NIST Workshop: High Throughput Analysis of Multicomponent Multiphase Diffusion Data

April 19-20

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&

Bill Boettinger

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, April 19, 2005

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

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

- Diffusion notation
- Progress on web access to Metallurgy Div. Diffusion Database (Campbell)
- Other

9:30-10:00 **Outside the Box on Diffusion Formalisms** (DeHoff)

10:00-10:30 **Intrinsic diffusion simulation for tests of Darken relations** (Kulkarni)

10:30-10:45 Break

10:45-11:15 **Results of NiAl/Superalloy Diffusion Couples** (Sohn)

11:15-11:45 **Multiphase Systems** (Morral)

11:45-12:15 **Analysis of Interdiffusion Microstructures** (Y. Wang)

12:15-1:15 **Lunch**

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Agenda

Thursday afternoon

1:15-1:45 **MultiDiflux Evaluation of Multicomponent Couples (n> 3)** (Dayananda)
1:45 –2:15 **Comparison of DICTRA and MultiDiflux Results**
2:15-2:30 Discussion
2:30-3:00 **Effective Diffusivity in Heterogeneous Systems** (Mishin)
3:00 – 3:30 **Kirkendall effect in multiphase planar layer systems** (Boettinger)
3:30 –3:45 Discussion/Break
3:45-4:00 **Modeling Diffusion in Ordered Phases** (Campbell)
4:00-4:30 **Diffusion Modeling in the $L1_2$ Phase** (T. Wang)
4:30-5:00 Discussion
5:00-5:15 **Viewpoint Discussion** (Perepezko)

6:00 Dinner: Café Mileto

Wednesday April 20

9:00-9:30 **RPI Teaching Modules** (Lupulescu, Glicksman)
9:30-10:00 **Update on High Throughput approach to Thermodynamics (NSF program)** (Liu)
10:00-11:00 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 $\beta = 1$ 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 (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
    - ME3/IN718
    - IN100/ME3
    - U720/IN718
    - IN100/ René-88
    - René-95/U720
    - IN718/IN100
    - U720/ME3
    - René-95/IN718
    - ME3/ René-95
    - ME3/ René-88
    - 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

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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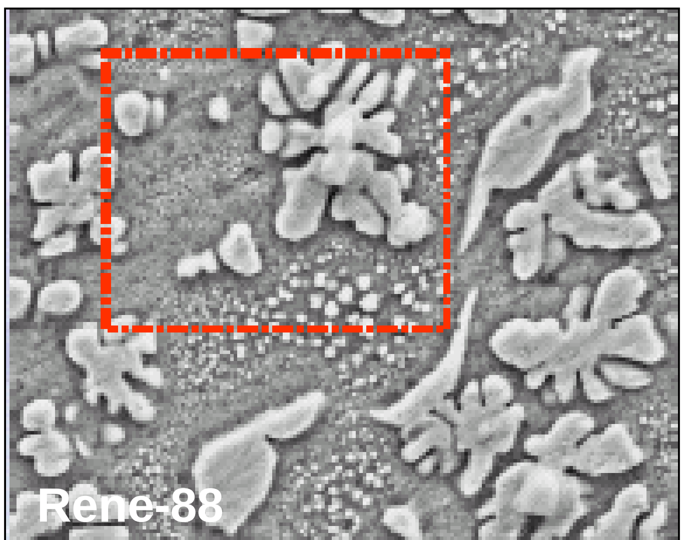
Thermodynamic Databases
Thermotech, UW, NIST

