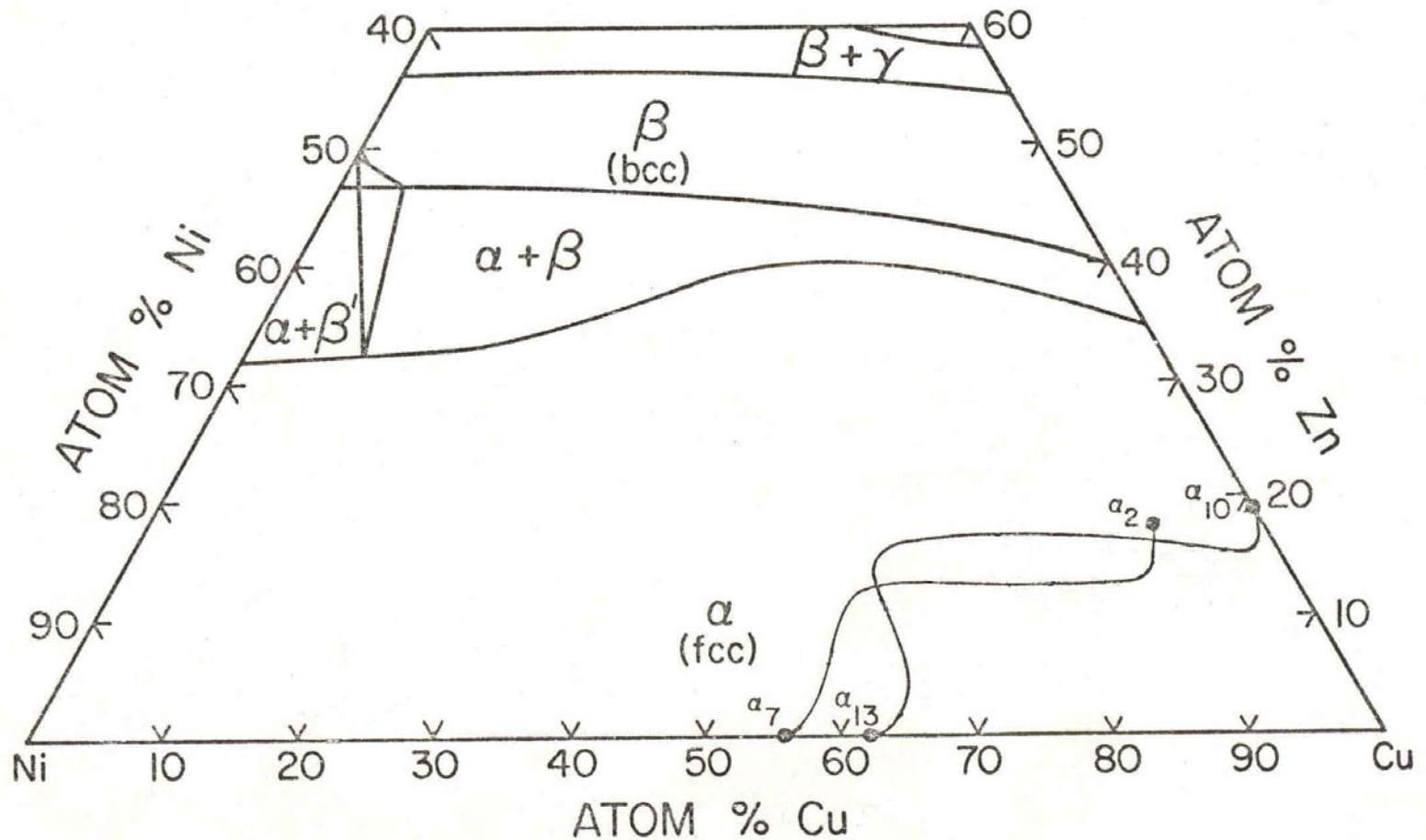
$$K_3 = \frac{1}{\tilde{D}} \left[ \left[ \tilde{D}_{21}^3 (C_{III} - C_{II}) \right] - \left( \tilde{D}_{11}^3 - \tilde{D}_{22}^3 - \tilde{D} \right) \left[ \frac{C_{2II} - C_{2I}}{2} \right] \right] \quad K_4 = \frac{1}{\tilde{D}} \left[ \left[ \tilde{D}_{21}^3 (C_{II} - C_{III}) \right] - \left( \tilde{D}_{11}^3 - \tilde{D}_{22}^3 + \tilde{D} \right) \left[ \frac{C_{2I} - C_{2II}}{2} \right] \right]$$

$$u = \tilde{D}_{11}^3 + 0.5 \left( \tilde{D}_{22}^3 - \tilde{D}_{11}^3 + \tilde{D} \right)$$

$$v = \tilde{D}_{22}^3 + 0.5 \left( \tilde{D}_{11}^3 - \tilde{D}_{22}^3 - \tilde{D} \right)$$

