NIST Workshop: High Throughput Analysis of Multicomponent Multiphase Diffusion Data February 7-8, 2006

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&
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Why a Workshop on Diffusion?

- Consensus of NIST Workshop held March 21-22, 2002 *Computational Thermodynamics and Diffusion Modeling*- Promotes continuing interest in thermodynamic databases
- Metallurgy Division participation in DARPA/AIM/GE program on Turbine Disks
- NIST interest in Combinatorial (High Thoughput) Measurement Methods
- Existence of legacy Diffusion in Metals Data base at NIST (J. R. Manning)

Goals

- Improve communication between experts in multicomponent diffusion measurement, analysis and simulation.
- Establish the most efficient method for extracting diffusion data (diffusion coefficients, fluxes, marker location) from multicomponent diffusion couple experiments.
- Provide a forum to solve common diffusion software execution problems.
- Agree on a common diffusion mobility data base assessment procedure.
- Establish a general approach to data handling and diffusion modeling in ordered phases.
- Develop standard problems and web site for inter-laboratory comparison of diffusion simulation methods and data extraction techniques

Agenda

Tuesday, February 7, 2006

8:30- 9:00 **Introduction** (Coffee and bagels)

9:00 –9:30 **Review of action items from last workshop**

9:30-10:00 Diffusion Barriers: Overview (Boettinger, Perepezko)

10:00-10:30 **Diffusion Barriers: Experimental Examples (Sohn, Josell)**

10:30-10:45 Break

10:45-11:15 Review of Horn Formation (Morral)

11:15-11:45 1-D Multiphase Diffusion Simulations (Larsson)

12:00-1:00 **Lunch**

Agenda

Tuesday afternoon

1:00-1:30 Hot topics in Grain Boundary Diffusion (Mishin)
1:30 –1:45 Discussion
1:45 - 2:15 Kirkendall effect in two phase systems (Boettinger)
2:15 – 2:45 Onsager relations and Kirkendall shift as a cross effect (Ågren)
2:45 – 3:00 Break
3:00 –3:30 Partial Thermodynamic Properties of γ'-$(Ni,Pt)_3Al$ and γ-(Ni,Pt,Al) in the Ni-Al-Pt-O system (Copland)
3:30-4:00 **Review and Assessment of Diffusion in B2 and γ' ($L1_2$) Phase** (Campbell)
4:00-4:30 Oxide Modeling (Höglund)
4:30-5:00 First Principle Calculations (Liu)

6:00 Dinner: Café Mileto

Wednesday February 8

9:00-9:30 **RPI Teaching Modules** (Lupulescu)
9:30-10:30 DICTRA Discussion: (Reference Frames, Comparisons with MultiDiflux, Order diffusion models, other suggestions)
10:30-10:45 Viewpoint Discussion (Perepezko)
10:45-11:30 Open discussion
11:00 –12:00 Action items

Lunch/Adjourn

Definitions

Coefficient	General Notation	DICTRA notation
Tracer Diffusivity	$D_i^* = \tilde{\nu}\beta a^2 f \exp\left(\frac{\Delta S_{Va}^f + \Delta S_{Va}^m}{k}\right)\exp\left(-\frac{\Delta H_{Va}^f + \Delta H_{Va}^m}{kT}\right)$ $\tilde{\upsilon}$ = vibration frequency a = lattice parameter β = 1 for FCC and BCC and 1/8 for diamond cubic f = correlation factor $D = D_0 \exp\left(\frac{-Q}{RT}\right)$	$D_k^* = RTM_k$ $M_k = \delta^2 \nu \exp\left(-\frac{\Delta G_{kVa}^*}{RT}\right)\frac{1}{RT}$
Intrinsic Diffusivity (partial chemical)	$D_i = D_i^*\left[1 + \frac{\partial \log \gamma}{\partial \log N}\right]$	${}^iD_{kj} = c_k M_{kVa}\frac{\partial \mu_k}{\partial c_j}$
Chemical Diffusivity (Interdiffusion)	$\tilde{D} = x_A D_B + x_B D_A$ (binary) D_i and $\tilde{D}$ are related by the velocity of Kirkendall frame, $v = -J_{Va}V_M$	$D_{kj} = \sum_{i=1}^{n}(\delta_{ik} - x_k)x_i M_i \frac{\partial \mu_i}{\partial x_j}V_m$

Further testing and refinement of database using GE Diffusion Couple Data (FY 2003)

- Binary Couples
  - Single phase couples
    - at 1100 °C for 1000 h : **Ni/Co**
  - Multiphase couples
    - at 1100 °C for 1000 h : Co/Cr, Co/Mo, Co/Nb, Co/W, Cr/Ta, Cr/W, Cr/Mo, Ni/W, Ni/Ta, Ni/Mo, Ni/NiAl(1150 °C)
    - at 850 °C for 4000 h: Ni/W, Co/Fe, Cr/Mo, Cr/Co, Mo/Fe
    - at 700 °C for 4000 h: Fe/Co, Mo/Cr
- Multicomponent Couples
  - Single Phase γ
    - at 1150 °C for 1000 h: René88 /IN718 and Ni/René88
  - γ / γ+γ' or γ+γ' / γ+γ' at 1150 °C for 1000 h
    - René-95/ René-88
    - U720/IN718
    - IN718/IN100
    - ME3/ René-95
    - ME3/IN718
    - IN100/ René-88
    - U720/ME3
    - ME3/ René-88
    - IN100/ME3
    - René-95/U720
    - René-95/IN718
    - IN100/U720
  - γ / B2 or γ+γ' /B2
    - at 1150 °C for 1000 h: NiAl/ René-88, NiAl/Ta
    - at 850 °C for 4000 h: NiAl/ René-88, NiAl/Ta
  - TCP Couples: (Rene88-X)
    - at 1150 °C for 1000 h: X= Ta, W
    - at 850 °C for 4000 h: X=Ta, W, Co, Cr, Fe, Mo, Ni, Ti
    - at 700 °C for 4000 h: X=Co, Cr, Fe, Mo

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Couples from UCF and RPI

- NiAl/Superalloy (UCF)
  - CM247/NiAl
  - GTD11/NiAl
  - IN738/NiAl
  - IN939/NiAl
  - Waspalloy/NiAl

- FeCrAl-Single Phase BCC (RPI)
  - X2/X3: Fe-18.5Cr-2.5Al/Fe-15.8Cr-35.7Al (at.%)
  - X5/X10: Fe-18.8Cr-25.8Al/Fe-20.6Cr-9.51Al (at.%)
  - X4/X6: Fe-5.7Cr-28.1Al/Fe-30.5Cr-18.7Al (at.%)

Multicomponent Mobility Database for FCC phase of Superalloys

Campbell, Boettinger & Kattner, Acta Mat.50 (2002) 775-792.