Lattice parameters
Questek

γ' precipitation
Questek, GE

Models for mechanical properties
GE



Linear cooling rate 0.2 °C/s

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

Multicomponent Mobility Database for FCC phase of Superalloys

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

Ni = solvent

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

René-N4 ($x10^{-14}$ m²/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

René-N5 ($x10^{-14}$ m²/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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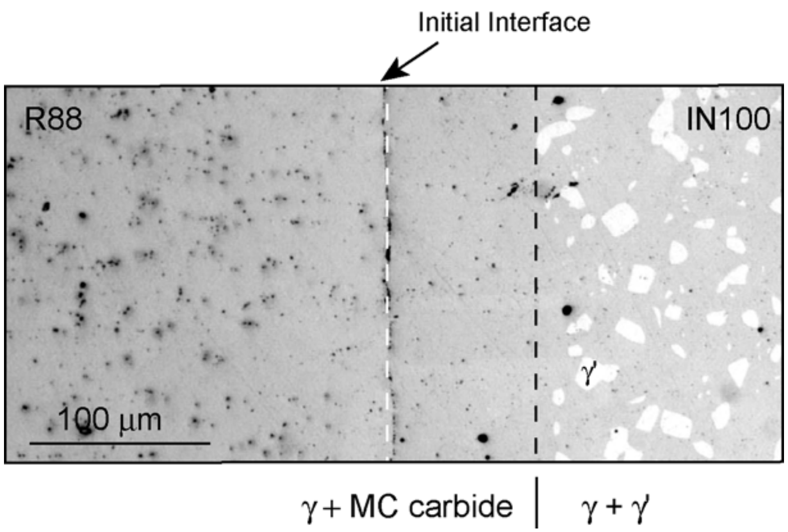
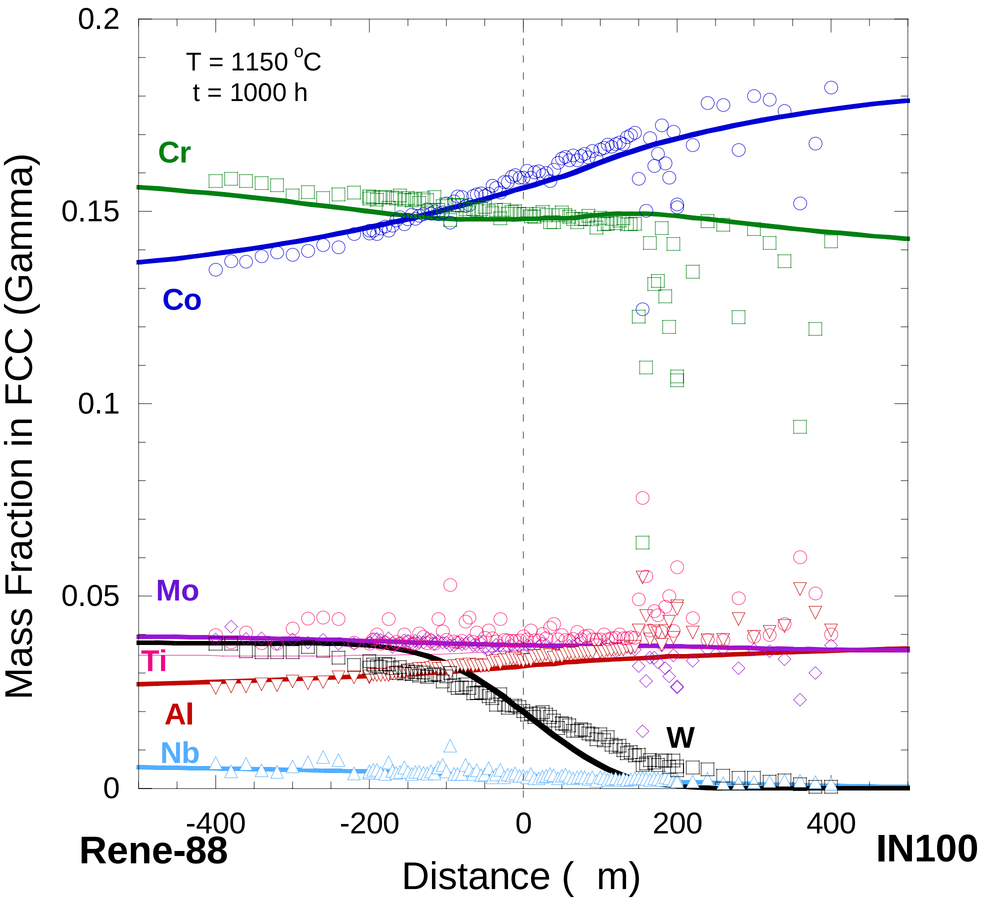
René-88/IN-100; 1000 h at 1150 °C