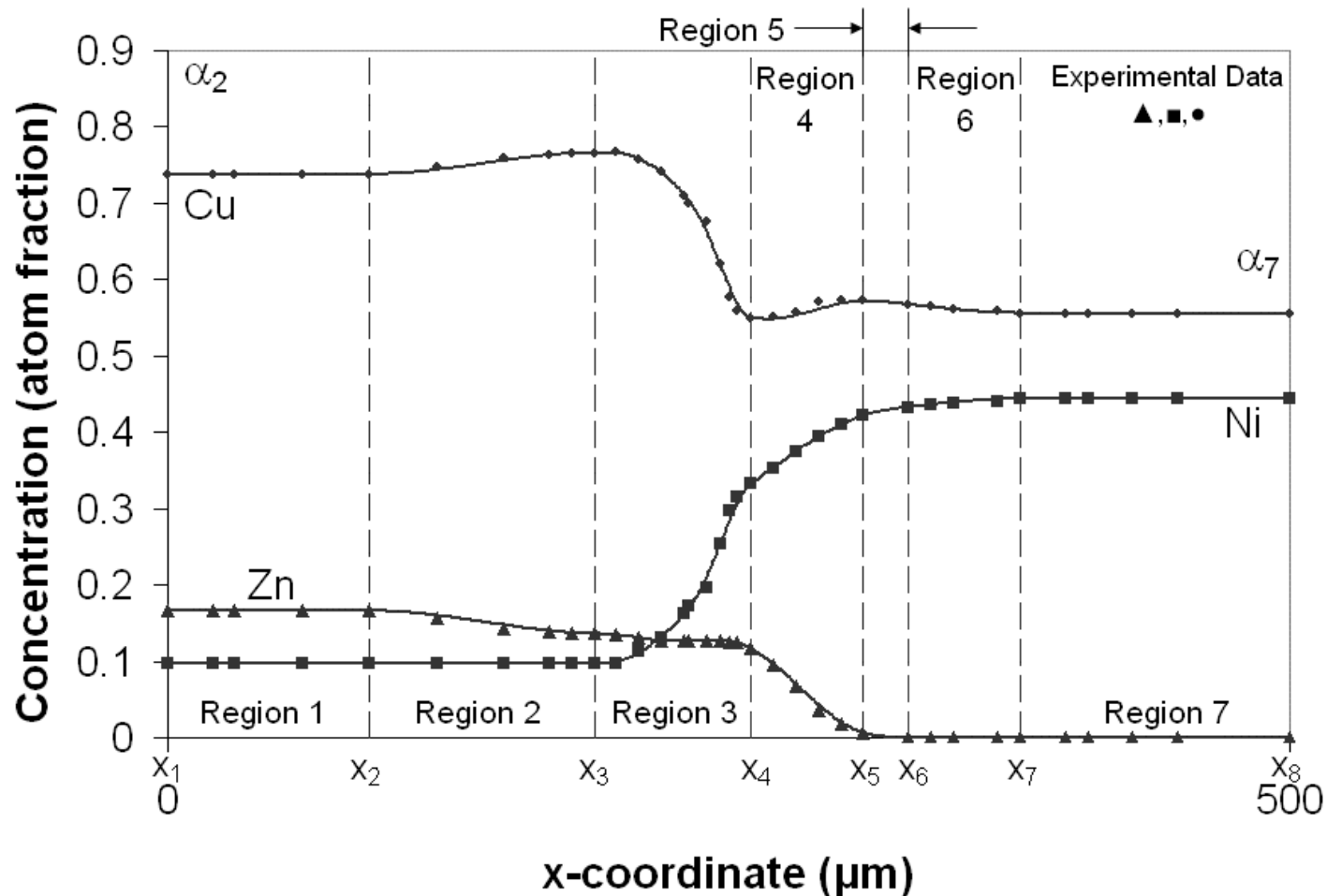
# Ternary Cu-Ni-Zn System at 775°C

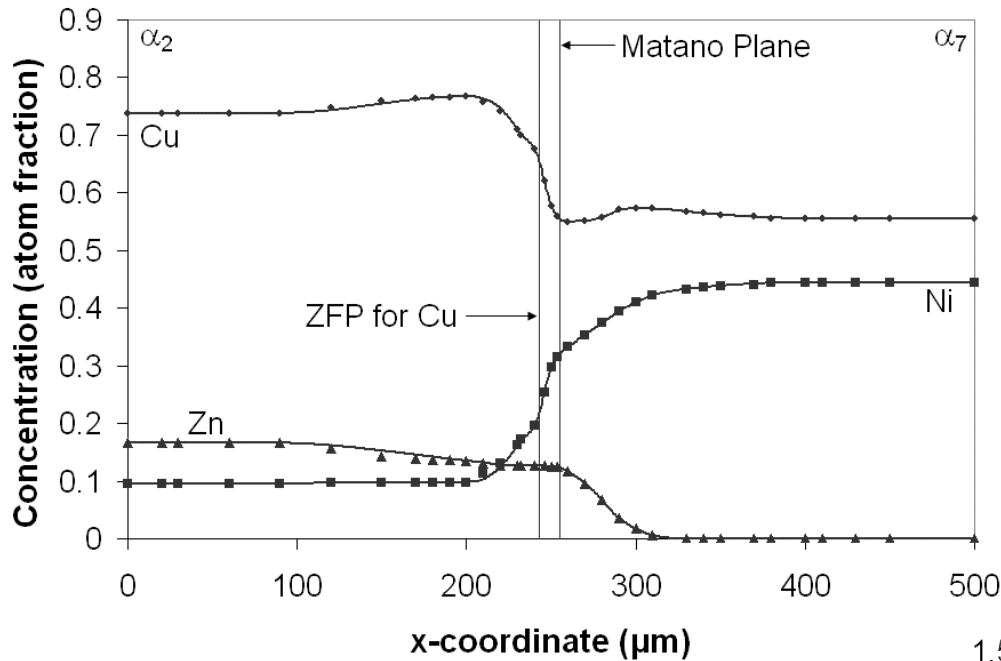
## Cu-Isoactivity couples



# Curve Fitting over Selected Regions of Concentration Profiles

$\alpha_2$  vs.  $\alpha_7$  couple; 775°C; 2 days

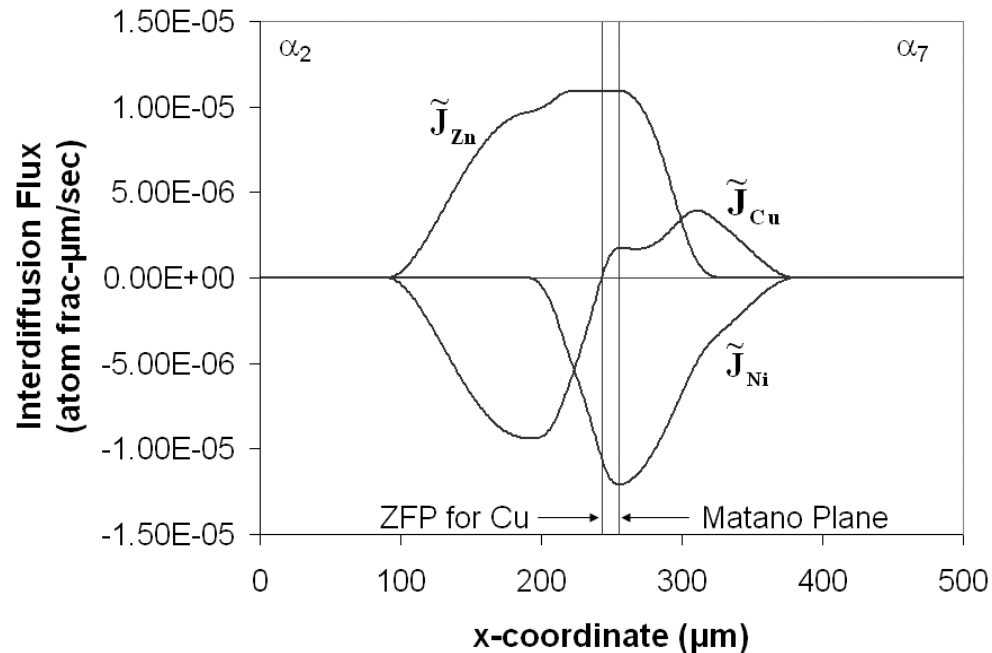




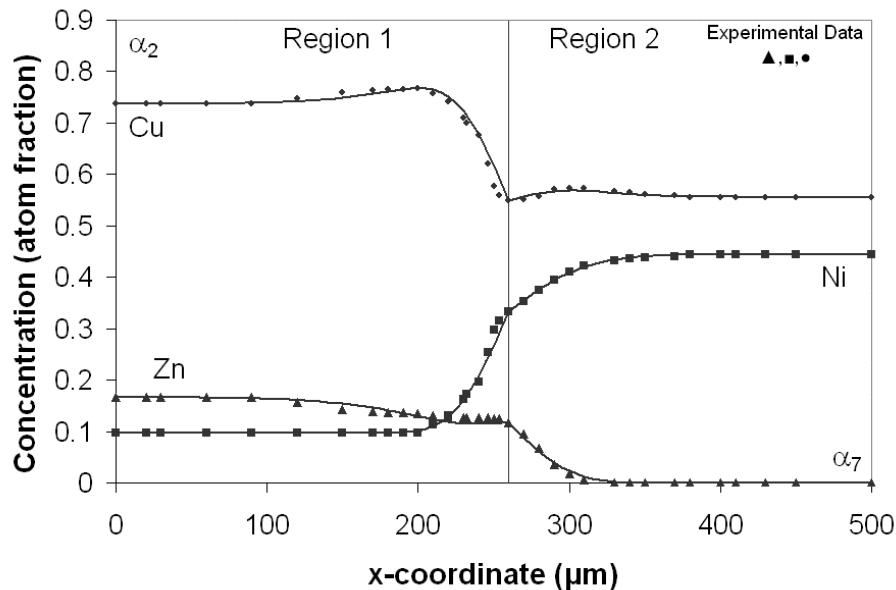
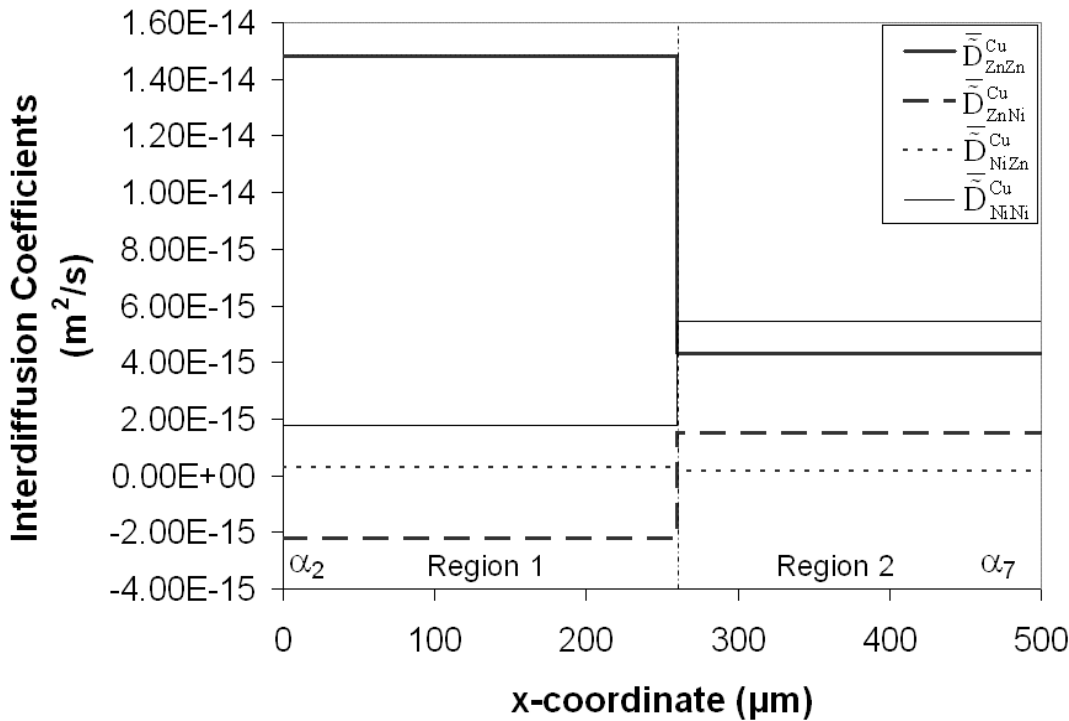
# Calculation of Interdiffusion Fluxes

$$\tilde{J}_i = \frac{1}{2t} \int_{C_i^- \text{ or } C_i^+}^{C_i(x)} (x - x_o) dC_i \quad (i = 1, 2, \dots, n)$$

$$\tilde{J}_i(x^*) = \frac{(C_i^+ - C_i^-)}{2t} \left[ Y_i^* \int_{-\infty}^{x^*} \frac{(1 - Y_i)}{V_m} dx + (1 - Y_i^*) \int_{x^*}^{+\infty} \frac{Y_i}{V_m} dx \right]$$

