NIST Workshop: High Throughput Analysis of Multicomponent Multiphase Diffusion Data March 27-28, 2003

Carelyn Campbell
&
Bill Boettinger

Introductory Remarks

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

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)

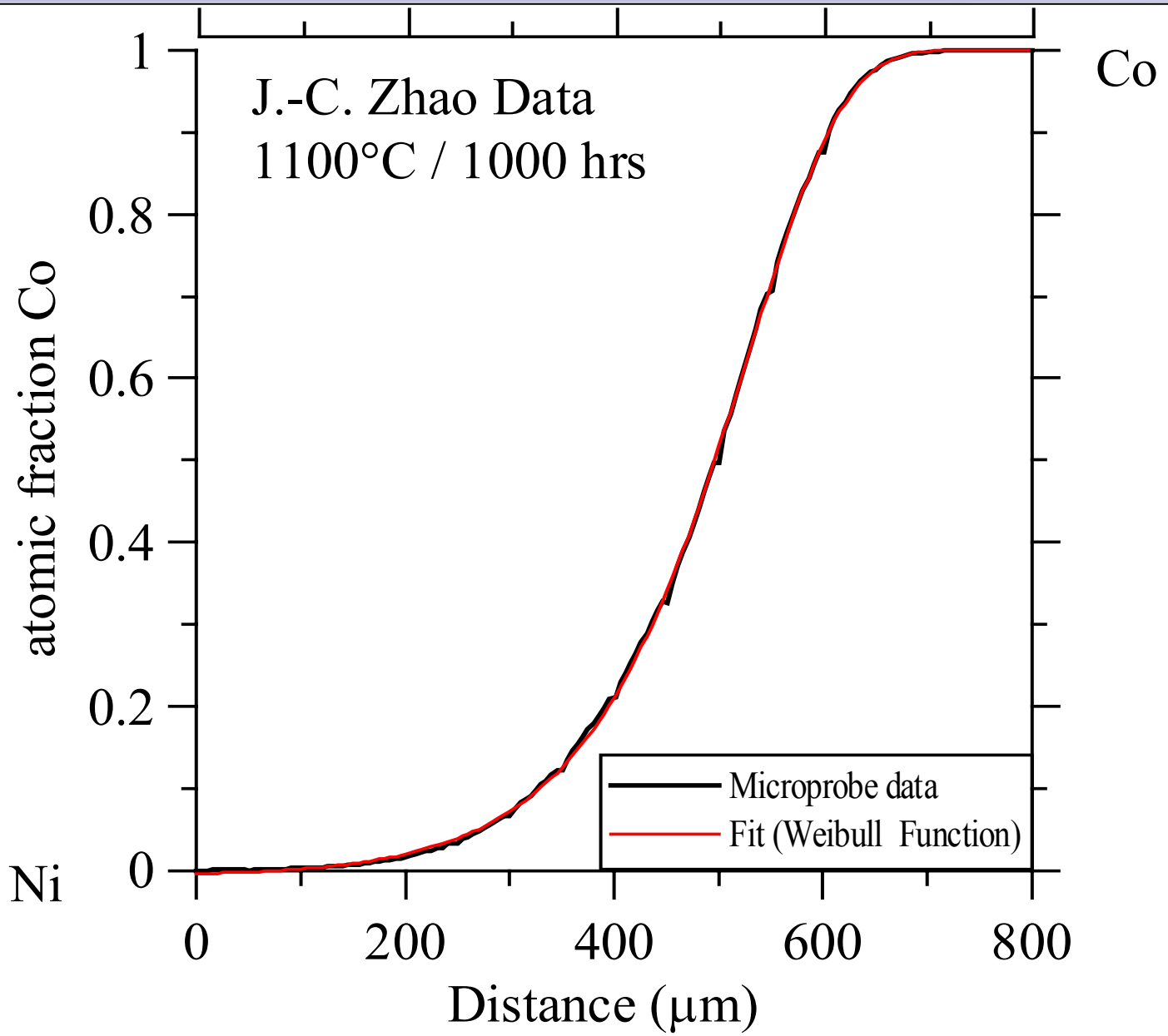
	Al	*Co*	*Cr*	*Hf*	*Mo*	*Re*	*Ta*	*W*
Al	+93.16	+13.92	+33.46	−6.51	+33.42	25.44	+48.63	+50.87
Co	−6.51	+27.22	−8.56	−27.64	−4.95	−5.11	+3.87	−9.21
Cr	+4.15	−4.23	+21.02	−6.25	−0.22	−0.78	+13.81	+6.89
Hf	0.86	+0.07	+1.70	+262.1	+1.52	0.87	+2.37	+1.84
Mo	−0.35	−0.30	−0.30	−1.905	+7.71	−0.25	−0.13	−0.19
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