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

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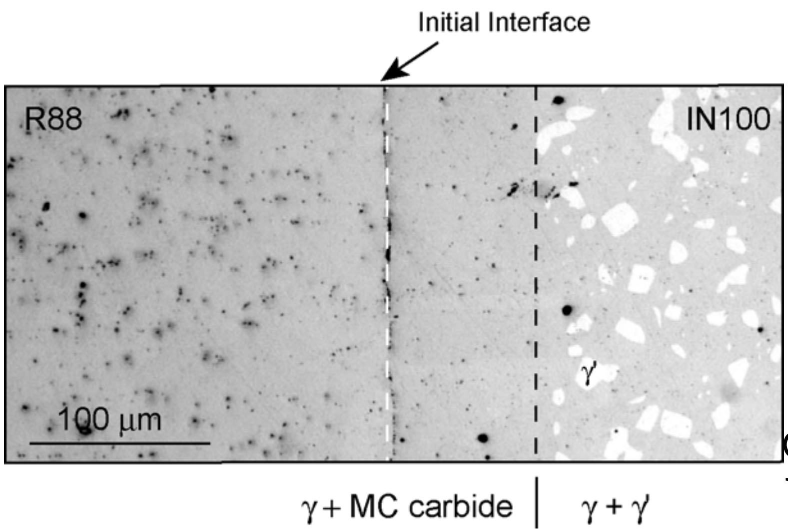
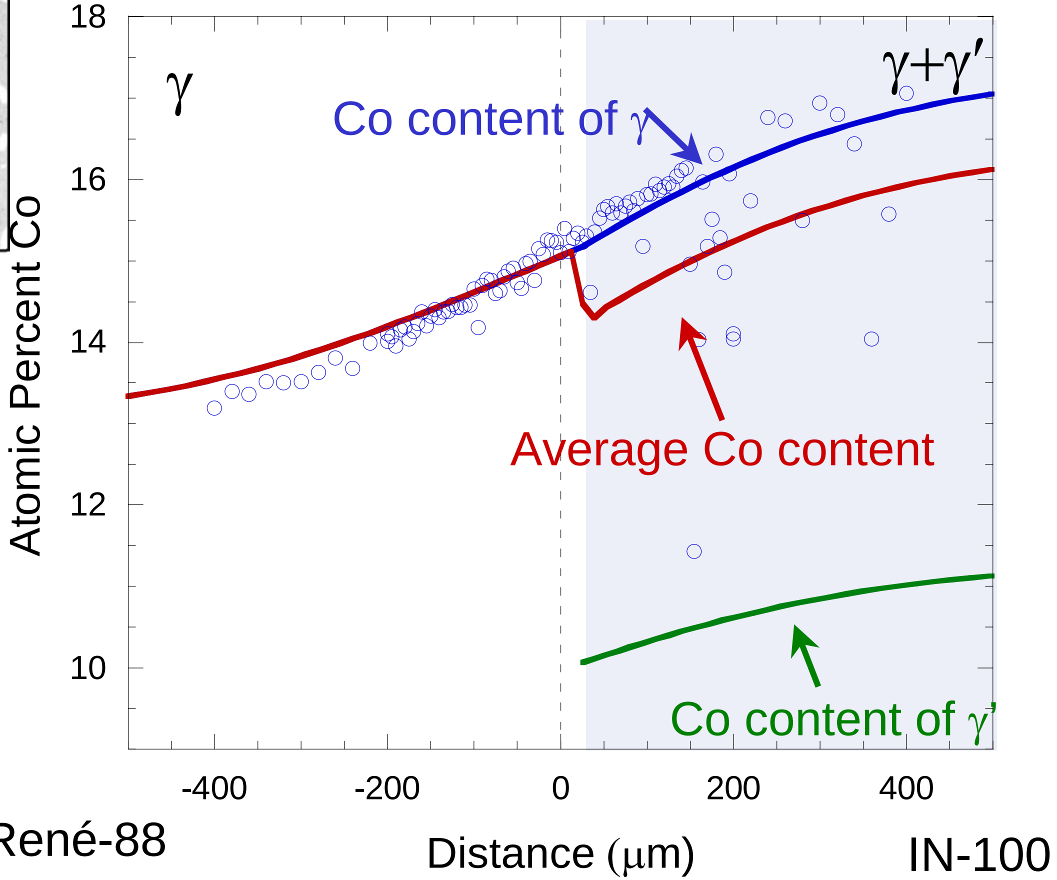
René-88/IN-100; 1000 h at 1150 °C