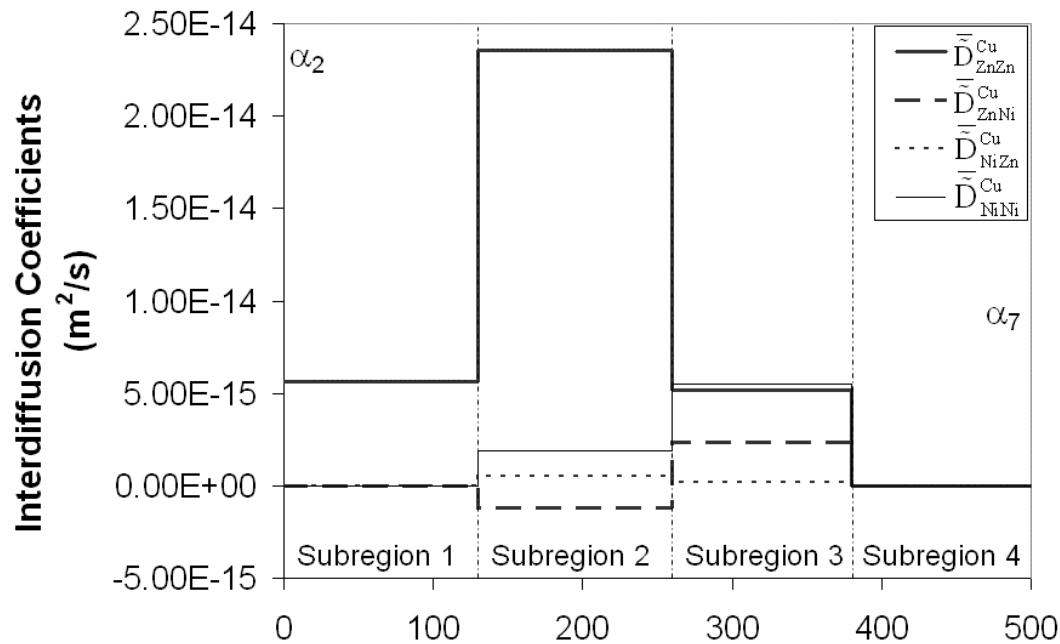


**Two sets of calculated interdiffusion coefficients, one on either side of the Matano plane**

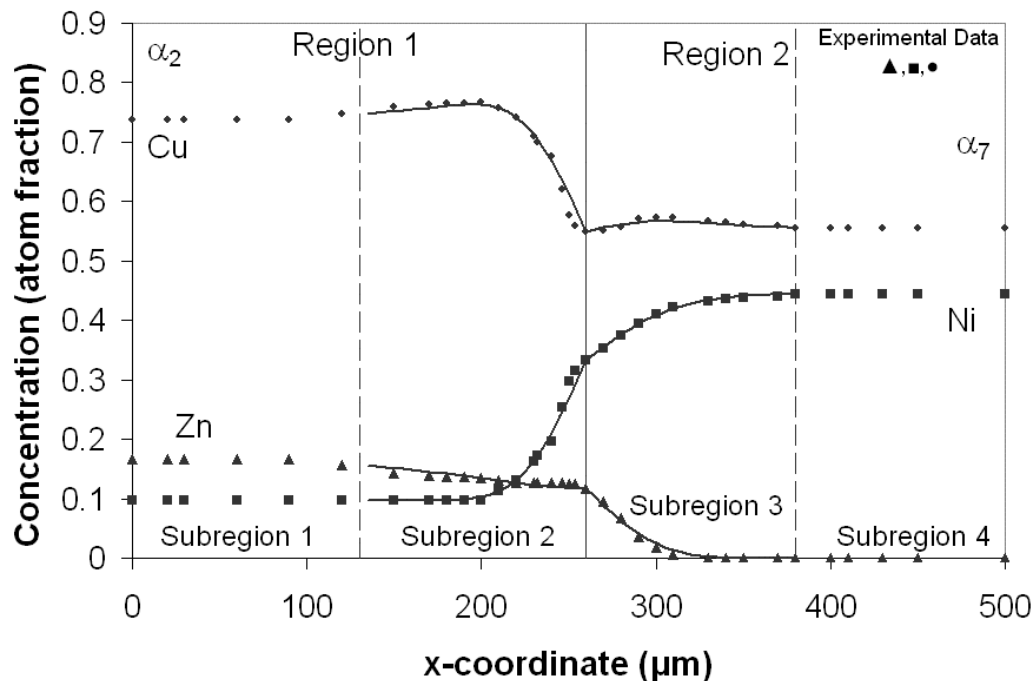


**Regenerated profiles with two sets of interdiffusion coefficient:**





**Four sets of calculated interdiffusion coefficients, two on either side of the Matano plane**



**Regenerated profiles with interdiffusion coefficients**

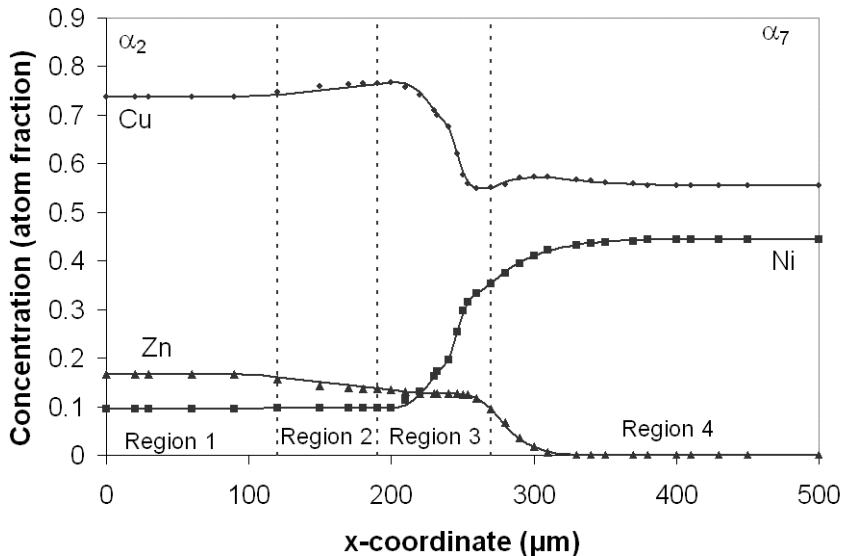
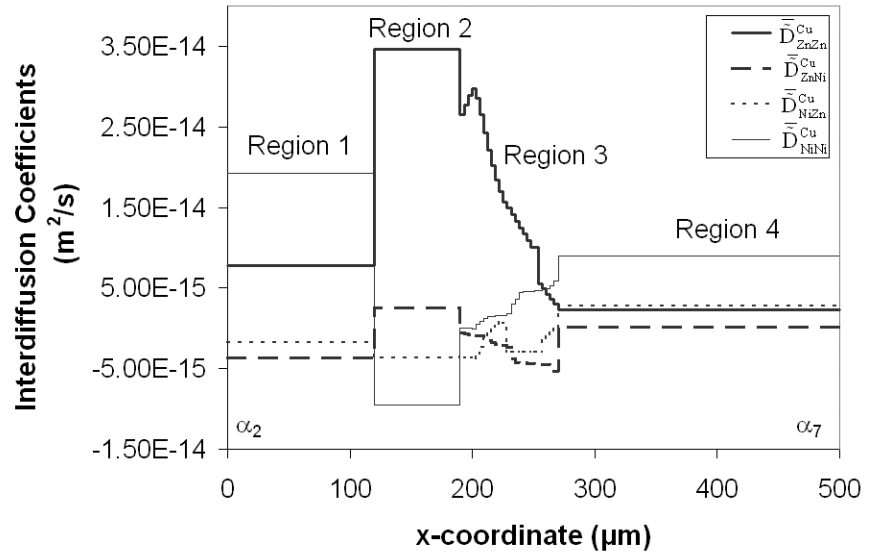
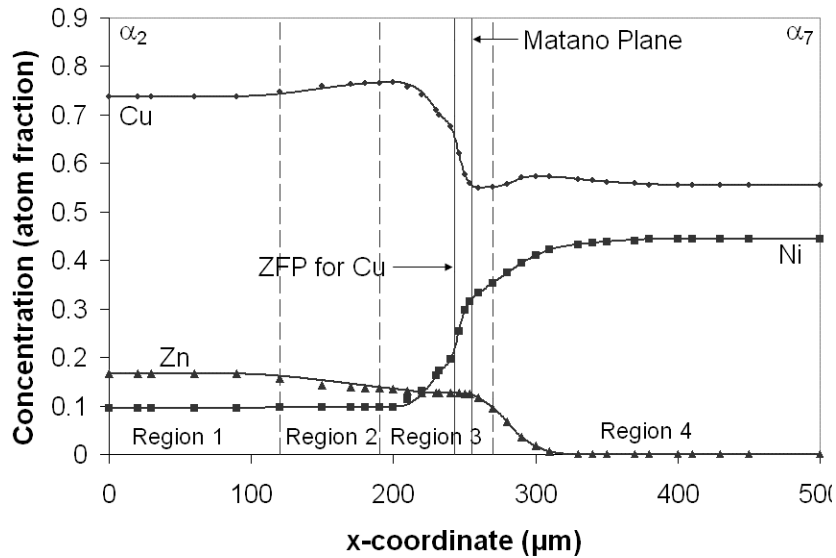