René-N4 (x10^{-14} m^2/s)

	Al	*Co*	*Cr*	*Mo*	*Nb*	*Ta*	*Ti*	*W*
Al	+119.5	+13.93	+34.83	+34.34	+42.43	+51.50	+49.51	+53.22
Co	−11.37	+17.00	−8.25	−5.67	−5.55	−1.83	−7.10	−9.69
Cr	−4.26	−5.37	+13.67	−3.21	+8.93	+9.91	+8.25	+2.49
Mo	−8.33	−0.280	−0.426	+7.57	−0.55	−0.36	−0.17	−0.45
Nb	+0.31	+0.25	+0.66	+0.27	+24.05	+0.74	+0.85	+0.31
Ta	−0.68	+0.33	+0.53	+0.24	+0.26	+0.76	+0.50	+0.23
Ti	+1.63	+1.35	+4.94	+4.94	+6.25	+6.57	+23.62	+5.41
W	−1.81	−0.62	−0.55	−0.60	−1.22	−0.83	−0.70	+3.40

Ni = solvent

Reduced (n-1)Diffusion Matrix at 1293 °C

René-N5 (x10^{-14} m^2/s)

	Al	*Co*	*Cr*	*Hf*	*Mo*	*Re*	*Ta*	*W*
Al	+93.16	+13.92	+33.46	−6.51	+33.42	25.44	+48.63	+50.87
Co	−6.51	+27.22	−8.56	−27.64	−4.95	−5.11	+3.87	−9.21
Cr	+4.15	−4.23	+21.02	−6.25	−0.22	−0.78	+13.81	+6.89
Hf	0.86	+0.07	+1.70	+262.1	+1.52	0.87	+2.37	+1.84
Mo	−0.35	−0.30	−0.30	−1.905	+7.71	−0.25	−0.13	−0.19
Re	−0.75	−0.32	−0.36	−2.59	−0.25	+0.08	−0.51	−0.32
Ta	−0.03	+0.33	+0.98	−4.17	+0.64	+0.86	+7.75	+0.87
W	−1.18	−0.57	−0.54	−4.51	−0.39	−0.11	−0.76	+0.59

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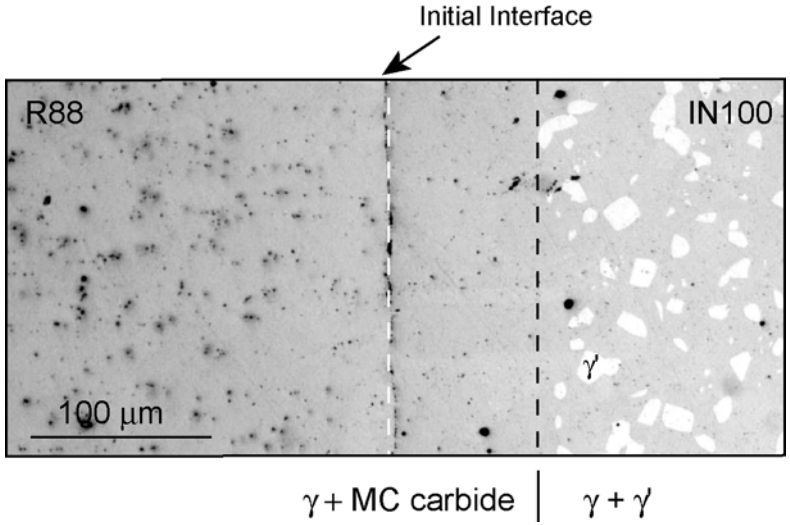
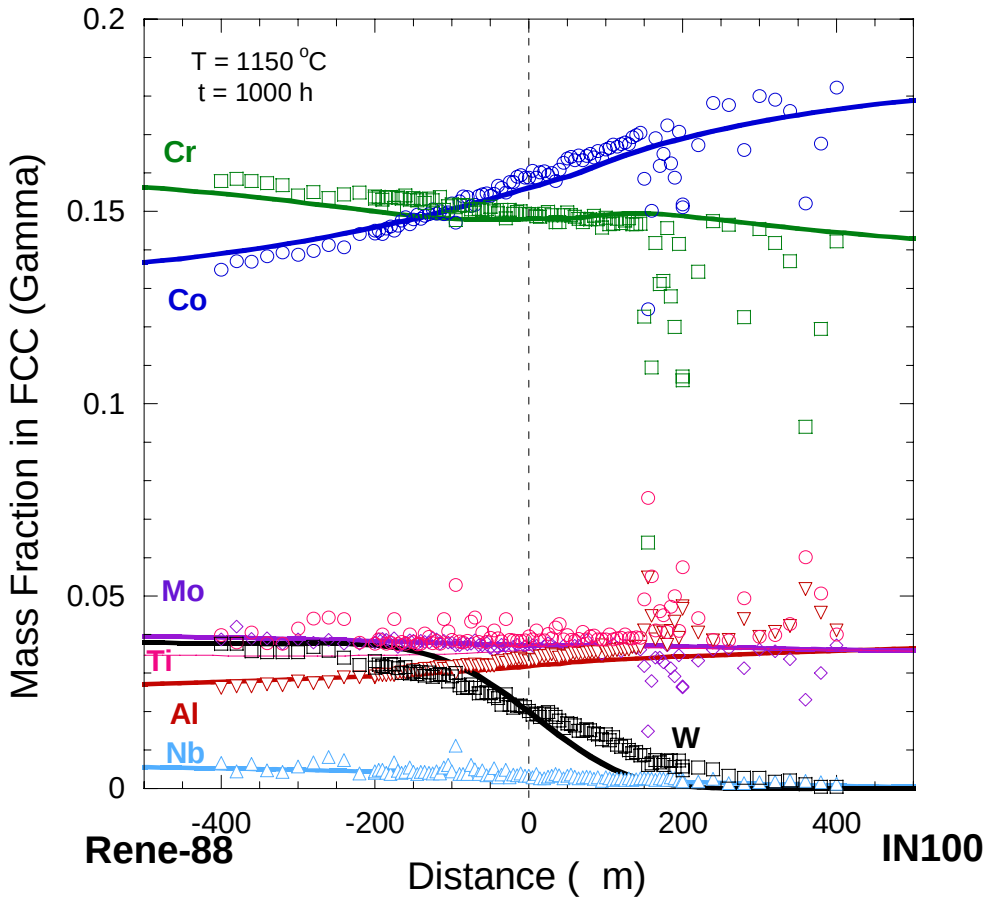
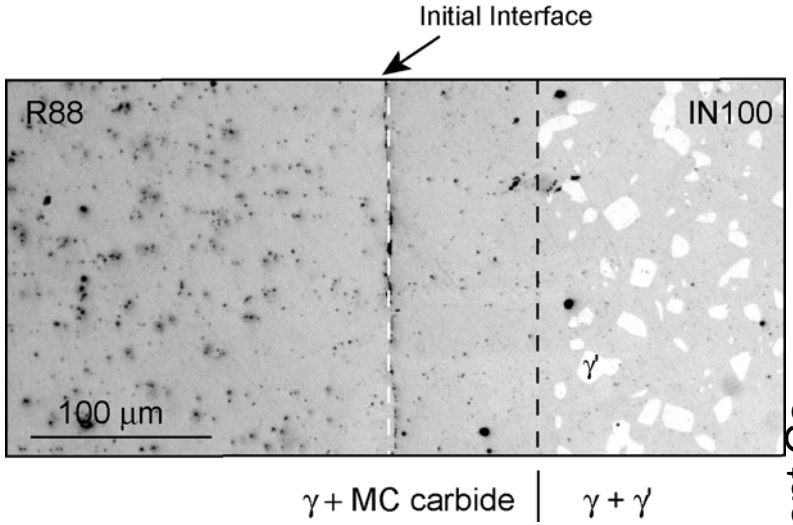
René-88/IN-100; 1000 h at 1150 °C