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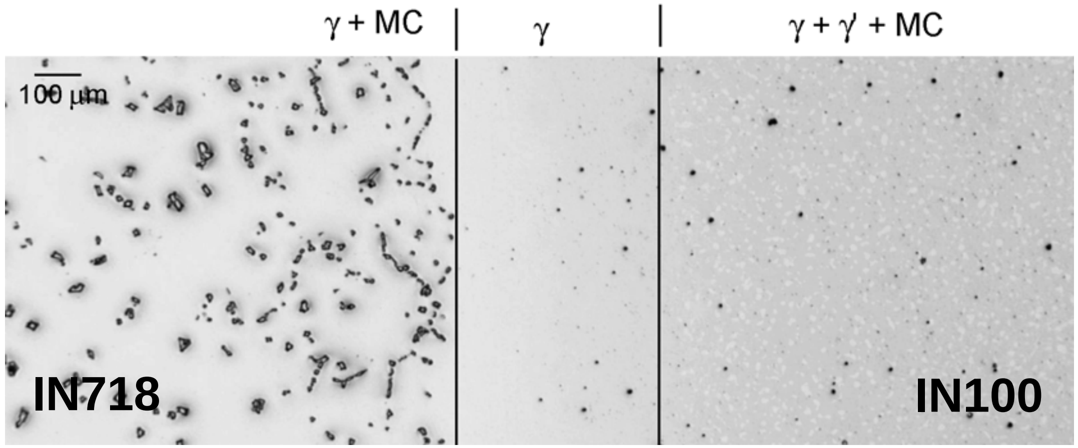
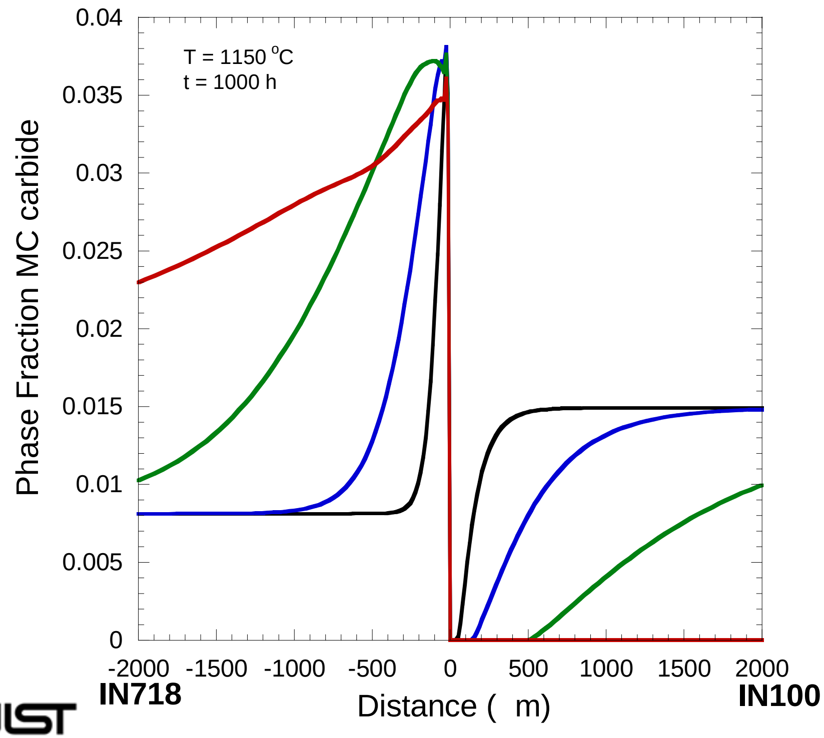