## Four sets of interdiffusion coefficients

	Interdiffusion Coefficients			
	$\bar{D}_{ij}^{\text{Cu}} (\times 10^{-14} \text{ m}^2/\text{s})$			
x-range	$\bar{D}_{\text{ZnZn}}^{\text{Cu}}$	$\bar{D}_{\text{ZnNi}}^{\text{Cu}}$	$\bar{D}_{\text{NiZn}}^{\text{Cu}}$	$\bar{D}_{\text{NiNi}}^{\text{Cu}}$
0-130	0.6	0	0	0
130-260	2.4	-0.1	0.05	0.2
260-380	0.5	0.2	0.02	0.6
380-500	0	0	0	0

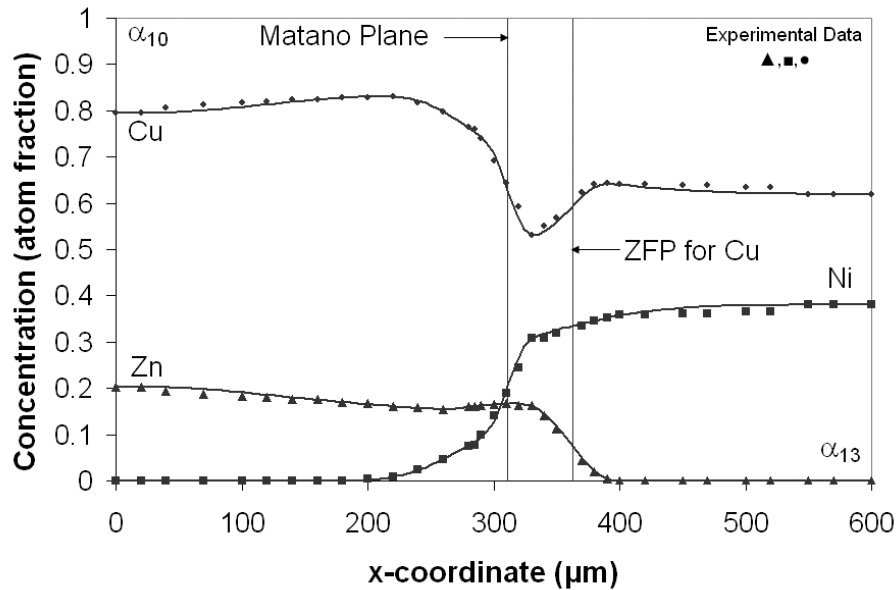


# Reproduction of Concentration Profiles with coefficients over many subregions



**Region 3: 25 Sub-regions**

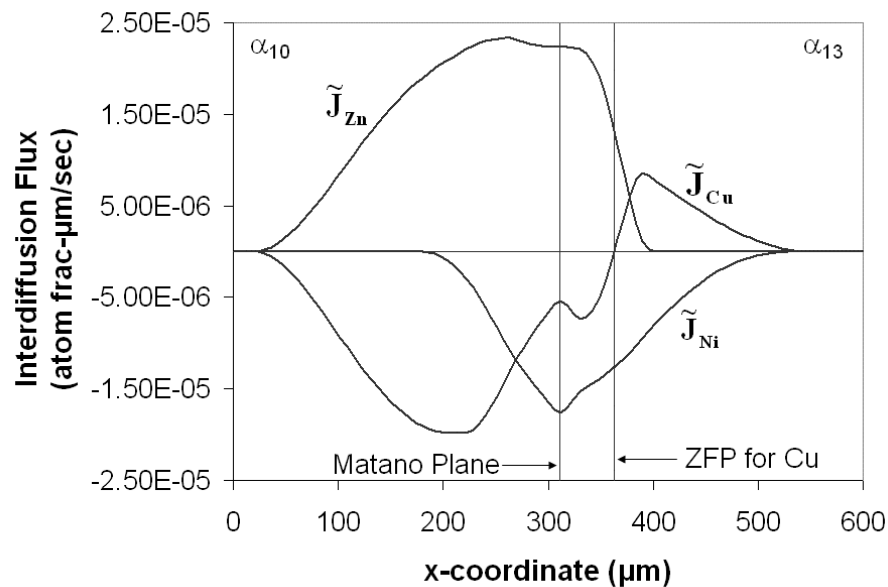




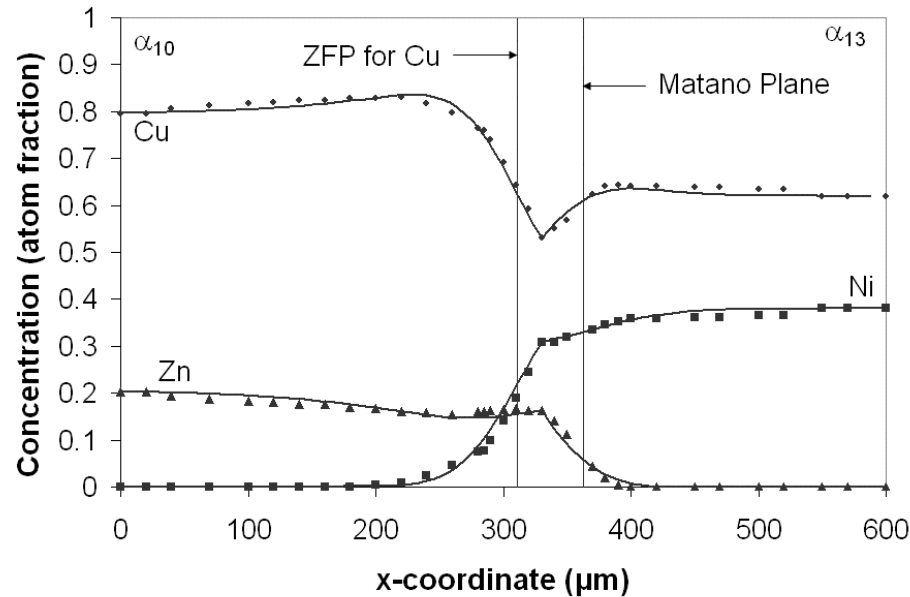
# Analysis of a second Cu-isoactivity couple

$\alpha_{10}$  VS.  $\alpha_{13}$ ;

775°C; 2 days



# Regeneration of Concentration profiles from two different sets of coefficients



Interdiffusion Coefficients for LHS of Minimum

$$\bar{\tilde{D}}_{ij}^{\text{Cu}} \left( \times 10^{-14} \text{ m}^2/\text{s} \right)$$

	$\bar{\tilde{D}}_{\text{ZnZn}}^{\text{Cu}}$	$\bar{\tilde{D}}_{\text{ZnNi}}^{\text{Cu}}$	$\bar{\tilde{D}}_{\text{NiZn}}^{\text{Cu}}$	$\bar{\tilde{D}}_{\text{NiNi}}^{\text{Cu}}$
LHS	4.9	-0.9	-0.2	0.4
RHS	0.6	0.2	-0.2	1.3

Interdiffusion Coefficients for RHS of Minimum

$$\bar{\tilde{D}}_{ij}^{\text{Ni}} \left( \times 10^{-14} \text{ m}^2/\text{s} \right)$$

	$\bar{\tilde{D}}_{\text{CuCu}}^{\text{Ni}}$	$\bar{\tilde{D}}_{\text{CuZn}}^{\text{Ni}}$	$\bar{\tilde{D}}_{\text{ZnCu}}^{\text{Ni}}$	$\bar{\tilde{D}}_{\text{ZnZn}}^{\text{Ni}}$
LHS	-0.5	-5.4	0.9	5.8
RHS	1.4	1.1	-0.2	0.4