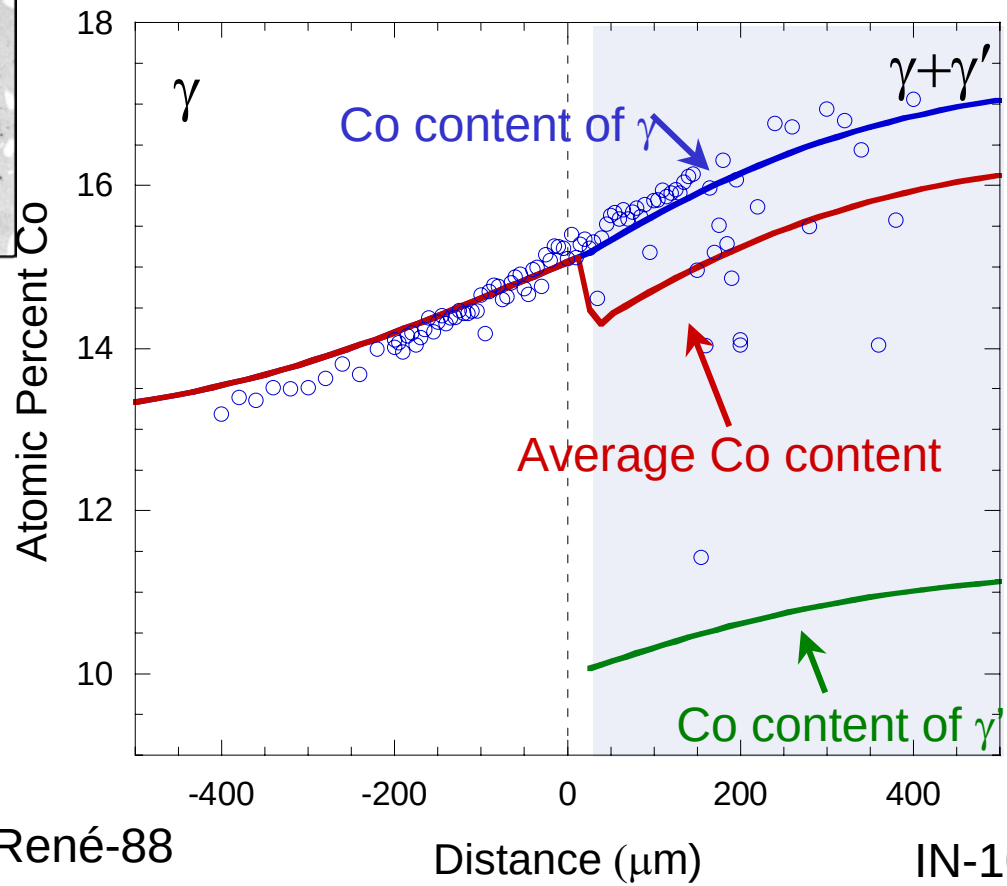




Experimental data from J-C. Zhao, GE Global Research

René-88/IN-100; 1000 h at 1150 °C





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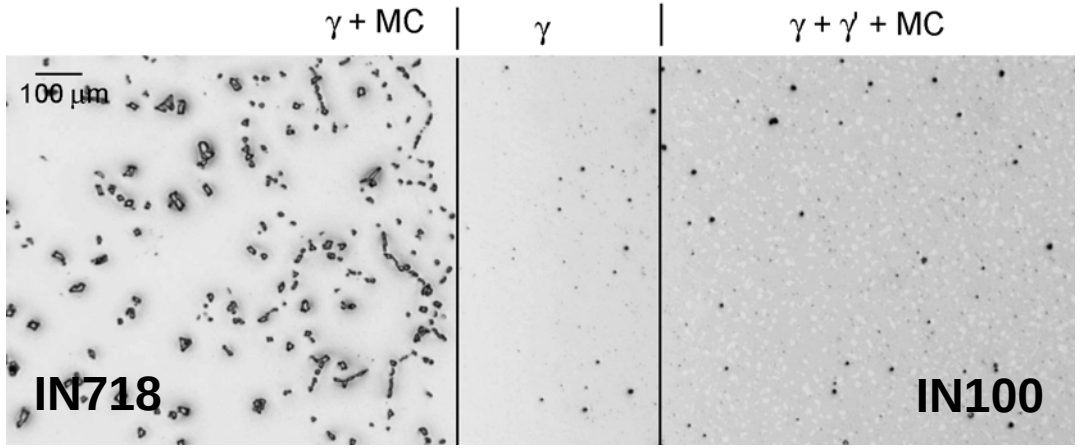
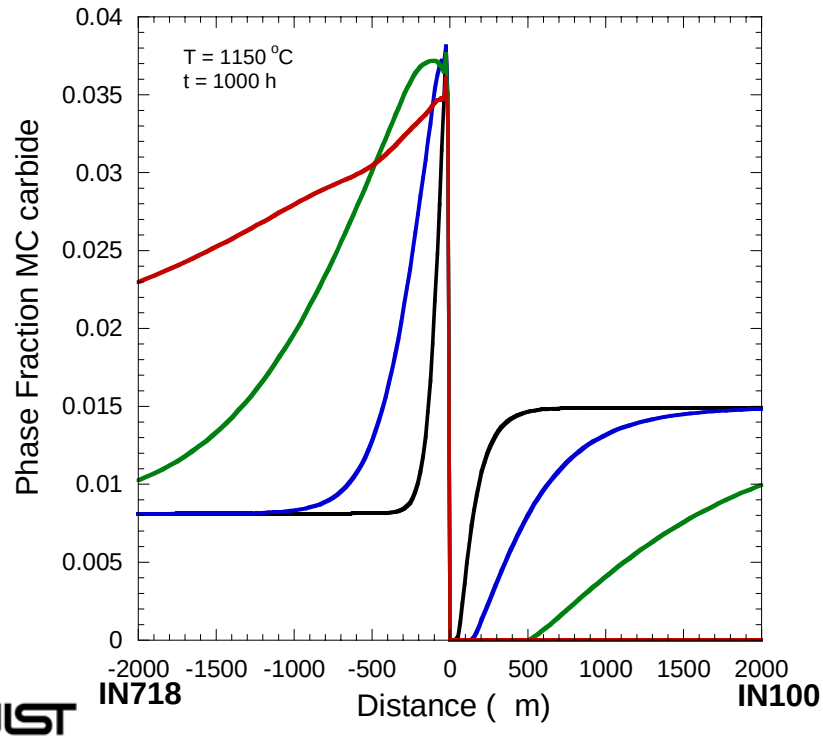
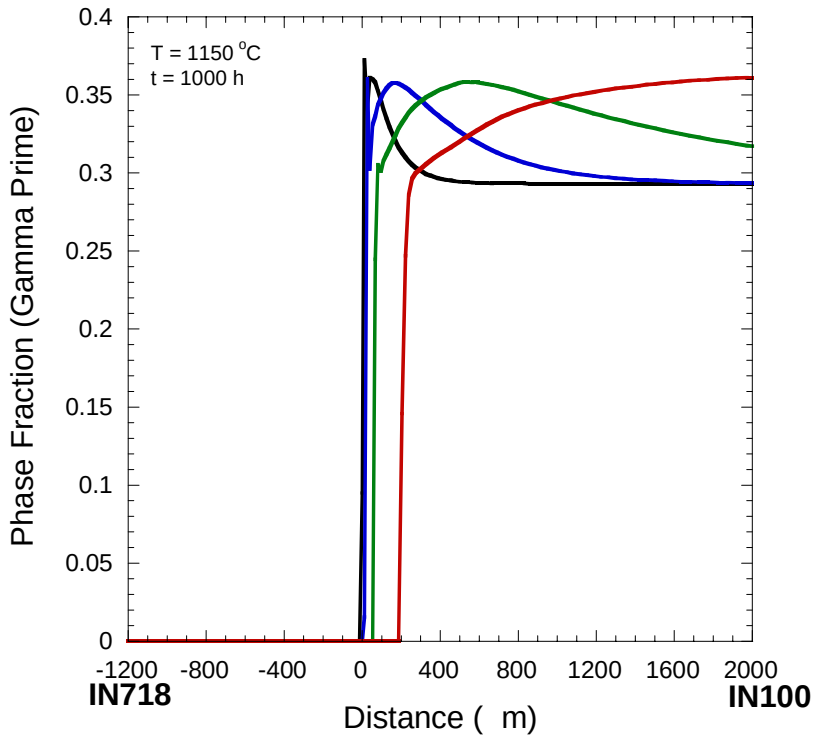
IN-718/IN-100; 1000 h at 1150 °C