NIST

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

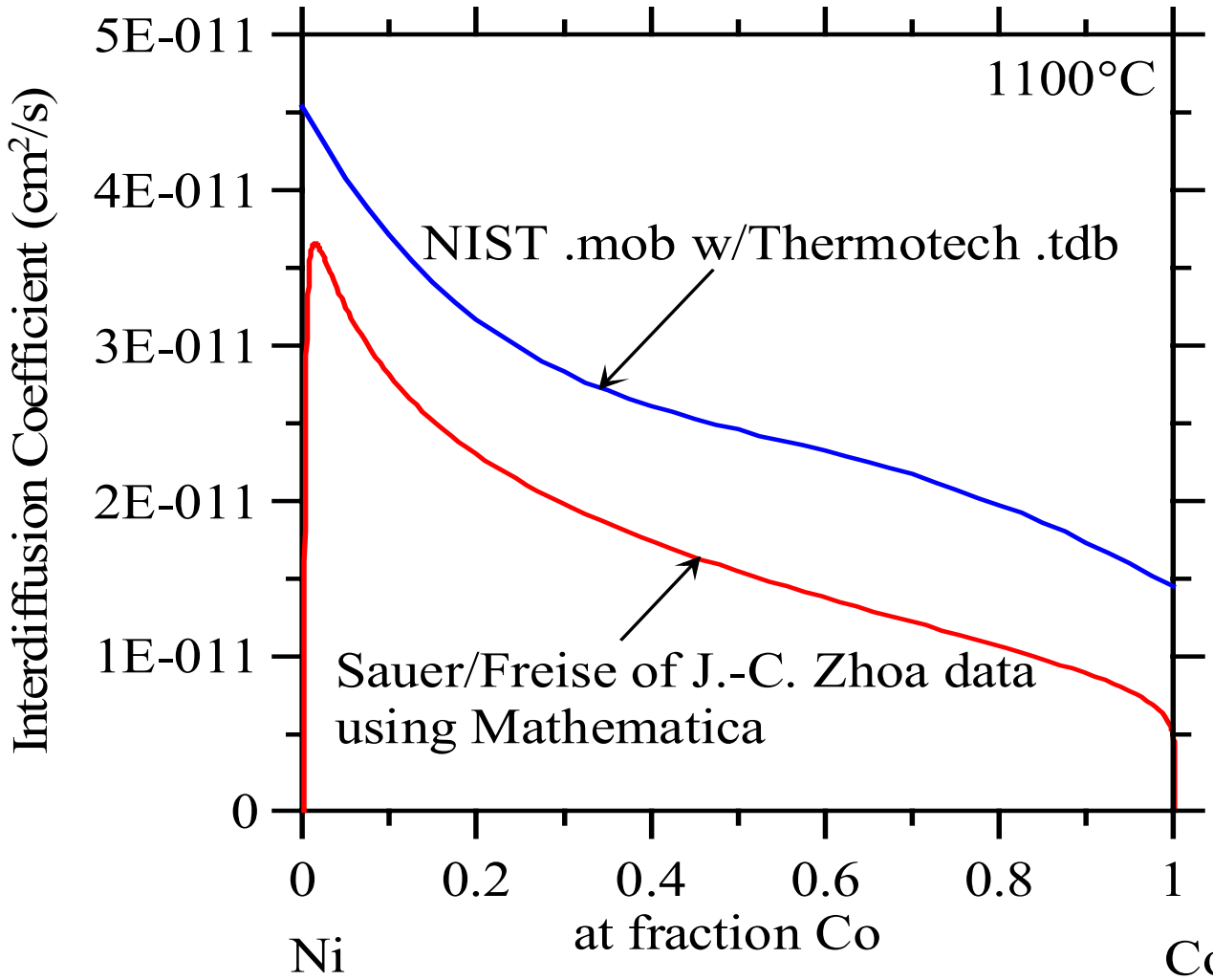
- Binary Couples
  - Single phase couples
    - at 1100 °C for 1000 h : **Ni/Co**
  - Multiphase couples
    - at 1100 °C for 1000 h : Co/Cr, Co/Mo, Co/Nb, Co/W, Cr/Ta, Cr/W, Cr/Mo, Ni/W, Ni/Ta, Ni/Mo, Ni/NiAl(1150 °C)
    - at 850 °C for 4000 h: Ni/W, Co/Fe, Cr/Mo, Cr/Co, Mo/Fe
    - at 700 °C for 4000 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