# Conversion of Interdiffusion coefficients from one dependent variable to another

$$\tilde{D}_{11}^2 = \tilde{D}_{11}^3 - \tilde{D}_{12}^3$$

$$\tilde{D}_{13}^2 = -\tilde{D}_{12}^3$$

$$\tilde{D}_{31}^2 = \tilde{D}_{22}^3 + \tilde{D}_{12}^3 - \tilde{D}_{11}^3 - \tilde{D}_{21}^3$$

$$\tilde{D}_{33}^2 = \tilde{D}_{22}^3 + \tilde{D}_{12}^3$$

$$\tilde{D}_{22}^1 = \tilde{D}_{22}^3 - \tilde{D}_{21}^3$$

$$\tilde{D}_{23}^1 = -\tilde{D}_{21}^3$$

$$\tilde{D}_{32}^1 = \tilde{D}_{11}^3 + \tilde{D}_{21}^3 - \tilde{D}_{22}^3 - \tilde{D}_{12}^3$$

$$\tilde{D}_{33}^1 = \tilde{D}_{11}^3 + \tilde{D}_{21}^3$$

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## Constraints

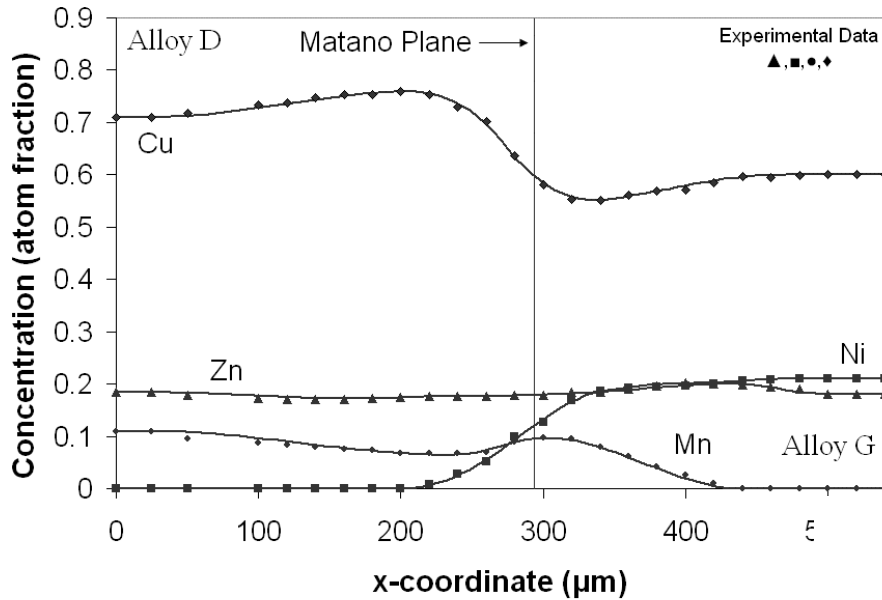
$$\tilde{D}_{11}^3 + \tilde{D}_{22}^3 > 0$$

$$\tilde{D}_{11}^3 \tilde{D}_{22}^3 - \tilde{D}_{12}^3 \tilde{D}_{21}^3 \geq 0$$

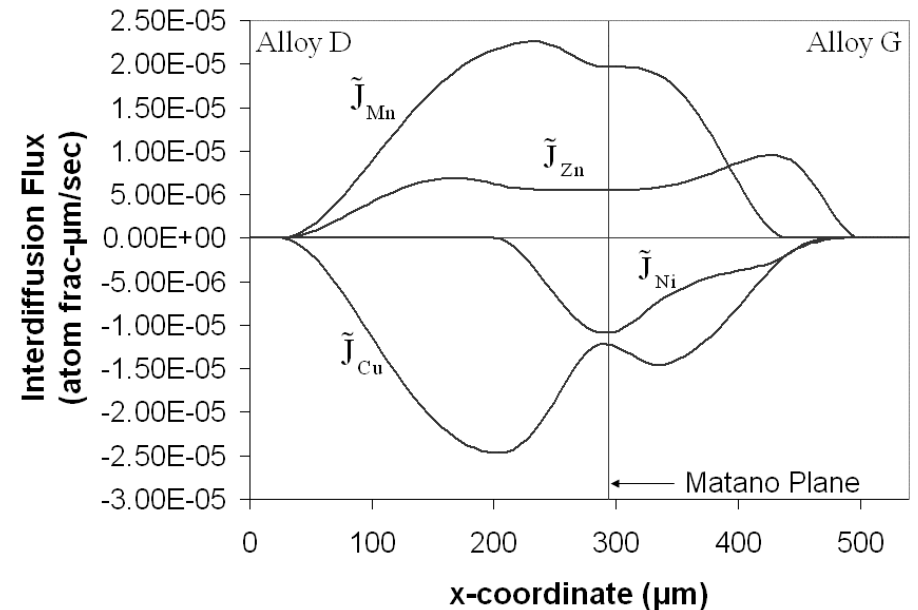
$$\left( \tilde{D}_{11}^3 - \tilde{D}_{22}^3 \right)^2 + 4 \tilde{D}_{12}^3 \tilde{D}_{21}^3 \geq 0$$



# Analysis of a Cu-Ni-Zn-Mn Couple



**Alloy D vs. Alloy G  
couple;  
775°C; 2 days**



# Quaternary Interdiffusion Coefficients for Alloy D vs Alloy G

Interdiffusion Coefficients (Dependent variable is Cu)								
$\bar{D}_{ij}^{Cu} (\times 10^{-13} \text{ m}^2/\text{s})$								
$\bar{D}_{ZnZn}^{Cu}$	$\bar{D}_{ZnNi}^{Cu}$	$\bar{D}_{ZnMn}^{Cu}$	$\bar{D}_{NiZn}^{Cu}$	$\bar{D}_{NiNi}^{Cu}$	$\bar{D}_{NiMn}^{Cu}$	$\bar{D}_{MnZn}^{Cu}$	$\bar{D}_{MnNi}^{Cu}$	$\bar{D}_{MnMn}^{Cu}$
4.6	-0.3	-1.4	0.6	0.01	-0.2	13.9	-1.0	-4.1
0.1	0.07	0.1	-0.005	0.05	-0.04	-0.6	-0.2	0.03

Interdiffusion Coefficients (Dependent variable is Ni)								
$\bar{D}_{ij}^{Ni} (\times 10^{-13} \text{ m}^2/\text{s})$								
$\bar{D}_{CuCu}^{Ni}$	$\bar{D}_{CuZn}^{Ni}$	$\bar{D}_{CuMn}^{Ni}$	$\bar{D}_{ZnCu}^{Ni}$	$\bar{D}_{ZnZn}^{Ni}$	$\bar{D}_{ZnMn}^{Ni}$	$\bar{D}_{MnCu}^{Ni}$	$\bar{D}_{MnZn}^{Ni}$	$\bar{D}_{MnMn}^{Ni}$
-0.8	-11.2	2.2	0.3	3.6	-0.7	0.7	8.7	-1.6
-0.8	-0.1	-0.6	-0.2	0.08	0.01	1.4	0.2	0.9

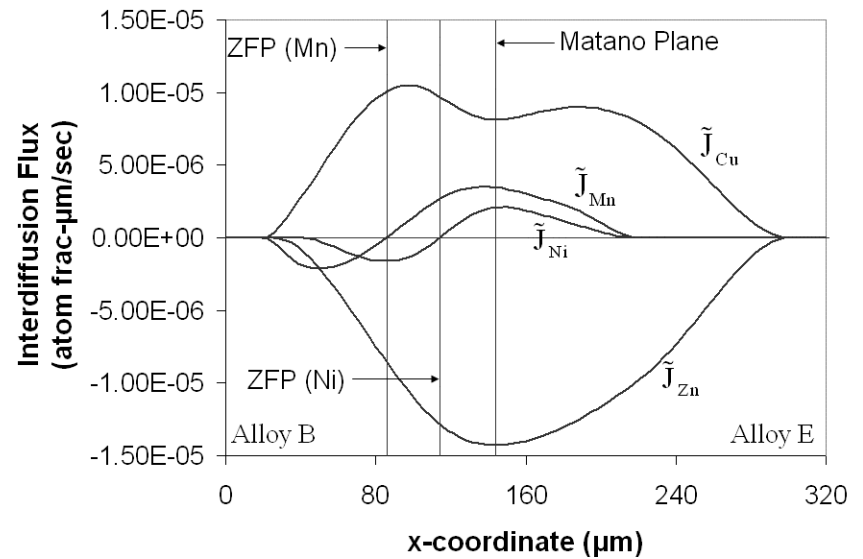
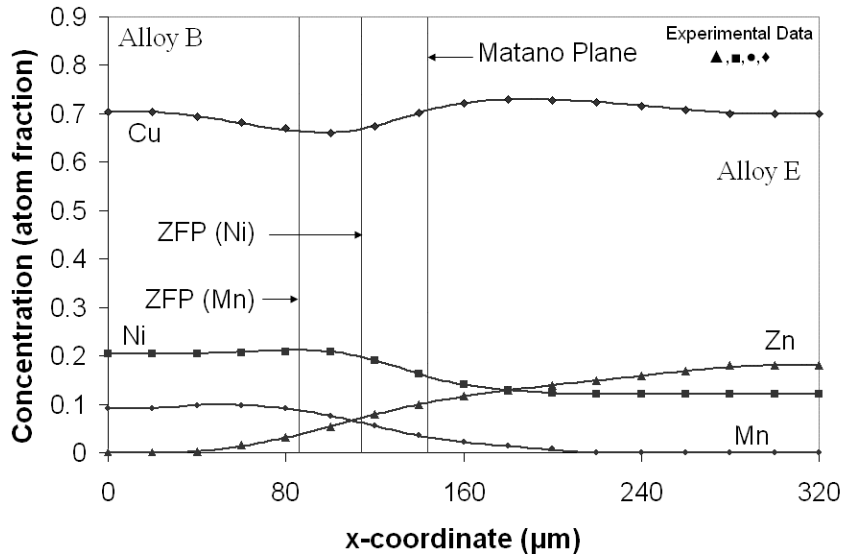
# Comparison of ternary to quaternary interdiffusion coefficients