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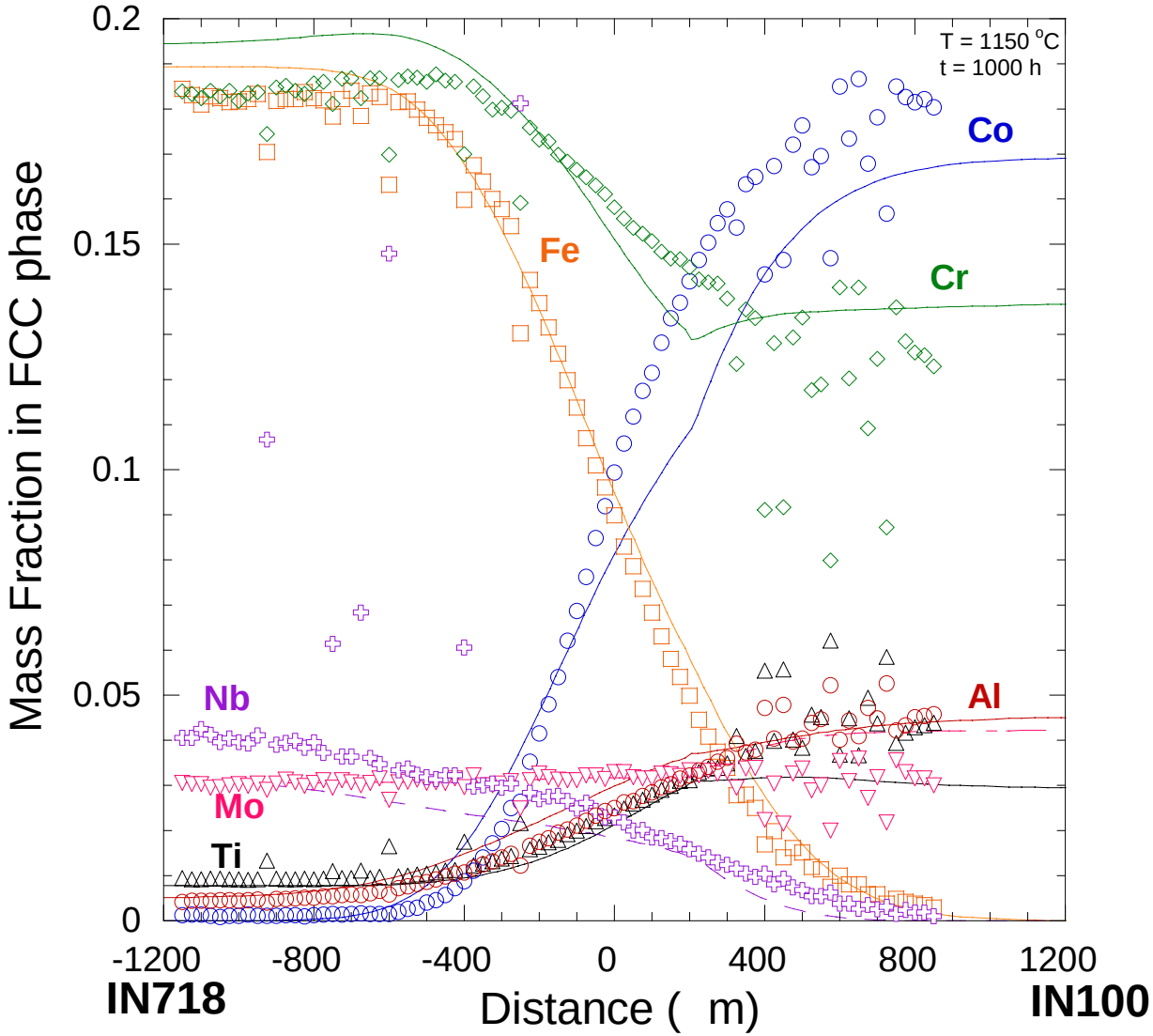
IN-718/IN-100; 1000 h at 1150 °C