Example of Simple Data Analysis



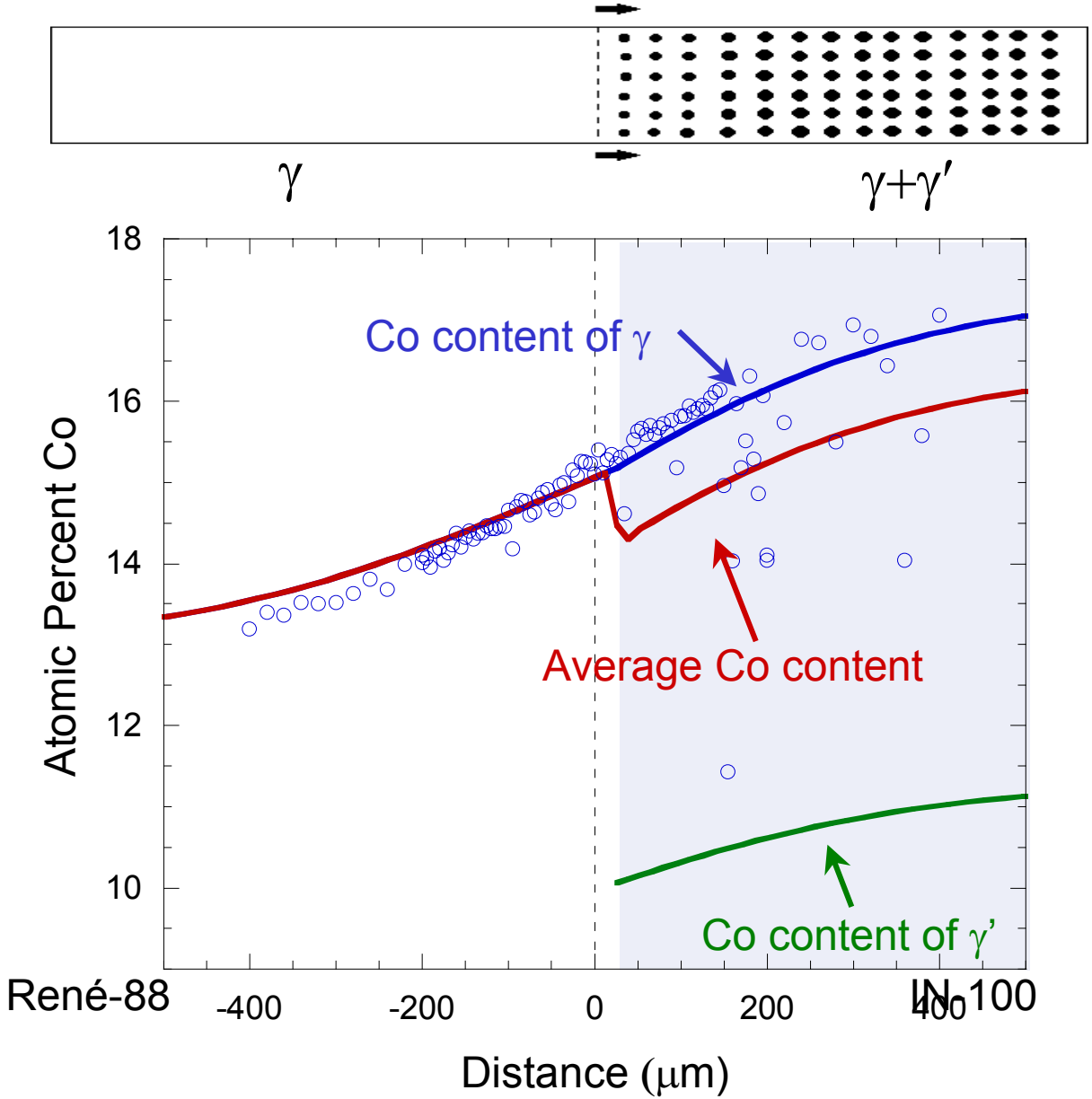
NIST

$$\widetilde{D}\Big|_{Y_i(x')} = \frac{V_M(x')}{2t}\left(\frac{dY_i}{dx}\Big|_{x=x'}\right)^{-1}\left[(1-Y_i(x'))\int_{-\infty}^{x'}\frac{Y_i}{V_M(x)}dx + Y_i(x')\int_{x'}^{+\infty}\frac{(1-Y_i)}{V_M(x)}dx\right] \quad \text{with} \quad Y_i = \frac{c_i - c_i^-}{c_i^+ - c_i^-}$$