Interdiffusion Coefficients for $\alpha_{10}$ vs $\alpha_{13}$			
$\bar{\tilde{D}}_{ij}^{Cu} (\times 10^{-14} \text{ m}^2/\text{s})$			
$\bar{\tilde{D}}_{ZnZn}^{Cu}$	$\bar{\tilde{D}}_{ZnNi}^{Cu}$	$\bar{\tilde{D}}_{NiZn}^{Cu}$	$\bar{\tilde{D}}_{NiNi}^{Cu}$
4.9	-0.9	-0.2	0.4
0.6	0.2	-0.2	1.3

Interdiffusion Coefficients for alloy D vs. alloy G (Dependent variable is Cu)								
$\bar{\tilde{D}}_{ij}^{Cu} (\times 10^{-13} \text{ m}^2/\text{s})$								
$\bar{\tilde{D}}_{ZnZn}^{Cu}$	$\bar{\tilde{D}}_{ZnNi}^{Cu}$	$\bar{\tilde{D}}_{ZnMn}^{Cu}$	$\bar{\tilde{D}}_{NiZn}^{Cu}$	$\bar{\tilde{D}}_{NiNi}^{Cu}$	$\bar{\tilde{D}}_{NiMn}^{Cu}$	$\bar{\tilde{D}}_{MnZn}^{Cu}$	$\bar{\tilde{D}}_{MnNi}^{Cu}$	$\bar{\tilde{D}}_{MnMn}^{Cu}$
4.6	-0.3	-1.4	0.6	0.01	-0.2	13.9	-1.0	-4.1
0.1	0.07	0.1	-0.005	0.05	-0.04	-0.6	-0.2	0.03



# Alloy B vs. Alloy E Quaternary Cu-Ni-Zn-Mn Diffusion Couple

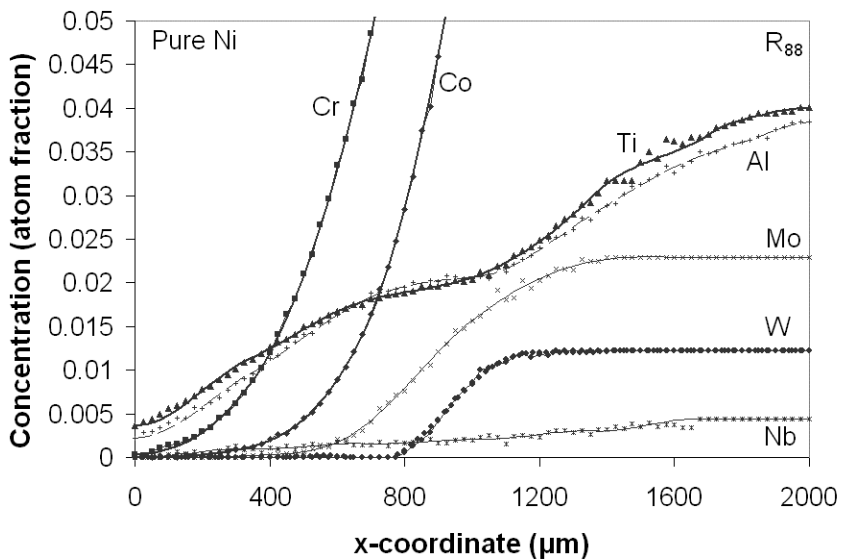
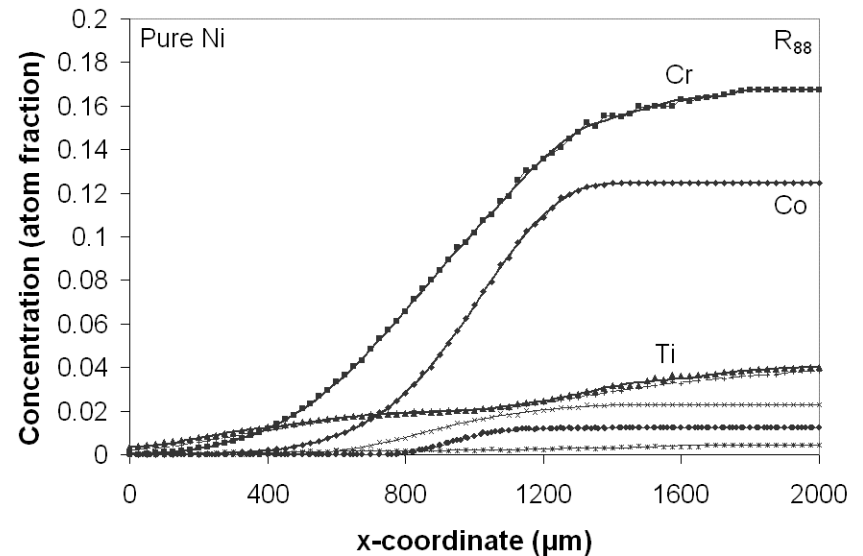
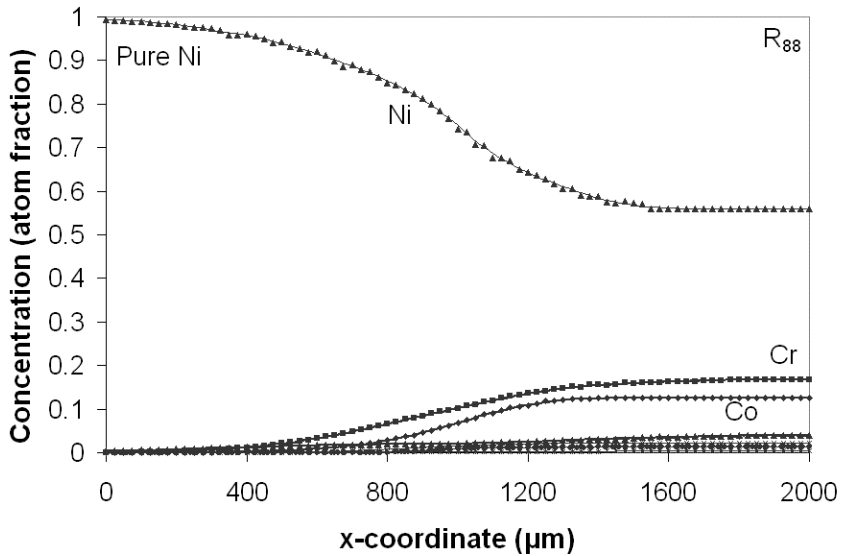


Interdiffusion Coefficients for alloy B vs. alloy E

$\bar{\tilde{D}}_{ij}^{\text{Cu}} \left( \times 10^{-14} \text{ m}^2/\text{s} \right)$								
$\bar{\tilde{D}}_{\text{ZnZn}}^{\text{Cu}}$	$\bar{\tilde{D}}_{\text{ZnNi}}^{\text{Cu}}$	$\bar{\tilde{D}}_{\text{ZnMn}}^{\text{Cu}}$	$\bar{\tilde{D}}_{\text{NiZn}}^{\text{Cu}}$	$\bar{\tilde{D}}_{\text{NiNi}}^{\text{Cu}}$	$\bar{\tilde{D}}_{\text{NiMn}}^{\text{Cu}}$	$\bar{\tilde{D}}_{\text{MnZn}}^{\text{Cu}}$	$\bar{\tilde{D}}_{\text{MnNi}}^{\text{Cu}}$	$\bar{\tilde{D}}_{\text{MnMn}}^{\text{Cu}}$
0.6	-0.4	-0.2	0.08	0.2	-0.1	0.2	0.2	0.3
0.8	3.0	-5.6	0.006	0.2	0.09	0.01	0.1	0.3