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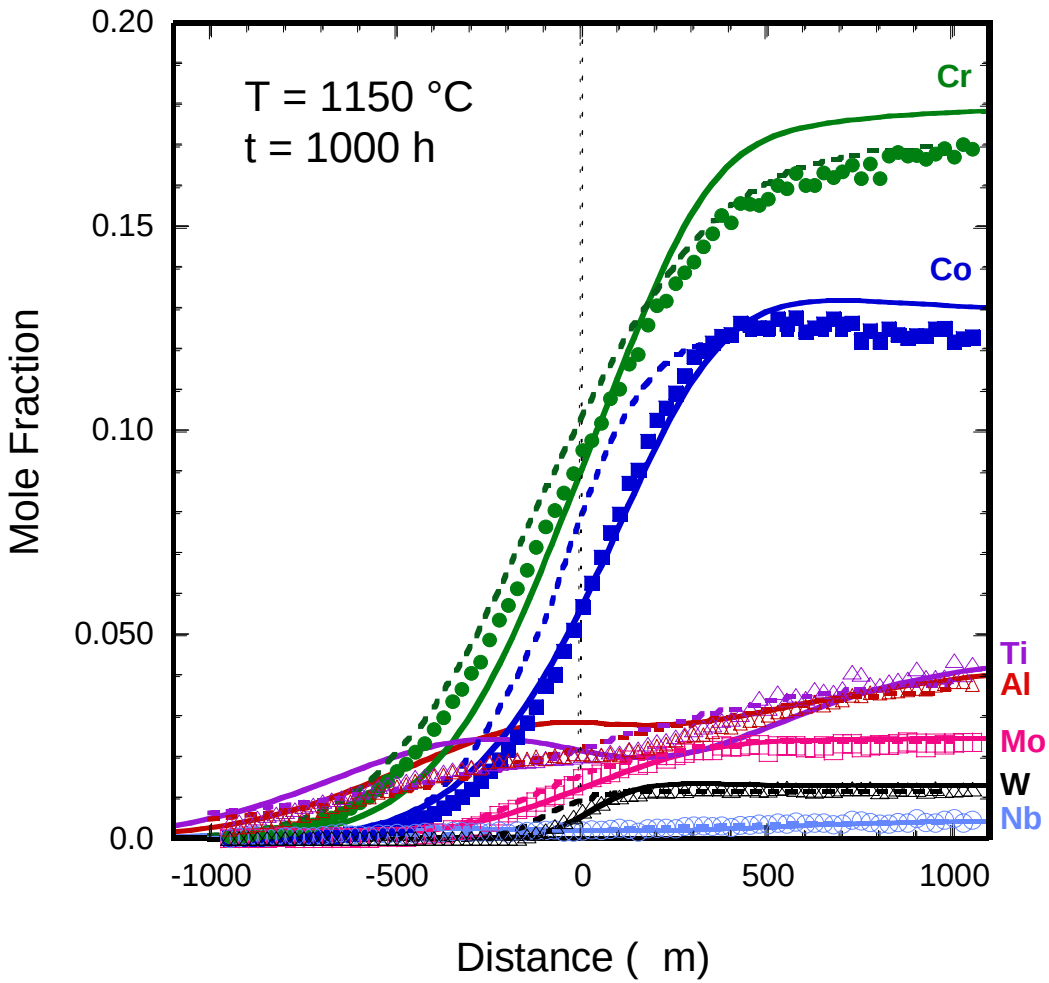
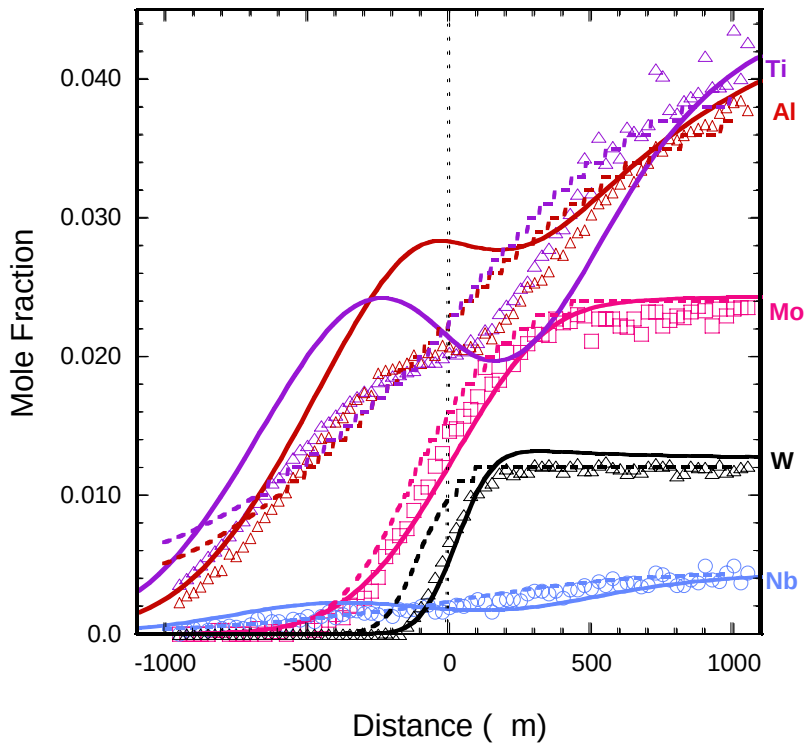
Comparison of DICTRA and MultiDiflux Results for Ni/René-88



- Symbols = GE exp. Data
- Solid lines = DICTRA simulation (only uses initial compositions as inputs)
- Dashed lines = MultiDiflux (uses experimental profiles as input)



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Comparison of DICTRA and MultiDiflux Results for Ni/René-88

$$\tilde{D}_{i,\Delta c}^{eff} = \frac{\sum_{j=1}^{n-1} \tilde{\bar{D}}_{ij}^{n} \left[c_j(x_1) - c_j(x_2) \right]}{\left[c_i(x_1) - c(x_2) \right]} \quad (i = 1,2,\ldots,n-1)$$

Component	-∞ (Ni) to 0 (x10^{-15}m^2/s)		0 to + ∞ (R88) (x10^{-15}m^2/s)	
	MultiDiflux	DICTRA	MultiDiflux	DICTRA
$\tilde{D}_{Co}^{eff}$	8.71	12.3	5.21	10.8
$\tilde{D}_{Cr}^{eff}$	15.5	12.9	16.9	11.9
$\tilde{D}_{Ti}^{eff}$	48.4	39.7	37.7	40.6
$\tilde{D}_{Mo}^{eff}$	6.52	10.6	7.19	9.92
$\tilde{D}_{Nb}^{eff}$	48.9	34.0	31.5	33.7
$\tilde{D}_{W}^{eff}$	1.05	3.06	1.72	1.56
$\tilde{D}_{Al}^{eff}$	42.8	35.3	46.5	58.0

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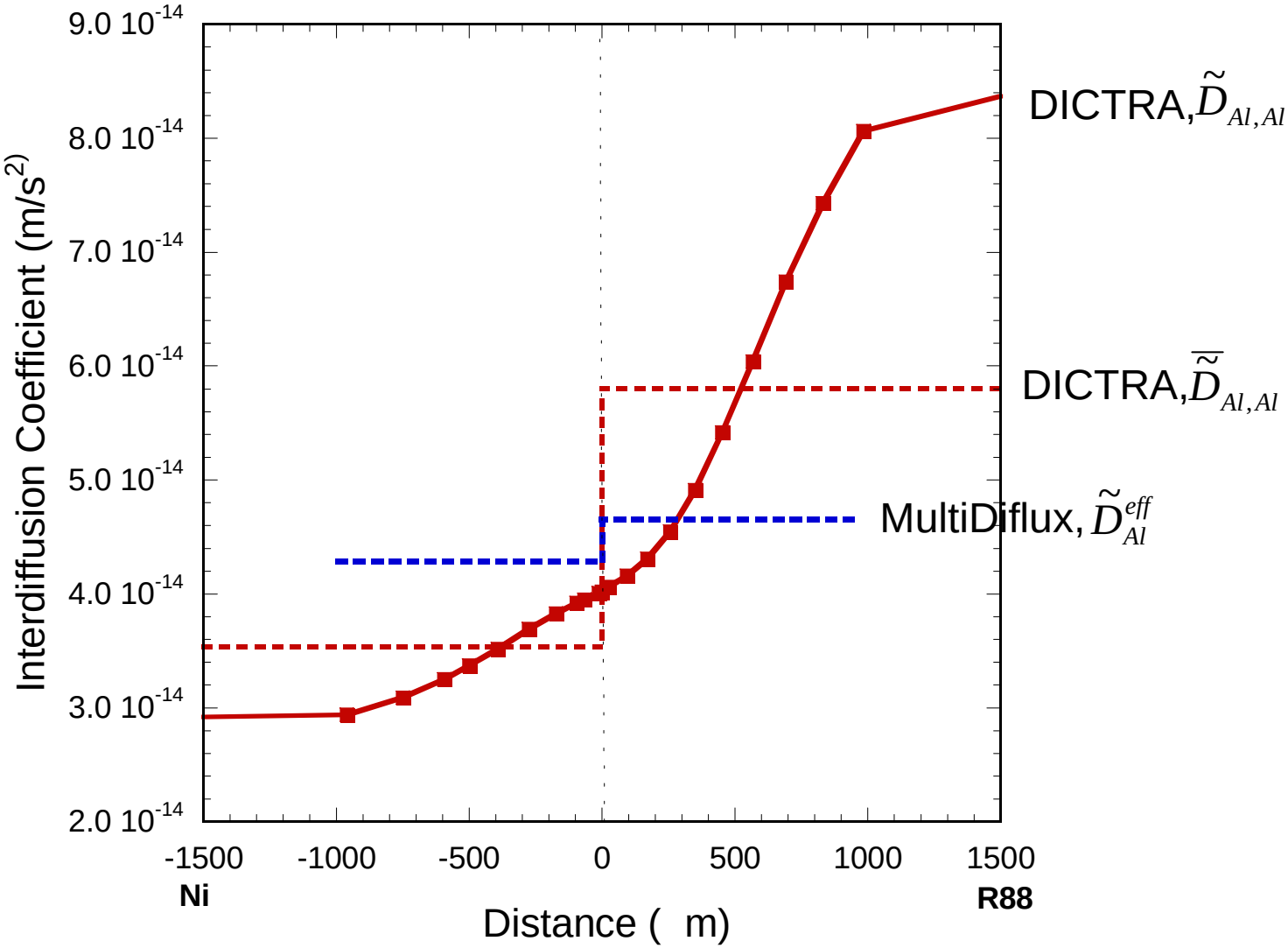
Comparison of Al Diffusion Coefficients for Ni/René-88