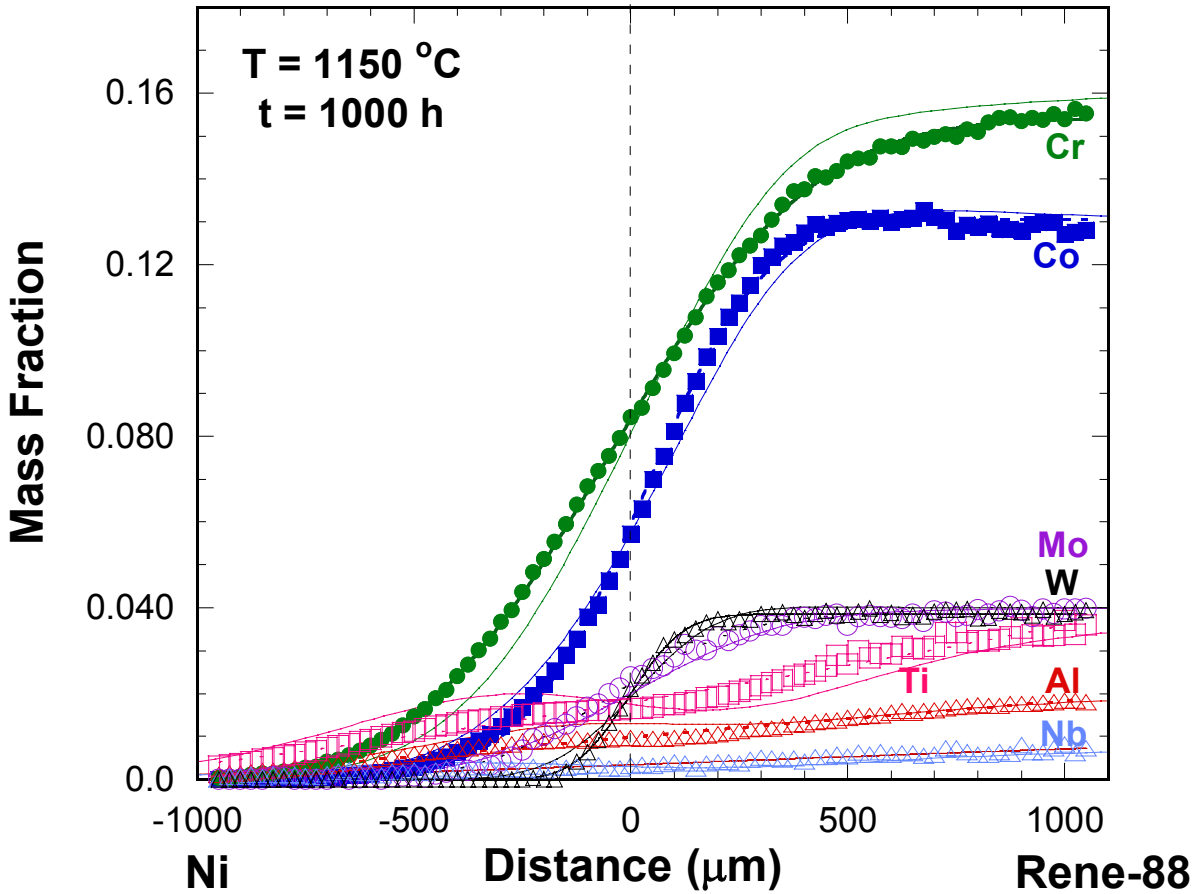


NIST

René-88/IN-100; 1000 h at 1150 °C



Ni-René88



Symbols = GE experimental data
Solid lines = NIST Database/DICTRA prediction

Dashed lines = Error function fit

NIST

Agenda

Thursday, March 27, 2003

8:00 *Coffee and Bagels*

8:30-9:00 **Introduction** (Boettinger, NIST)

NIST motivation

Participant's idea of purpose

Modify agenda by consensus

9:00-9:30 **Review of Multicomponent Diffusion** (Campbell, NIST)

- Definitions: Tracer, Intrinsic, Chemical (Interdiffusion) and Data Sources
- Types of diffusion experiments
- Methods to extract diffusion coefficients (for a review of some of the methods see Bouchet and Mevrel, *Acta Mat*. **50** (2002) 4887)

9:30-11:00 **Summary of Availabe Software Tools for Calculating Concentration Profiles**

9:30 Profiler- Morral, U Conn.

9:45 DICTRA – Liu, Penn State

10:00 NIST Multiphase, Boettinger, NIST

10:15 Other work summary

10:30-11:00 **Computer demonstrations**

11:00-11:30 **Discussion: Evaluation of current approaches: What are the limits of the Darken approach?**

11:30–12:00 **High Throughput approach to Thermodynamics,** Zi-Kui Liu, Penn State

12:00-1:00 Lunch NIST Cafeteria

Agenda

Thursday afternoon

1:00-1:30 **MultiDiflux**, Dayananda, Purdue

1:30-3:00 **Discussion of Inverse Methods for Determining Interdiffusion Coefficients from Multicomponent Data**

3:00-4:00 **Detailed Description of DICTRA and DICTRA format Database** (Campbell, and Boettinger)
Description of DICTRA, Diffusion Data format and Assessment, Examples