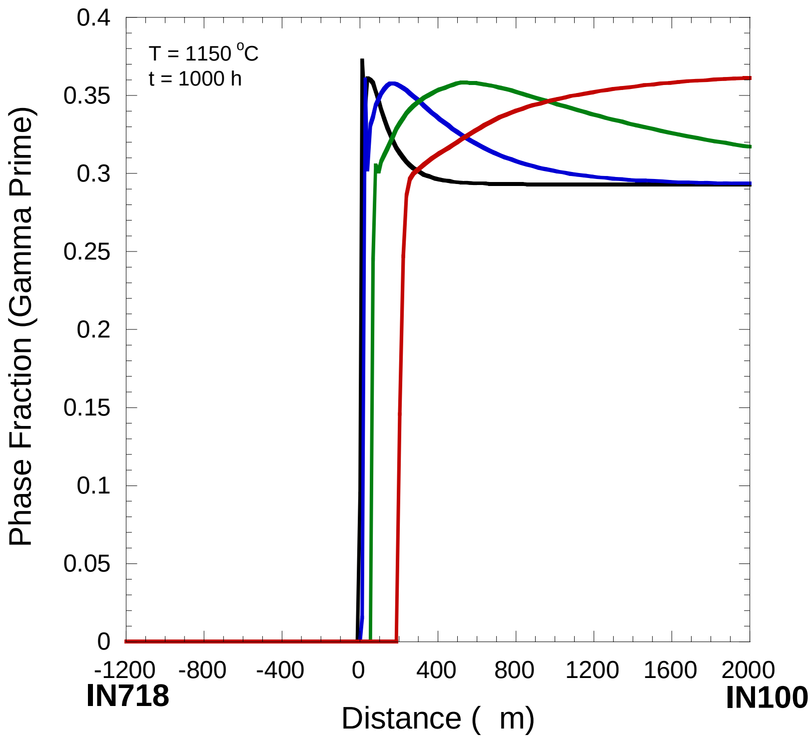
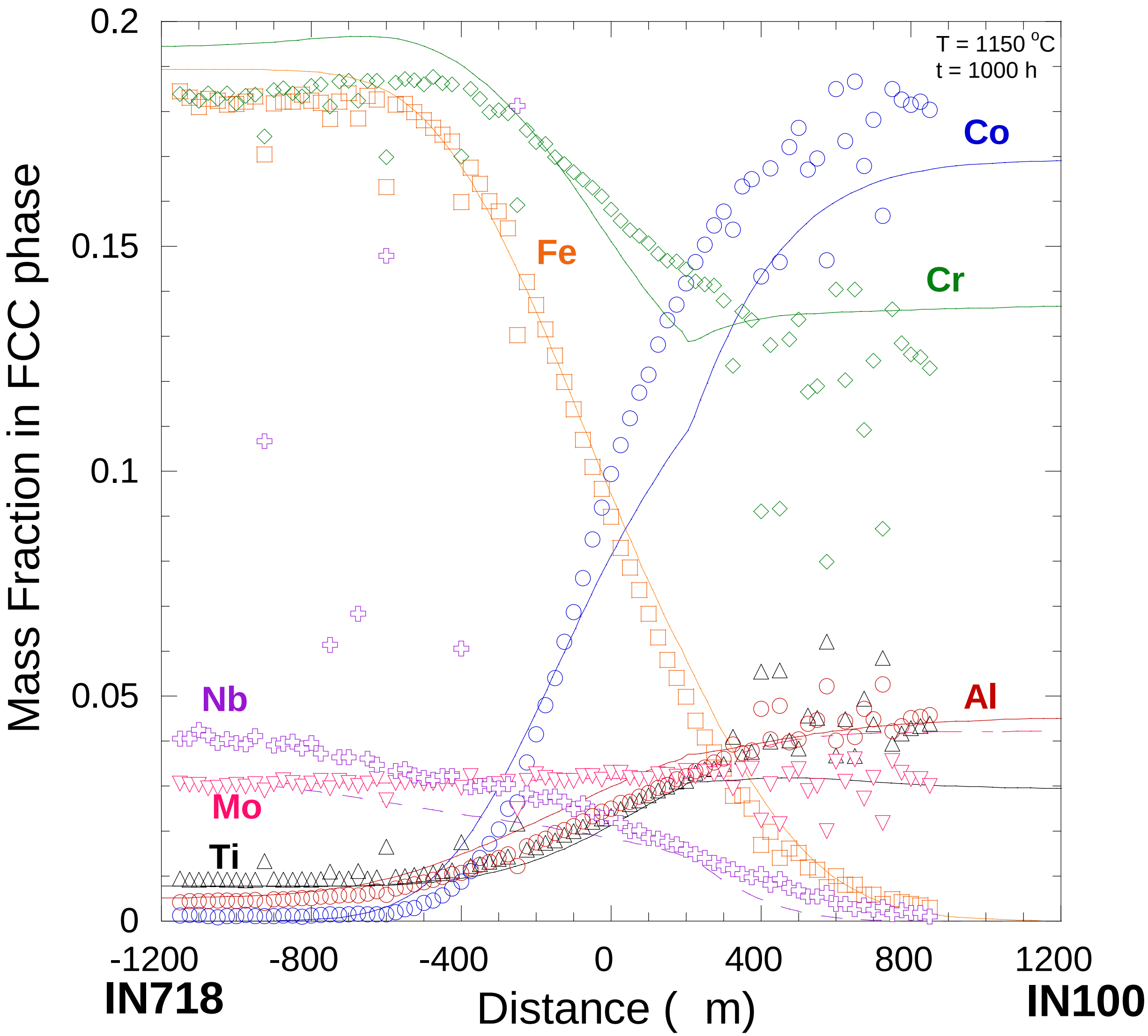
IN-718/IN-100; 1000 h at 1150 °C