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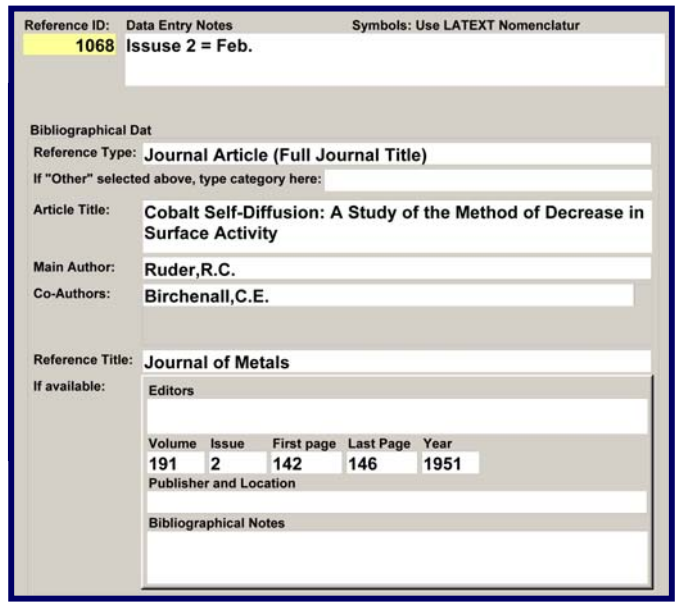
Diffusion Database Center

C. E. Campbell, U.R. Kattner, C. Beauchamp, K. Dotterer, H. Gates, S. Tobery

- ✯ Goal: To make the NIST paper-based diffusion database center publicly available.
  - ➢ Convert to a searchable electronic form to be access over the internet
- ❖ Motivation
  - Industrial and academic support: GE $5K initiation
  - Center represents an unique collection summarizing the diffusion work between 1965-1980
- ➢ Task:
  - Need to enter bibliographic and diffusion system cards
  - Convert paper documents to electronic documents
  - Develop searchable database
- ✓ Accomplishments (2006)
  - Developed database entry strategy
  - Entered 14000 bibliographic and system cards
  - Database available online



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Diffusion Database Center

C. E. Campbell, U.R. Kattner, C. Beauchamp, K. Dotterer, H. Gates, S. Tobery, L. Souders

Web site: http://winweb.nist.gov/diffusion/

- ✯ **Goal:** To make the NIST paper-based diffusion database center publicly available.

Can search by author or diffusion element

Materials Science and Engineering Laboratory
Metallurgy Division
NIST National Institute of Standards and Technology

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20 record(s) found with manning as Author

Index	Authors	Document Title	Medium Title
12033	Manning, D. L. Mamantov, G.	Determination of the Diffusion Coefficient of Nickel (II) in Molten Lif-BeF{_2}-ZrF{_4} by Linear Sweep Voltammetry and Chronopotentiometry	High Temp. Sci.
1212	Manning, J. R.	Correlation effects and activation energies for diffusion in alloys	Z. Naturforschg. A
1348	Manning, J. R.	Diffusion in a Chemical Concentration Gradient	Phys. Rev.
2565	Manning, J. R.	Diffusion and the Kirkendall Shift in Binary Alloys	Acta. Met.
5175	Manning, J. R.	Drift Mobility and Diffusion for Impurities in Ionic Crystals	Phys. Rev.
5773	Manning, J. R.	15 0544 Cross Terms in the Thermodynamic Diffusion Equations for Multicomponent Alloys	Met. Trans.
8124	Manning, J. R.	Correlation Factors for Diffusion of Dilute Impurities	American Physical Society, Subject Index Number 43.4 (1971) 1 pp.
51	Manning, J. R.	Tracer Diffusion in a Chemical Concentration Gradient in Silver-Cadmium	Phys. Rev.
11277	Manning, J. R.	Correlation factors for non-dilute alloys	Phys. Rev. B
18686	Manning, J. R.	Transport Properties in Fluids.	Proc. Appl. Space Flight & Mat. Sci. Tech.

Current tasks:

- Testing implementation
- Scanning unpublished reports

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Ternary A-B-C System

In the lattice fixed frame of reference, assuming a substitutional solid solution for a given phase:

$$M_{kVa} = M_k^0 \exp\left(\frac{-\Delta G_{kVa}}{RT}\right)\frac{1}{RT}$$

Assume: $M_k^0 = 1$

Then the activation energy, Q_k:

$$\Delta G^*_{AVa} = x_A y_{Va}\Delta G_A^{A:Va} + x_B y_{Va}\Delta G_A^{B:Va} + x_C y_{Va}\Delta G_A^{C:Va} + \Delta G^{excess}$$
$$\Delta G^*_{BVa} = x_A y_{Va}\Delta G_B^{A:Va} + x_B y_{Va}\Delta G_B^{B:Va} + x_C y_{Va}\Delta G_B^{C:Va} + \Delta G^{excess}$$
$$\Delta G^*_{CVa} = x_A y_{Va}\Delta G_C^{A:Va} + x_B y_{Va}\Delta G_C^{B:Va} + x_C y_{Va}\Delta G_C^{C:Va} + \Delta G^{excess}$$

Note x_i = mole fraction of component *i*
y_i = site fraction of component *i* on a given sublattice

Since this is a substitutional solid solution with no interstitials, $y_{Va} = 1$:

Concentration variables: $c_k = \frac{x_k}{V_m} = \frac{x_k}{\sum_{j=1}^{n} x_j V_j}$ *and* $V_j = \left(\frac{\partial V}{\partial N_j}\right)_{P,T,N_k}$

Where x_k is the mole fraction of component *k*, V_j is the partial molar volume and N_j is the number of moles of component *k*.