4:00-5:00 Computer Demonstrations

6:30 Dinner: Sir Walter Raleigh Inn

Friday, March 28, 2003

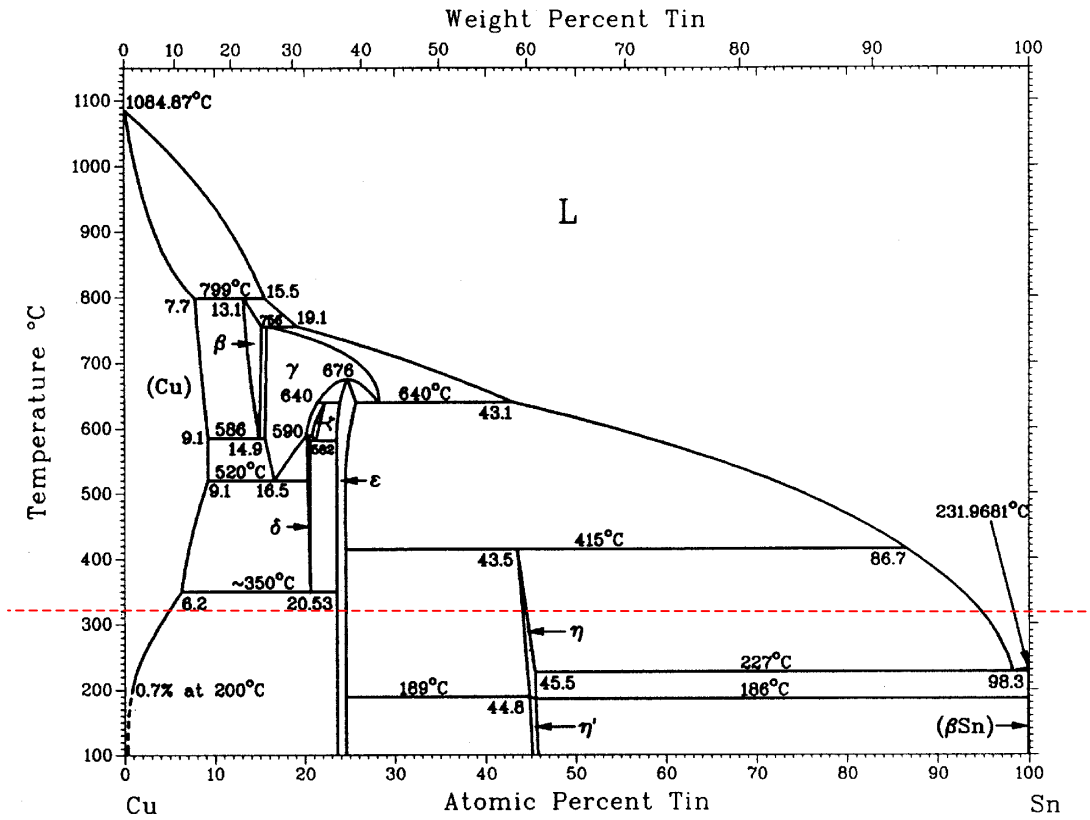
8:00-9:00 Discussion on development of a web site, file sharing, teaching tools
"Teaching Inverse Diffusion Methods" Lupulescu, RPI
9:00-10:00 DICTRA operation issues: Grid resolution etc.,
10:00-11:00 Computer time for small discussions/demos
11:00-12:00 Action Items