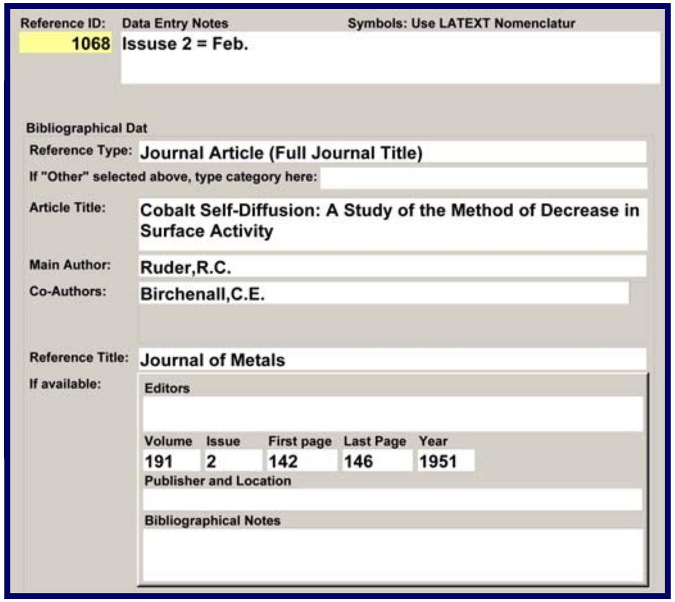
IN-718/IN-100; 1000 h at 1150 °C



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 25000 bibliographic and diffusion system cards
  - Convert paper documents to electronic documents
  - Develop searchable database
- **Accomplishments (2003)**
  - Developed database entry strategy
  - Entered 6000 bibliographic cards