Assume all the substitutional components have the same partial molar volume: $V_j = V_s$ then for the A-B-C system: $V_m = x_A V_s + x_B V_s + x_C V_s$

Ternary A-B-C System

In the lattice fixed frame of reference: $\sum_{k=1}^{n} J_k = -J_{Va} = J_A + J_B + J_C$

$$J_k = -\sum_{j=1}^{n} {}^{i}D_{kj} \frac{\partial c_j}{\partial z} = -\sum_{j=1}^{n-1} L_{kk} \frac{\partial \mu_k}{\partial c_j} \frac{\partial c_j}{\partial z}$$

$${}^{i}D_{kj} = L_{kk} \frac{\partial \mu_k}{\partial c_j} = c_k y_{Va} M_{kVa} \frac{\partial \mu_k}{\partial c_j}$$

Note y_{Va} =1 and for simplicity drop the *Va* from $M_{kVa} = M_k$

$$L_{AA} = x_A M_A \qquad L_{BB} = x_B M_B \qquad L_{CC} = x_C M_C$$

$$c_i = \frac{x_i}{V_m}$$

$${}^{i}D_{AA} = L_{AA} \frac{\partial \mu_A}{\partial c_A} \qquad {}^{i}D_{AB} = L_{AA} \frac{\partial \mu_A}{\partial c_B} \qquad {}^{i}D_{AC} = L_{AA} \frac{\partial \mu_A}{\partial c_C}$$

$${}^{i}D_{BA} = L_{BB} \frac{\partial \mu_B}{\partial c_A} \qquad {}^{i}D_{BB} = L_{BB} \frac{\partial \mu_B}{\partial c_B} \qquad {}^{i}D_{BC} = L_{BB} \frac{\partial \mu_B}{\partial c_C}$$

$${}^{i}D_{CA} = L_{CC} \frac{\partial \mu_C}{\partial c_A} \qquad {}^{i}D_{CB} = L_{CC} \frac{\partial \mu_C}{\partial c_B} \qquad {}^{i}D_{CC} = L_{CC} \frac{\partial \mu_C}{\partial c_C}$$

Ternary A-B-C System

In the volume-fixed frame of reference: $\sum_{k=1}^{n} J_k V_k = 0 = \left(J_A + J_B + J_C\right)\cdot V_s$

$$J_k = -\sum_{i=1}^{n} L'_{ki}\frac{\partial \mu_i}{\partial z} = -\sum_{i=1}^{n} L'_{ki}\sum_{j=1}^{n}\frac{\partial \mu_i}{\partial c_j}\frac{\partial c_j}{\partial z} = -\sum_{j=1}^{n} D_{kj}\frac{\partial c_j}{\partial z}$$

$$D_{kj} = -\sum_{i=1}^{n} L'_{ki}\frac{\partial \mu_i}{\partial c_j} = \sum_{i=1}^{n}\left(\delta_{ik} - x_k\right)x_i M_i \frac{\partial \mu_i}{\partial x_j}V_m$$

See next page for expansion

$$L'_{kj} = \sum_{i=1}^{n}\left[\delta_{ik} - x_k\left(\frac{V_i}{V_m}\right)\right]L_{ij} \qquad L_{kk} = c_k y_{Va} M_{kVa}$$

Equivalent forms

Or $J_k = -\sum_{i=1}^{n} L''_{ki}\left[\nabla \mu_i - \left(\frac{V_i}{V_m}\right)\nabla \mu_n\right]$

$$L''_{ki} = \sum_{j=1}^{n}\left[\delta_{ij} - x_i\left(\frac{V_i}{V_m}\right)\right]L'_{kj} = \sum_{j=1}^{n}\sum_{r=1}^{n}\left[\delta_{ir} - x_i\left(\frac{V_r}{V_m}\right)\right]\left[\delta_{jk} - x_k\left(\frac{V_j}{V_m}\right)\right]L_{jr}$$

$$D_{kj} = \sum_{i=1}^{n} L''_{ki}\frac{\partial\left[\mu_i - \left(V_i/V_m\right)\mu_n\right]}{\partial c_j} = \sum_{i=1}^{n} L'_{ki}\frac{\partial \mu_i}{\partial c_j} - \sum_{i=1}^{n} x_i\frac{\partial \mu_i}{\partial c_j}\sum_{r=1}^{n}\left(\frac{V_r}{V_m}\right)L'_{kr}$$

Recall that the Gibbs–Duhem equations provides that: $\sum_{i=1}^{n} x_i\frac{\partial \mu_i}{\partial c_j} = 0$ thus, $D_{kj} = \sum_{i=1}^{n} L'_{ki}\frac{\partial \mu_i}{\partial c_j}$

Reduce diffusivities when $V_k = V_s$: $D^n_{kj} = D_{kj} - D_{kn}$ $\quad J_k = -\sum_{j=1}^{n-1} D^n_{kj}\frac{\partial c_j}{\partial z}$

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Ternary A-B-C

$$D_{kj} = -\sum_{i=1}^{n} L'_{ki} \frac{\partial \mu_i}{\partial c_j} = \sum_{i=1}^{n} \left(\delta_{ik} - x_k\right) x_i M_i \frac{\partial \mu_i}{\partial x_j} V_m$$

$$D_{AA} = \left(1 - x_A\right) x_A M_A \frac{\partial \mu_A}{\partial x_A} V_m + \left(0 - x_A\right) x_B M_B \frac{\partial \mu_B}{\partial x_A} V_m + \left(0 - x_A\right) x_C M_C \frac{\partial \mu_C}{\partial x_A} V_m$$

$$D_{AB} = \left(1 - x_A\right) x_A M_A \frac{\partial \mu_A}{\partial x_B} V_m + \left(0 - x_A\right) x_B M_B \frac{\partial \mu_B}{\partial x_B} V_m + \left(0 - x_A\right) x_C M_C \frac{\partial \mu_C}{\partial x_B} V_m$$

$$D_{AC} = \left(1 - x_A\right) x_A M_A \frac{\partial \mu_A}{\partial x_C} V_m + \left(0 - x_A\right) x_B M_B \frac{\partial \mu_B}{\partial x_C} V_m + \left(0 - x_A\right) x_C M_C \frac{\partial \mu_C}{\partial x_C} V_m$$

$$D_{BA} = \left(0 - x_B\right) x_A M_A \frac{\partial \mu_A}{\partial x_A} V_m + \left(1 - x_B\right) x_B M_B \frac{\partial \mu_B}{\partial x_A} V_m + \left(0 - x_B\right) x_C M_C \frac{\partial \mu_C}{\partial x_A} V_m$$

$$D_{BB} = \left(0 - x_B\right) x_A M_A \frac{\partial \mu_A}{\partial x_B} V_m + \left(1 - x_B\right) x_B M_B \frac{\partial \mu_B}{\partial x_B} V_m + \left(0 - x_B\right) x_C M_C \frac{\partial \mu_C}{\partial x_B} V_m$$