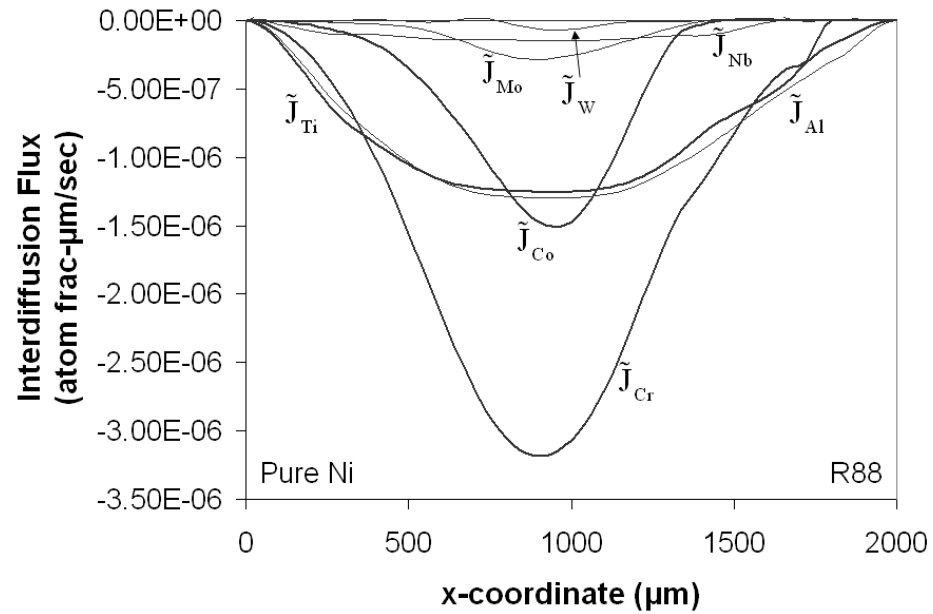
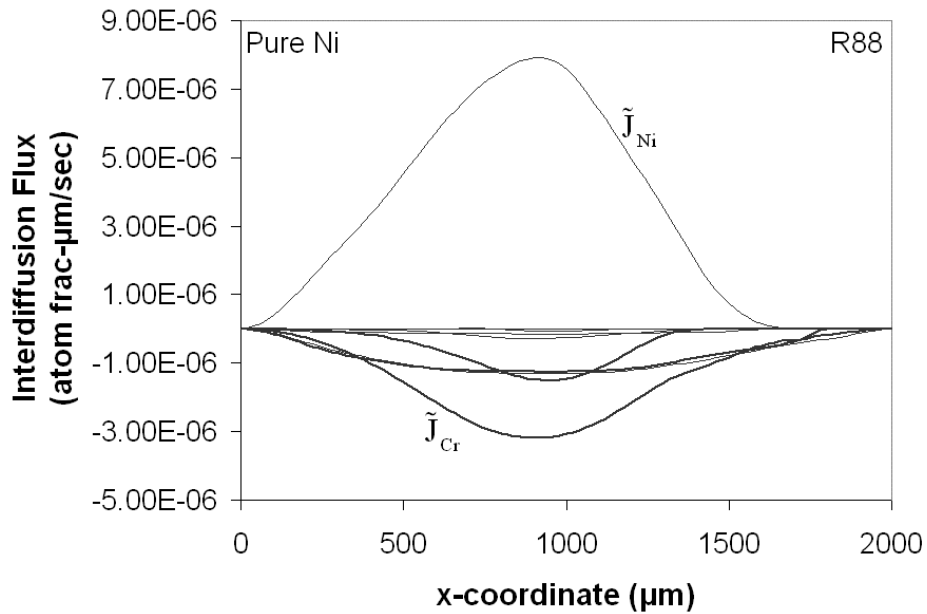
# Pure Ni vs R88 ---- 1150oC;1000 hrs (GE)



Composition (wt. %) of Rene 88							
<u>Co</u>	<u>Cr</u>	<u>Ti</u>	<u>Mo</u>	<u>Nb</u>	<u>W</u>	<u>Al</u>	<u>Ni</u>
13	16	3.7	4	0.7	4	2.1	55.72



# Pure Ni vs. R88



# Calculation of Effective Interdiffusion Coefficients

$$\tilde{D}_{i,\Delta C}^{\text{int}} = \int_{x_1}^{x_2} \tilde{J}_i(x) dx \quad \tilde{D}_{i,\Delta C}^{\text{Int}} = \sum_{j=1}^{n-1} \overline{\tilde{D}_{ij}^n} [C_j(x_1) - C_j(x_2)]$$

$$\tilde{D}_{i,\Delta C}^{\text{eff}} = \frac{\sum_{j=1}^{n-1} \overline{\tilde{D}_{ij}^n} [C_j(x_1) - C_j(x_2)]}{[C_i(x_1) - C_i(x_2)]} \quad (i=1,2,\dots,n-1)$$