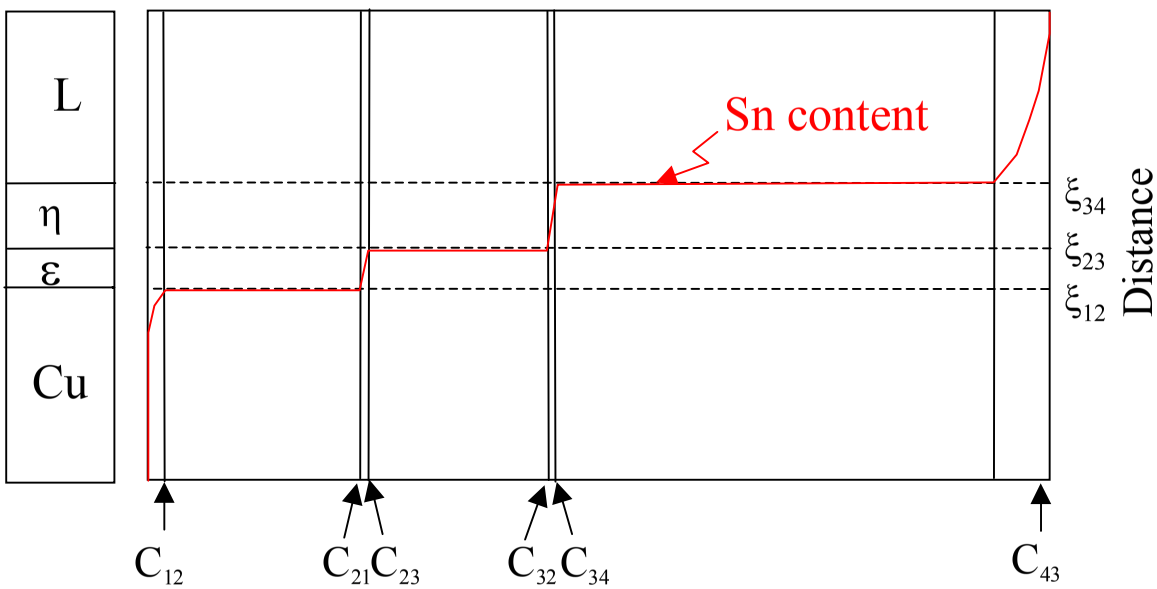
Lunch/Finish

End

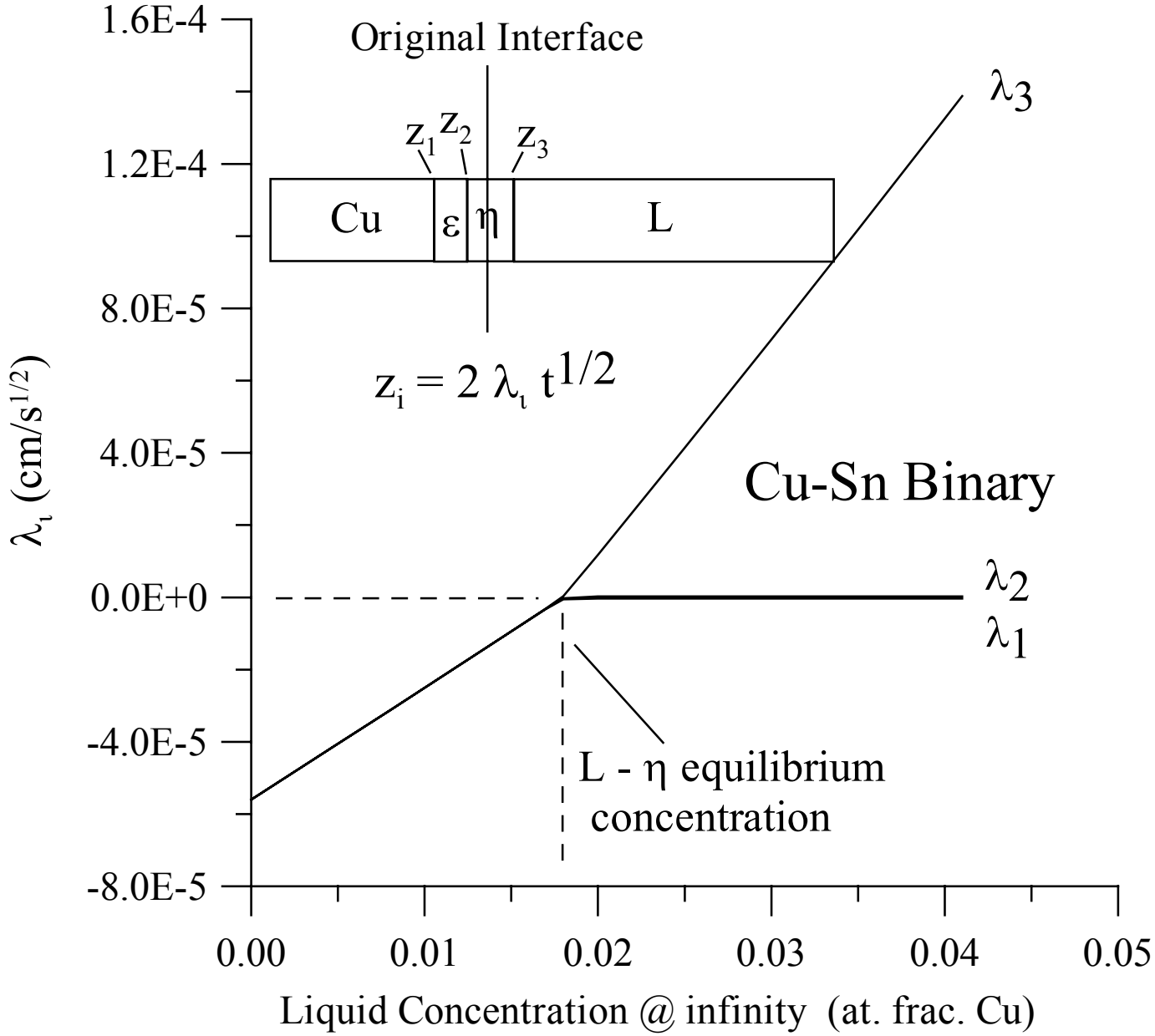
Multiphase 1-D Binary $t^{1/2}$ Growth Code

S. R. Coriell & W. J. Boettinger


Weight Percent Tin
Temperature °C
Atomic Percent Tin
Cu
Sn
1084.87°C
L
799°C
15.5
7.7
13.1
19.1
β
γ
676
640
640°C
43.1
(Cu)
9.1
586
590
14.9
562
520°C
9.1
16.5
ε
δ
231.9681°C
415°C
43.5
86.7
~350°C
6.2
20.53
η
227°C
0.7% at 200°C
189°C
45.5
186°C
98.3
44.8
η'
(βSn)


L
η
ε
Cu
Sn content
ξ34
ξ23
ξ12
Distance
C12
C21
C23
C32
C34
C43

Results from Fortran Code for 4 phase Erf solution (S. Corriel)



NIST

End

Are we missing anything Important?