  - Purchase high speed scanner and software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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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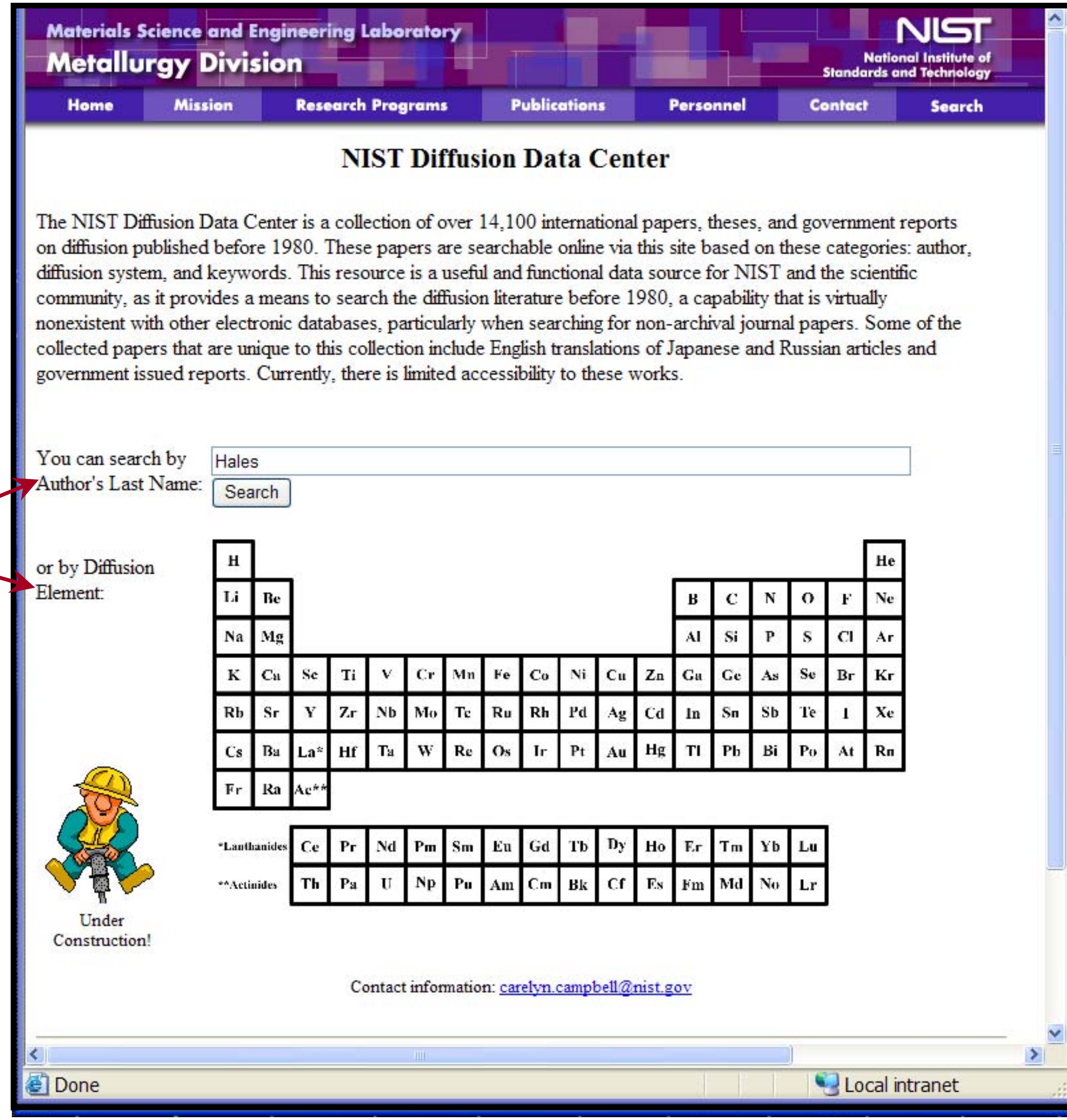
C. E. Campbell, U.R. Kattner, C. Beauchamp, K. Dotterer, H. Gates, S. Tobery, L. Souders

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



Current tasks:

- Testing implementation
- Scanning unpublished reports