•Dayananda, M.A. Metall. Trans. A,1996, vol. 27A, pp 2504-2509

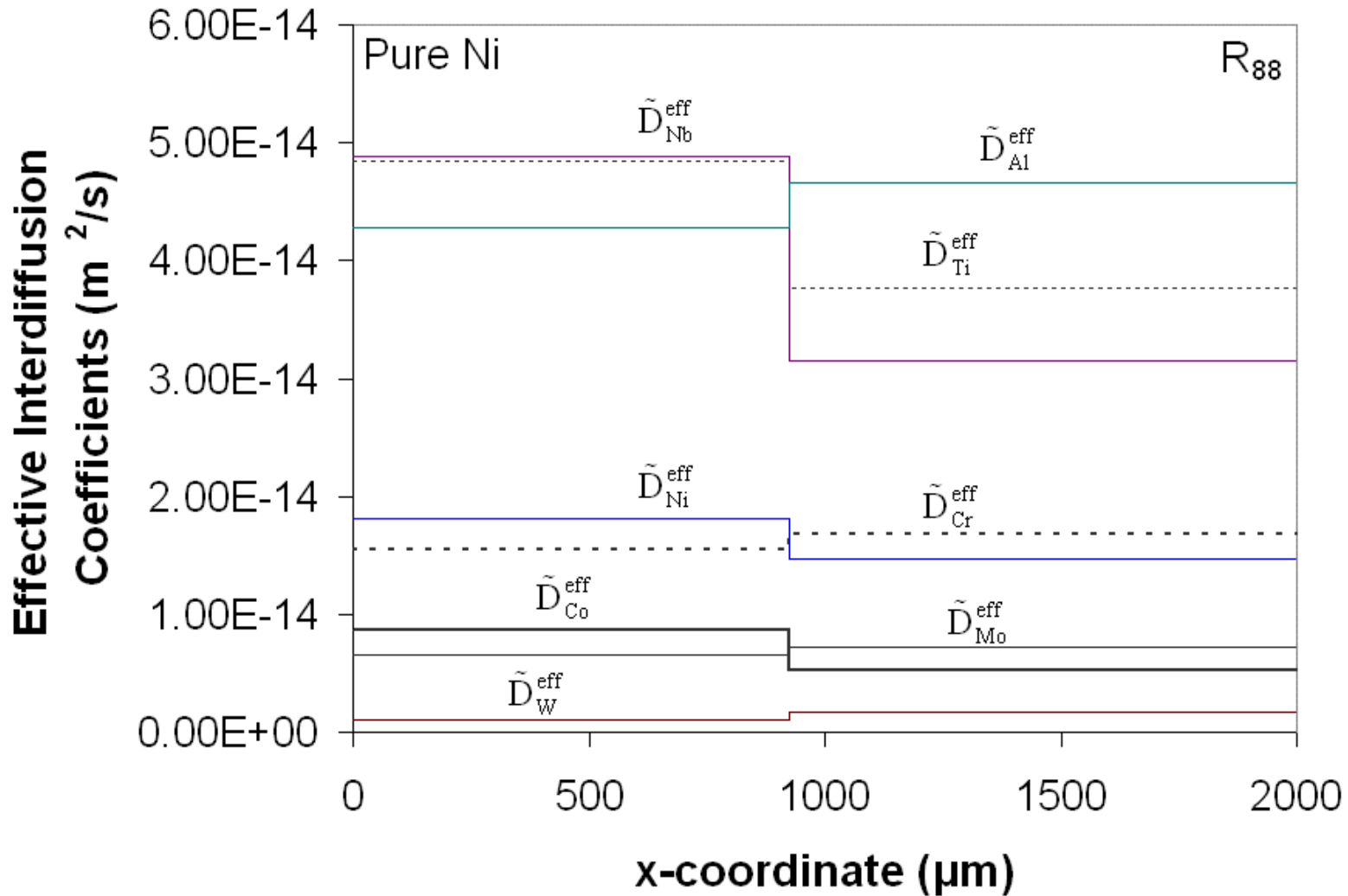


# Pure Ni vs R88

	<b>Calculated Effective Interdiffusion Coefficients</b>							
	$\tilde{D}_{i,\Delta C}^{\text{eff}} \left( \times 10^{-15} \text{ m}^2/\text{s} \right)$							
	$\tilde{D}_{\text{Co}}^{\text{eff}}$	$\tilde{D}_{\text{Cr}}^{\text{eff}}$	$\tilde{D}_{\text{Ti}}^{\text{eff}}$	$\tilde{D}_{\text{Mo}}^{\text{eff}}$	$\tilde{D}_{\text{Nb}}^{\text{eff}}$	$\tilde{D}_{\text{W}}^{\text{eff}}$	$\tilde{D}_{\text{Al}}^{\text{eff}}$	$\tilde{D}_{\text{Ni}}^{\text{eff}}$
$-\infty$ to $x_0$	8.71	15.5	48.4	6.52	48.9	1.05	42.8	18.1
$x_0$ to $+\infty$	5.21	16.9	37.7	7.19	31.5	1.72	46.5	14.7



# Pure Ni vs R88



# Equations used to regenerate the profiles from average effective interdiffusion coefficients in an n-component system

$$\tilde{D}_{i,L} = \frac{\int_{C_i^o}^{C_i^-} (x - x_o)^2 dC_i}{2t[C_i^- - C_i^o]}$$

$$S = \frac{2\sqrt{\tilde{D}_{i,L}t} (C_i^- - C_i^o)}{\alpha_{i,L}}$$

$$C_i = [C_i^o - C_i^-] \left[ 1 - \operatorname{erf} \left( \frac{\alpha_{i,L}(x_o - x)}{2\sqrt{\pi D_{i,L}t}} \right) \right] + C_i^-$$

$$\tilde{D}_{i,R} = \frac{\int_{C_i^+}^{C_i^o} (x - x_o)^2 dC_i}{2t(C_i^o - C_i^+)}$$

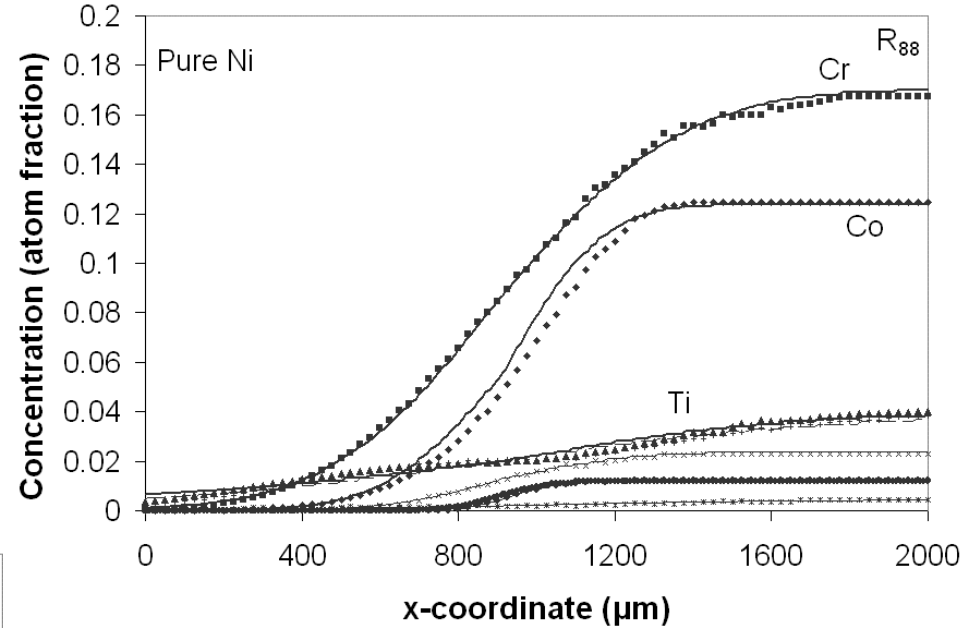
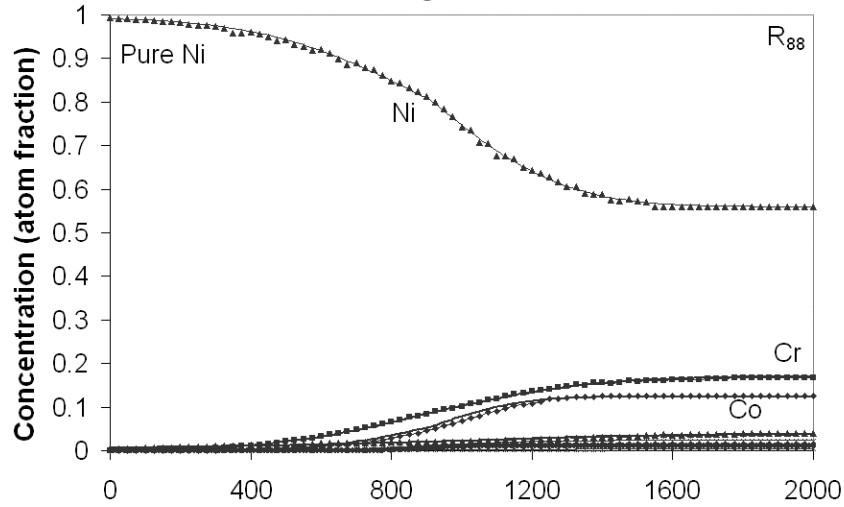
$$S = \frac{2\sqrt{\tilde{D}_{i,R}t} (C_i^o - C_i^+)}{\alpha_{i,R}}$$

$$C_i = (C_i^o - C_i^+) \left[ 1 - \operatorname{erf} \left( \frac{\alpha_{i,R}(x - x_o)}{2\sqrt{\pi D_{i,R}t}} \right) \right] + C_i^+$$

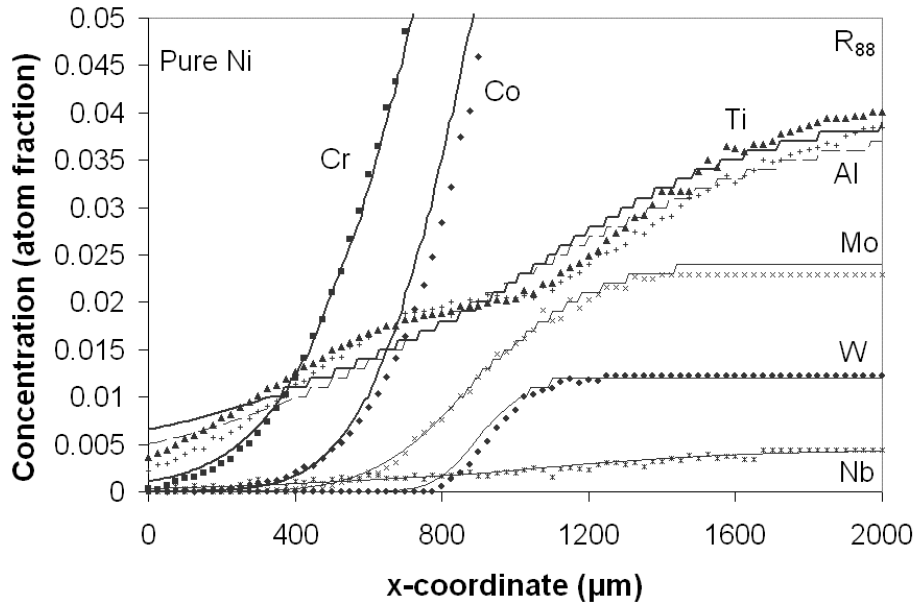


# Error Function Representation with Average Effective Interdiffusion Coefficients

Conc Range: 0-1



Conc Range: 0-0.2



Conc Range: 0-0.05



# Conclusions

- *The MultiDiflux* program can be used to analyze binary and multicomponent systems ( $n > 2$ ) for interdiffusion fluxes and  $(n-1)^2$  interdiffusion coefficients over selected composition ranges.
- All profiles in ternary couples can be analyzed for interdiffusion coefficients and reproduced from the calculated coefficients based on error function solutions.
- The program also calculates an Integrated and an effective interdiffusion coefficient for each component.
- The effective coefficients may also be used to generate concentration profiles in an  $n$ -component system.