Effects usually ignored

- **Is Darken analysis good enough?**

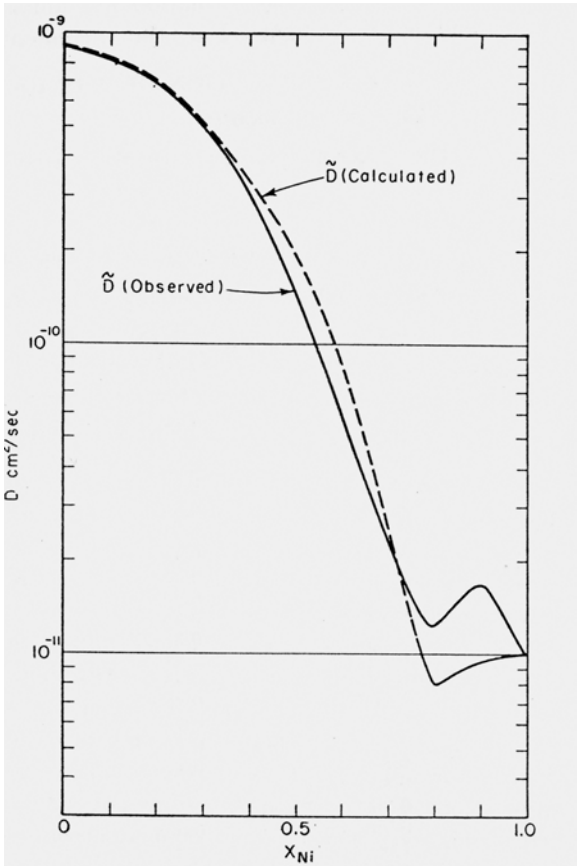


FIG. 4. Calculated and observed interdiffusion coefficients in gold-nickel alloys at 900°C.

Reynolds, Averbach & Cohen, Acta Met. 2 (1957) 29

Effects usually ignored

- **Nonequilibrium vacancy content**

$$\frac{\partial c_v}{\partial t} + \nabla \cdot J_v = s_v$$

$$s_v = -L(\mu_v - \mu_v^0)$$

Vacancy source/sink constitutive law
L→∞ (vacancy equilibrium)

- **Molar Volume**

$$\overline{D} = D_2 C_1 \overline{V}_1 + D_1 C_2 \overline{V}_2$$

- **Vacancy Wind**

$$J_i^{lattice} = -x_i M_i \frac{\partial \mu_i}{\partial z}$$

Only "diagonal" mobility terms

$$J_i^{lattice} = -\sum_{j=1}^{n} x_j M_j \left[\delta_{ij} + \frac{\alpha\, x_j M_j}{1 - \alpha \sum_{p=1}^{n} x_p M_p} \right] \frac{\partial \mu_j}{\partial z}$$

"off-diagonal" mobility terms

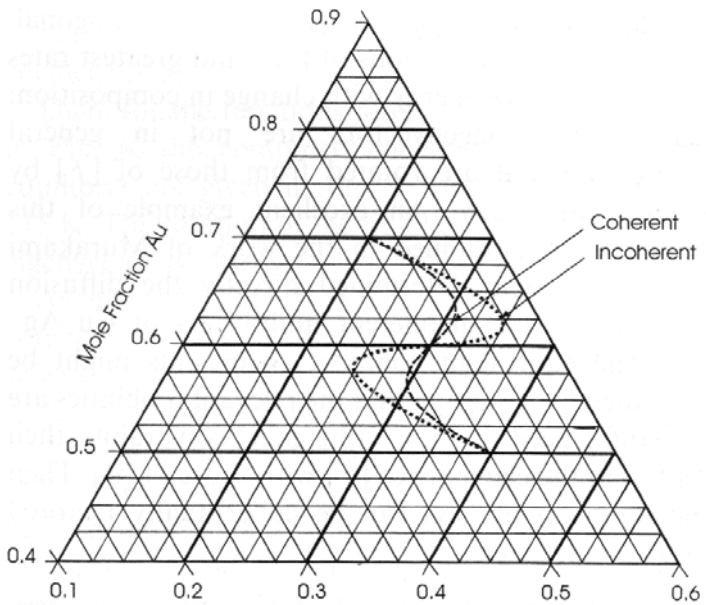
single parameter α depends on composition, temperature