$$D_{BC} = \left(0 - x_B\right) x_A M_A \frac{\partial \mu_A}{\partial x_C} V_m + \left(1 - x_B\right) x_B M_B \frac{\partial \mu_B}{\partial x_C} V_m + \left(0 - x_B\right) x_C M_C \frac{\partial \mu_C}{\partial x_C} V_m$$

$$D_{CA} = \left(0 - x_C\right) x_A M_A \frac{\partial \mu_A}{\partial x_A} V_m + \left(0 - x_C\right) x_B M_B \frac{\partial \mu_B}{\partial x_A} V_m + \left(1 - x_C\right) x_C M_C \frac{\partial \mu_C}{\partial x_A} V_m$$

$$D_{CB} = \left(1 - x_C\right) x_A M_A \frac{\partial \mu_A}{\partial x_B} V_m + \left(0 - x_C\right) x_B M_B \frac{\partial \mu_B}{\partial x_B} V_m + \left(1 - x_C\right) x_C M_C \frac{\partial \mu_C}{\partial x_B} V_m$$

$$D_{CC} = \left(1 - x_C\right) x_A M_A \frac{\partial \mu_A}{\partial x_C} V_m + \left(0 - x_C\right) x_B M_B \frac{\partial \mu_B}{\partial x_C} V_m + \left(1 - x_C\right) x_C M_C \frac{\partial \mu_C}{\partial x_C} V_m$$

NIST

Relation between Intrinsic and Interdiffusion Coefficients

From Sohn and Dayananda (*Met. Mat. Trans* **33A** (2002) 3375)

Published notation:

$$\tilde{D}_{ij}^{n} = D_{ij}^{n} - N_i \sum_{k=1}^{n} D_{kj}^{n}$$

$\tilde{D}_{ij}^{n}$ = interdiffusion coefficient

D_{ij}^{n} = intrinsic diffusion coefficient (reduced)

N_i = atom fraction

DICTRA notation:

$$\tilde{D}_{ij}^{n} = {}^{i}D_{ij}^{n} - x_i \sum_{k=1}^{n} {}^{i}D_{kj}^{n}$$

Example:

$$\tilde{D}_{AA}^{C} = {}^{i}D_{AA}^{C} - x_A\left({}^{i}D_{AA}^{C} + {}^{i}D_{BA}^{C} + {}^{i}D_{CA}^{C}\right)$$

$$\tilde{D}_{AA}^{C} = D_{AA} - D_{AC}$$ (see previous slide for expansion of D_{AA} and D_{AC})

$$\tilde{D}_{AA}^{C} = x_A V_m\left[(1-x_A)M_A\frac{\partial\mu_A}{\partial x_A} - x_B M_B\frac{\partial\mu_B}{\partial x_A} - x_C M_C\frac{\partial\mu_C}{\partial x_A}\right] - x_A V_m\left[(1-x_A)M_A\frac{\partial\mu_A}{\partial x_C} - x_B M_B\frac{\partial\mu_B}{\partial x_C} - x_C M_C\frac{\partial\mu_C}{\partial x_C}\right]$$

Note $${}^{i}D_{kj} = x_k M_k\frac{\partial\mu_k}{\partial x_j}$$

$$\tilde{D}_{AA}^{C} = x_A V_m\left[M_A\frac{\partial\mu_A}{\partial x_A} - {}^{i}D_{AA} - {}^{i}D_{BA} - {}^{i}D_{CA}\right] - x_A V_m\left[M_A\frac{\partial\mu_A}{\partial x_C} - {}^{i}D_{AC} - {}^{i}D_{BC} - {}^{i}D_{CC}\right]$$

$$\tilde{D}_{AA}^{C} = x_A V_m M_A\frac{\partial\mu_A}{\partial x_A} - x_A V_m M_A\frac{\partial\mu_A}{\partial x_C} - x_A V_m\left[\left({}^{i}D_{AA} - {}^{i}D_{AC}\right) + \left({}^{i}D_{BA} - {}^{i}D_{BC}\right) + \left({}^{i}D_{CA} - {}^{i}D_{CC}\right)\right]$$

$$\tilde{D}_{AA}^{C} = \left({}^{i}D_{AA} - {}^{i}D_{AC}\right) - x_A V_m\left[\left({}^{i}D_{AA} - {}^{i}D_{AC}\right) + \left({}^{i}D_{BA} - {}^{i}D_{BC}\right) + \left({}^{i}D_{CA} - {}^{i}D_{CC}\right)\right]$$

Rewrite in terms of reduce diffusivities

$$\tilde{D}_{AA}^{C} = {}^{i}D_{AA}^{C} - x_A V_m\left[{}^{i}D_{AA}^{C} + {}^{i}D_{BA}^{C} + {}^{i}D_{CA}^{C}\right]$$

Note:

$${}^{i}D_{kj}^{n} = {}^{i}D_{kj} - {}^{i}D_{kn}$$

$${}^{i}D_{AA}^{C} = {}^{i}D_{AA} - {}^{i}D_{AC}$$

$${}^{i}D_{BA}^{C} = {}^{i}D_{BA} - {}^{i}D_{BC}$$

$${}^{i}D_{CA}^{C} = {}^{i}D_{CA} - {}^{i}D_{CC}$$

NIST participation in GE-AIM (DARPA) Program
γ′ Precipitation Model

Experimental diffusion data (Binary data)
J.C. Zhao, GE-CRD
NIST Diffusion Data Center

Multicomponent diffusion data
B. Mueller, Howmet
J-C. Zhao, GE-CRD

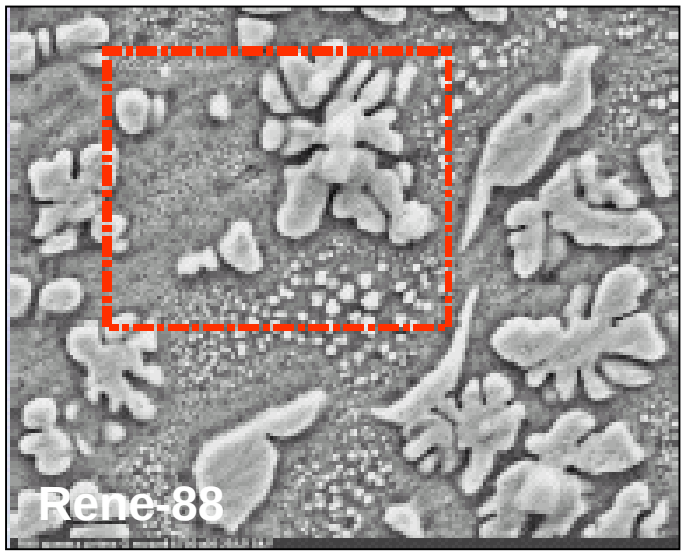
Diffusion Mobility Database
NIST

Thermodynamic Databases
Thermotech, UW, NIST

Lattice parameters
Questek

γ′ precipitation
Questek, GE

Models for mechanical properties
GE



Linear cooling rate 0.2 °C/s

NIST also providing guidance on γ′ precipitation modeling, simple coding for thermodynamic calculations, modeling interfacial energies.