NIST Workshop: High Throughput Analysis of Multicomponent Multiphase Diffusion Data
May 14 & 15, 2007

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NIST

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

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Agenda

Monday May 14, 2007

8:45-9:15 **Introduction** (Coffee and bagels)

9:15 –9:30 **Review of action items from last workshop**

9:30-10:15 Calculating diffusion coefficients in non-dilute multi-component solids from first principles (van der Ven)

10:15-11:00 First-principles Calculations of Diffusion Coefficients and Migration Entropy (Liu)

11:00-11:15 Break

11:15-12:00 Dislocation diffusion in metals (Mishin)

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

Agenda

Monday May 14, 2007

1:30 Modeling of Diffusion-induced transformations in Ni superalloys (Mirsa)

2:00 Composition-Dependent Ternary Interdiffusion Coefficients in Ni_3Al ($L1_2$) with Ir, Ta or Re alloying additions (Sohn)

2:30 Effects of solute concentrations on kinetic pathways in Ni-Al-Cr alloys (Booth-Morrison)

3:00 The kinetic pathway of coarsening morphology in a Ni-Al-Cr alloy by Lattice Kinetic Monte Carlo simulation (Mao)

3:30-3:45 Break

3:45 Modeling Diffusion mobilities in the L12 and B2 phases (Campbell)

4:15 Modeling of oxidation and diffusion in oxides (Ågren)

5:45 Dinner

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Agenda

Tuesday, May 15

9:00 Welcome to Day 2

9:15-9:45 Educational Tools developed at Union College (Lupulescu)

9:45-10:15 Composition-Dependent Growth Kinetics of Intermetallic Phases in U- Mo vs. Al Alloy Diffusion Couples Annealed at 550 C and 600 C (Sohn)

10:15-10:45 Single Phase Layer Formation at the Initial Interface of Ternary Diffusion Couples (Morral)

10:45-11:00 Break

11:00-11:30 New Models in DICTRA (Mason)

11:30 –12:00 Discussion

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, $v = -J_{Va} V_M$	$D_{kj} = \sum_{i=1}^{n} (\delta_{ik} - x_k) x_i M_i \frac{\partial \mu_i}{\partial x_j} V_m$

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Further testing and refinement of database using GE Diffusion Couple Data

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.%)

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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
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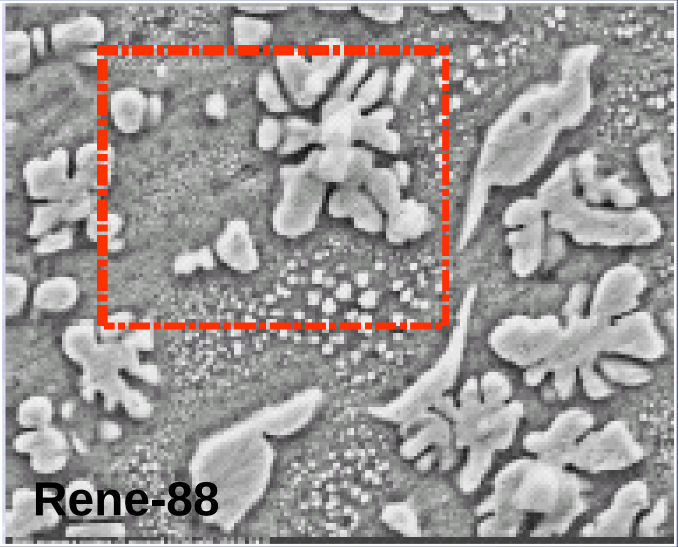
Thermodynamic Databases
Thermotech, UW, NIST