Effects usually ignored

- Stress (Coupled diffusion / deformation)
  - Elastic network solid (e.g. Cahn & Larche)

$$\bar{J} = -M\nabla\left(\mu_2^{SF} - \mu_1^{SF} - V_0\eta\sigma_{kk}\right) \quad \text{for isotropic network solid}$$

$$\text{with} \quad \eta = \frac{1}{a_o}\frac{da}{dc}\bigg|_{c=c_0} \quad \text{"solute expansion coefficient"}$$



Purdy & Brechet, Acta Mater. 44 (1996) 4853
Calculation Cu-Ag-Au couple

Effects usually ignored

- Stress (Coupled diffusion / deformation) continued
  - Non- network solid (i.e. lattice sites not conserved)

(e.g. G. B. Stephenson, Acta Met. 36 (1988) 2663)

J. Philibert (1988)

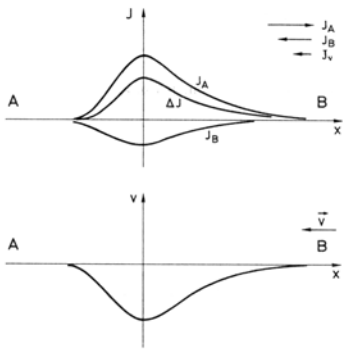


Fig. VI.1. — Interdiffusion of A and B, assuming $D_A > D_B$ everywhere.

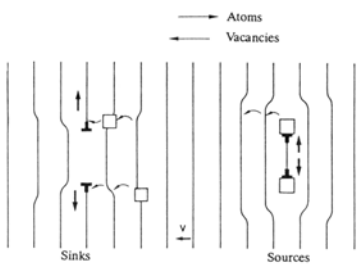
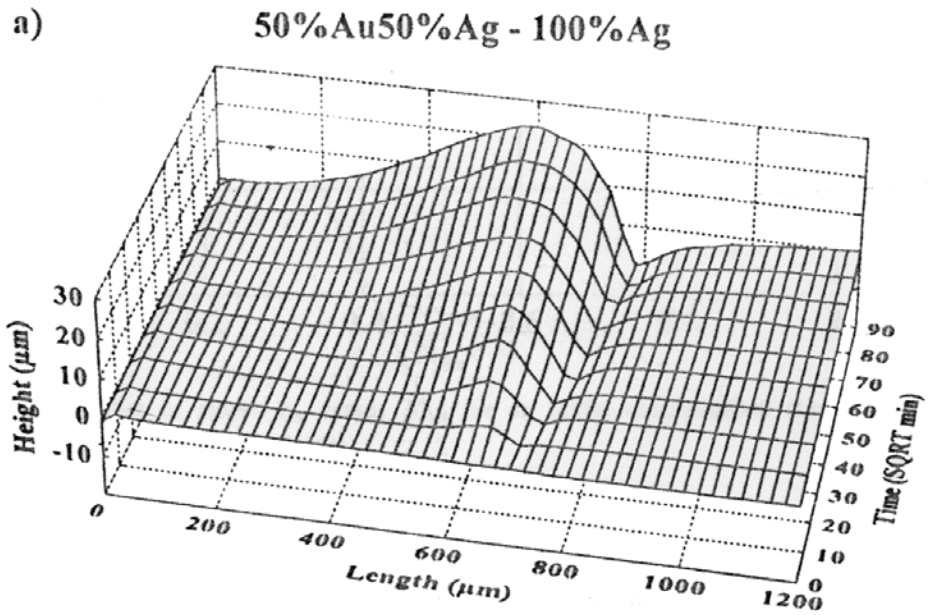


Fig VI.2 — Kirkendall effect: displacement of atomic planes resulting from a flux of vacancies. Vacancy sources are on the right, sinks on the left. The vertical arrows indicate dislocation climb.



R. Voigt & V. Ruth, J. Condens. Matter 7 91995) 2655
Surface deformation in diffusion zone

NIST

Transfer of Diffusion Mobility Parameters to Phase-Field Calculations for Multicomponent alloys

- Phase field models are usually derived in a volume fixed frame.
- A particular component, say '*n*', is picked to be the solvent.
- One needs mobilities, $L_{ij}''(\phi)$, for the dynamic constitutive law.

$$J_i = -\sum_{j=1}^{n-1} L_{ij}'' \frac{\delta F}{\delta X_i} = \sum_{j=1}^{n-1} L_{ij}'' \nabla \left(\frac{\partial f(X_1, \ldots, X_{n-1})}{\partial X_j} \right) = \sum_{j=1}^{n-1} L_{ij}'' \nabla \left(\mu_j - \mu_n \right)$$

- Using the mobility matrix, M, obtained by the current approach for each phase, the L'' matrix for that phase is given by

$$L'' = PMP^T \qquad \text{(matrix multiplication)}$$

where

$$P_{ij} = \delta_{ij} - X_i$$

- Then $L''(\phi) = \phi L_1'' + (1-\phi) L_2''$ where L_1'' and L_2'' are for each phase.

End