Lattice parameters
Questek

γ' precipitation
Questek, GE

Models for mechanical properties
GE

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



Linear cooling rate 0.2 C/s

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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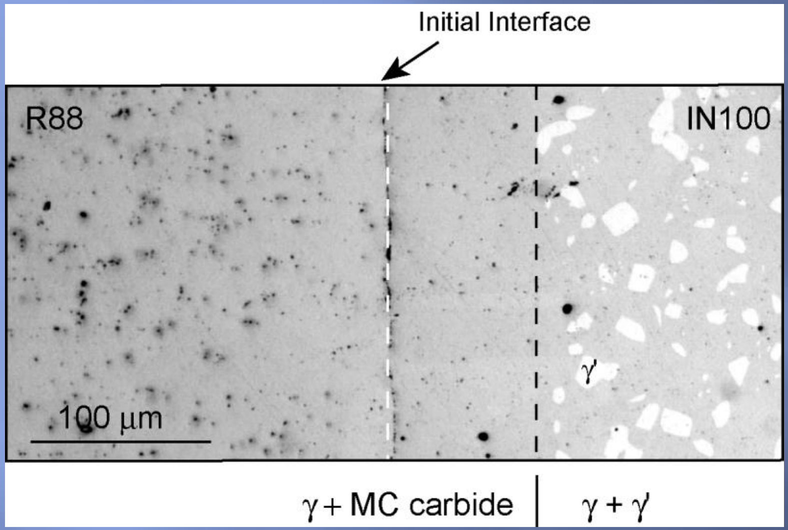
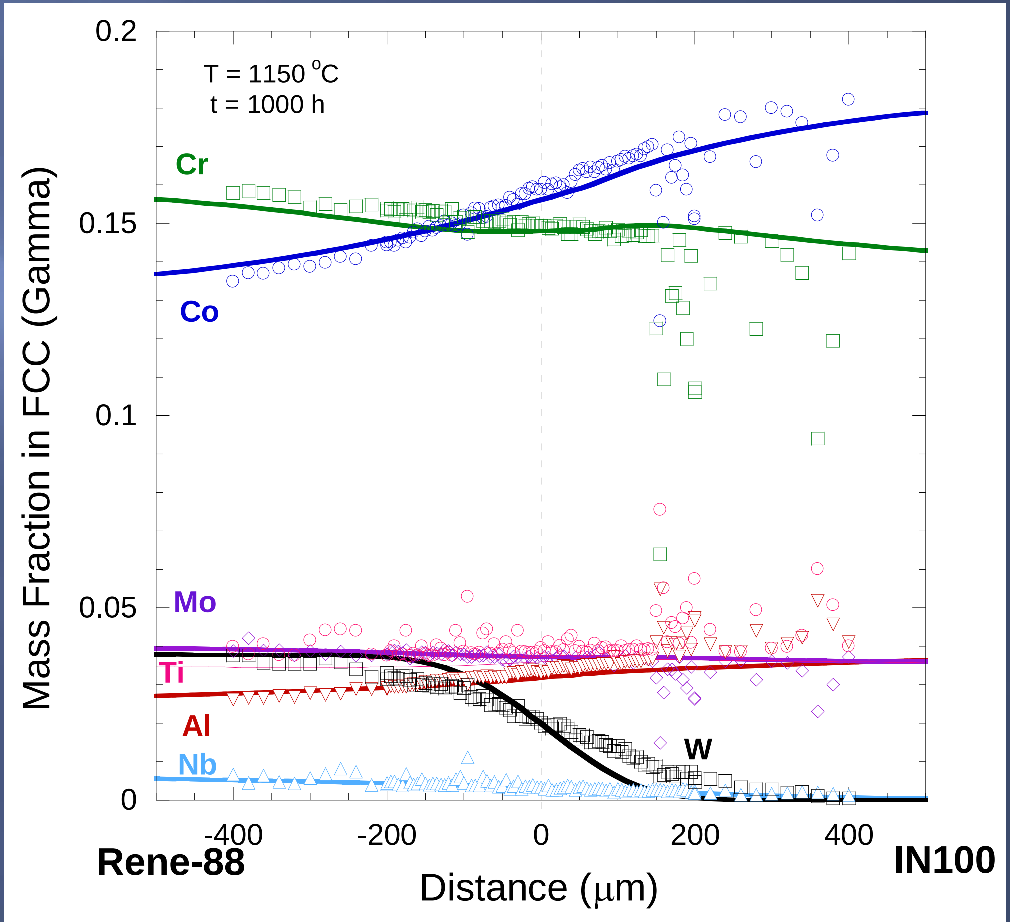
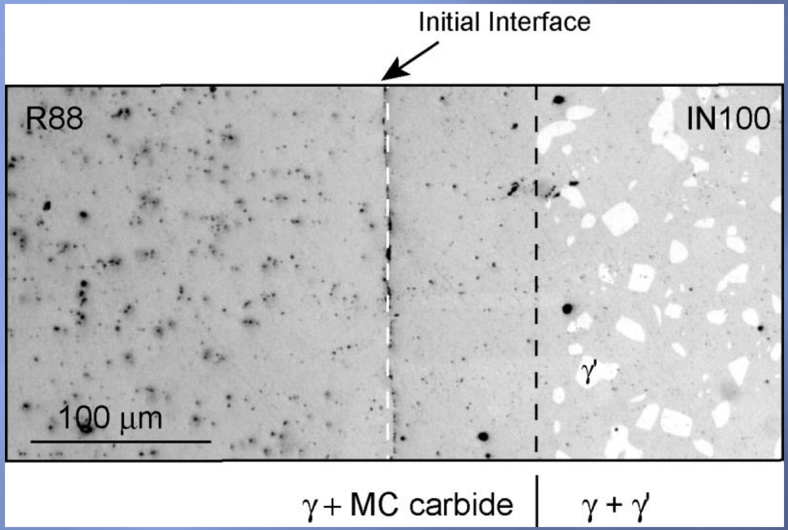
René-88/IN-100; 1000 h at 1150 °C

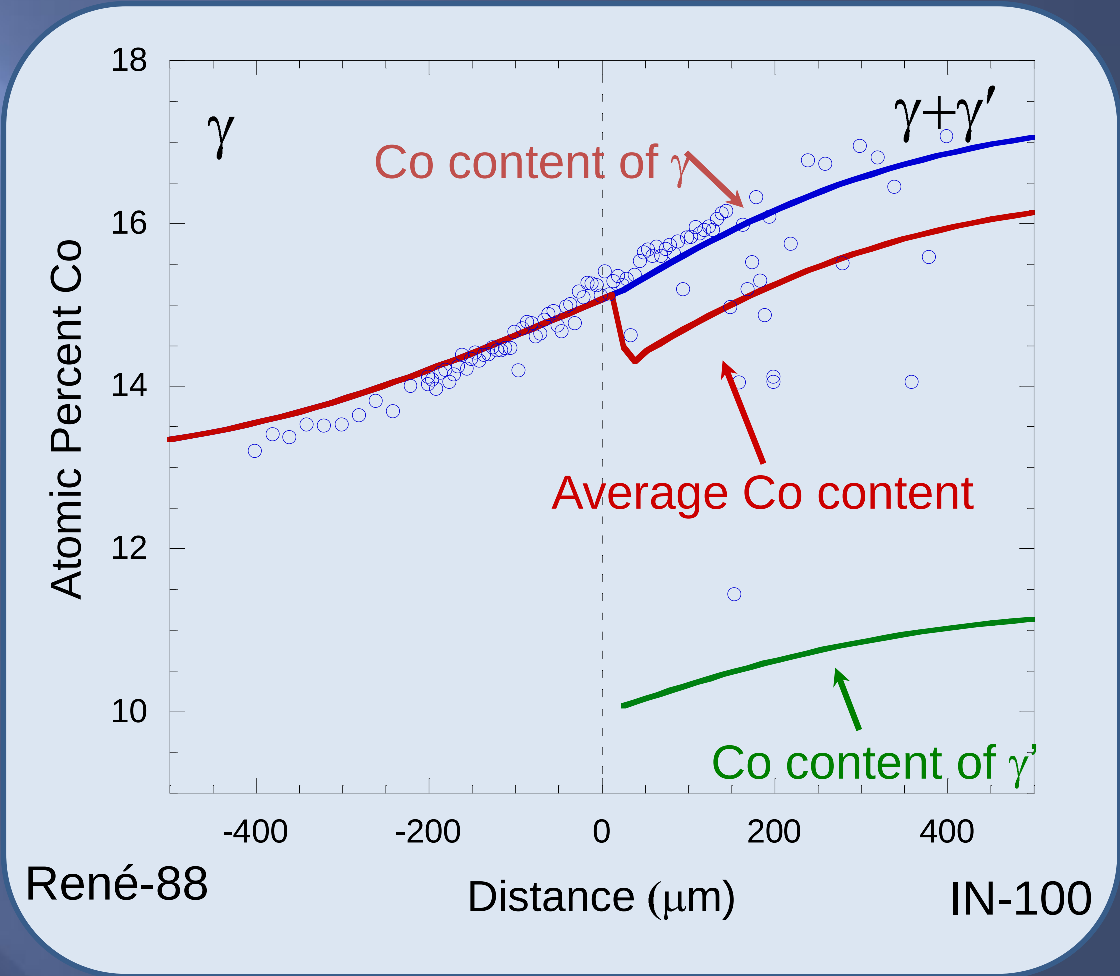




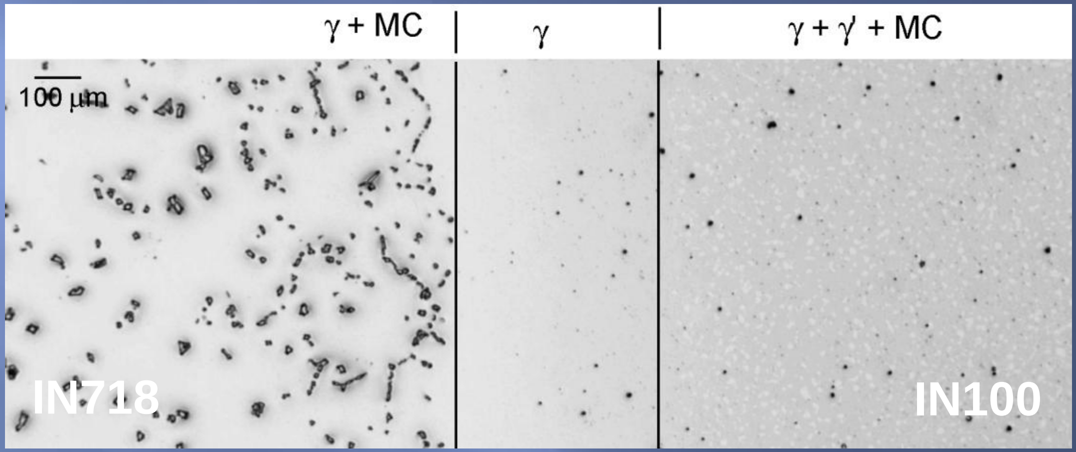
Experimental data from J-C. Zhao, GE Global Research

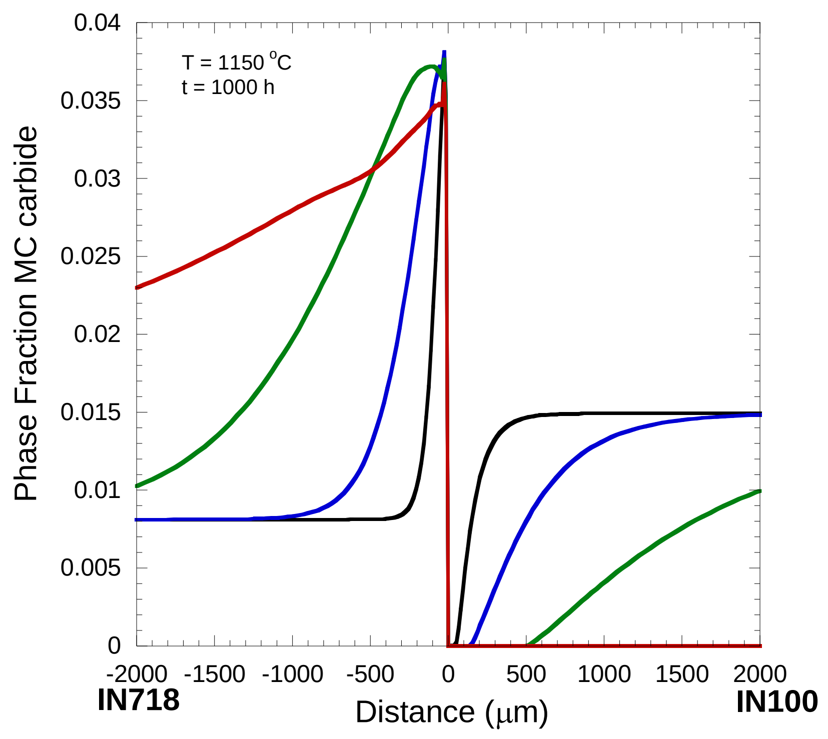
René-88/IN-100; 1000 h at 1150 °C

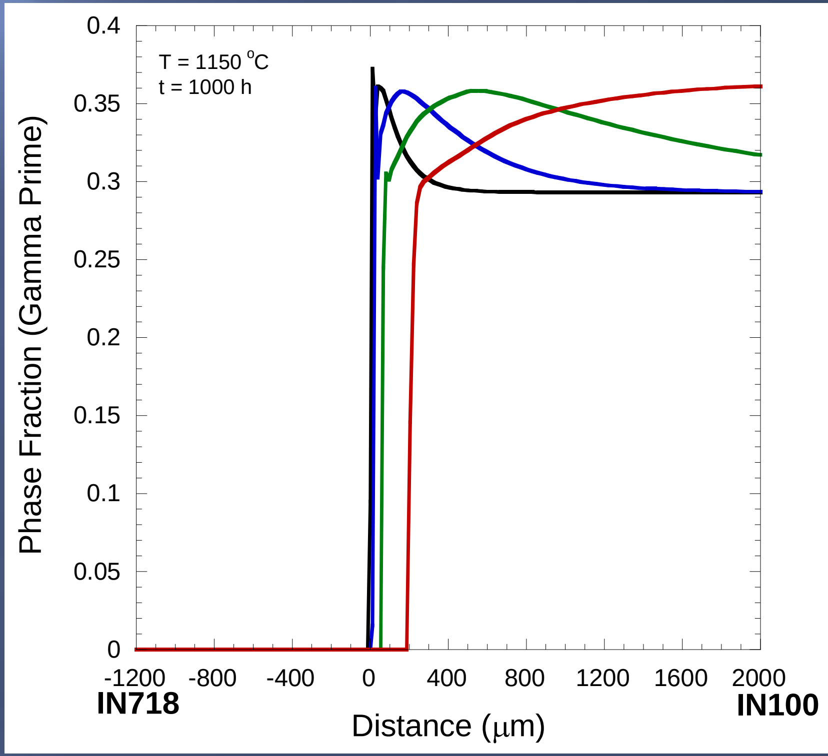




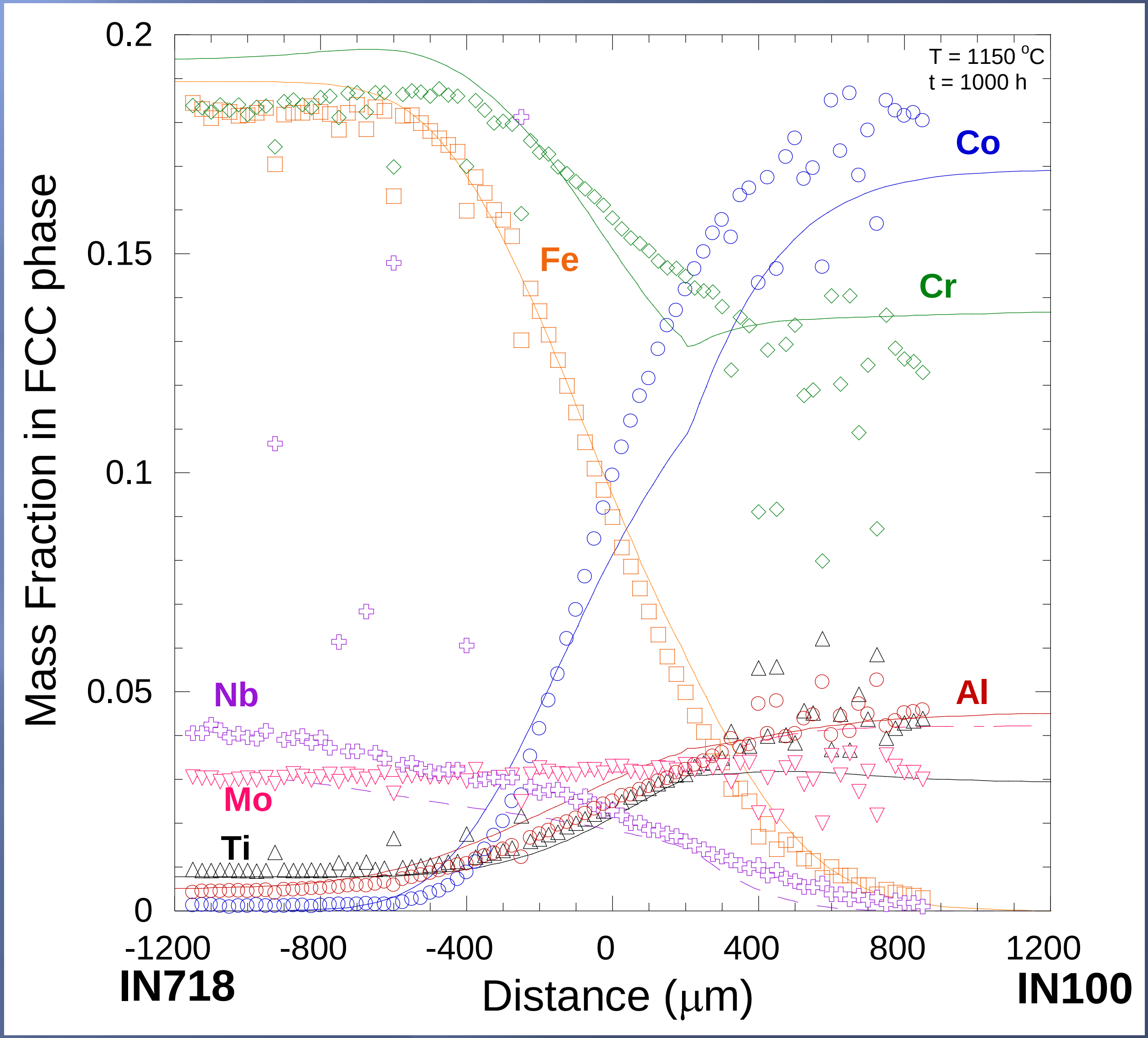
IN-718/IN-100; 1000 h at 1150 °C







IN-718/IN-100; 1000 h at 1150 °C



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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

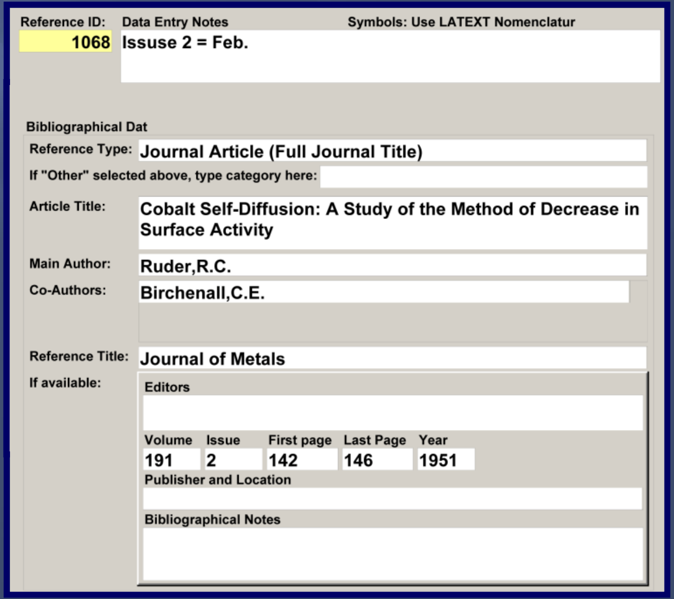
- Industrial and academic support: GE $5K initiation
- Center represents an unique collection summarizing the diffusion work between 1965-1980

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



Reference ID: 1068
Data Entry Notes: Issuse 2 = Feb.
Symbols: Use LATEXT Nomenclatur

Bibliographical Dat

Reference Type: Journal Article (Full Journal Title)
If "Other" selected above, type category here:
Article Title: Cobalt Self-Diffusion: A Study of the Method of Decrease in Surface Activity
Main Author: Ruder,R.C.
Co-Authors: Birchenall,C.E.
Reference Title: Journal of Metals
If available: Editors

Volume	Issue	First page	Last Page	Year
191	2	142	146	1951

Publisher and Location

Bibliographical Notes

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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