NIST Diffusion Workshop: Diffusion Challenges in Sustainable Energy Applications

May 12 & 13, 2008

MSEL, Metallurgy Division

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 Throughput) Measurement Methods

• Existence of legacy Diffusion in Metals Data base at NIST (J. R. Manning)

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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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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

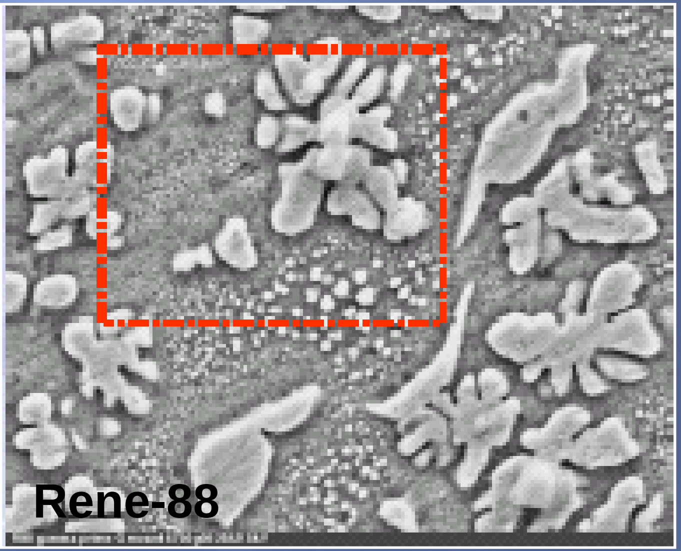
Diffusion Mobility Database
NIST

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.

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

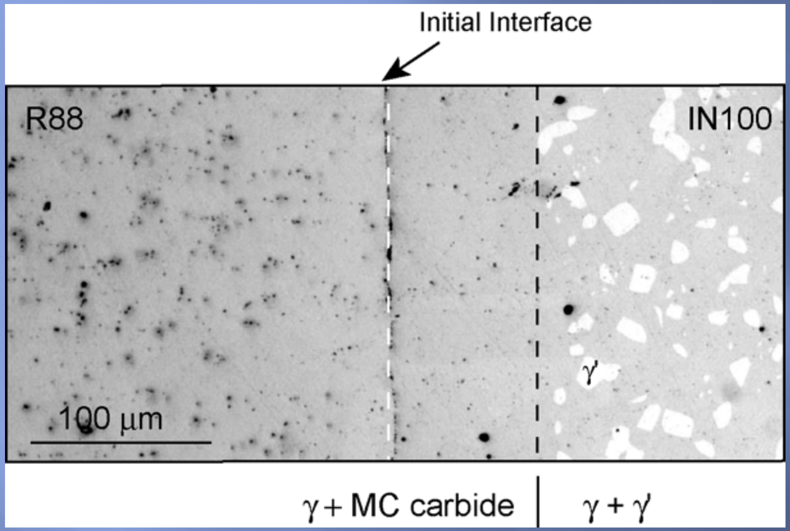
René-N4 ($\times 10^{-14}$ m^2/s)

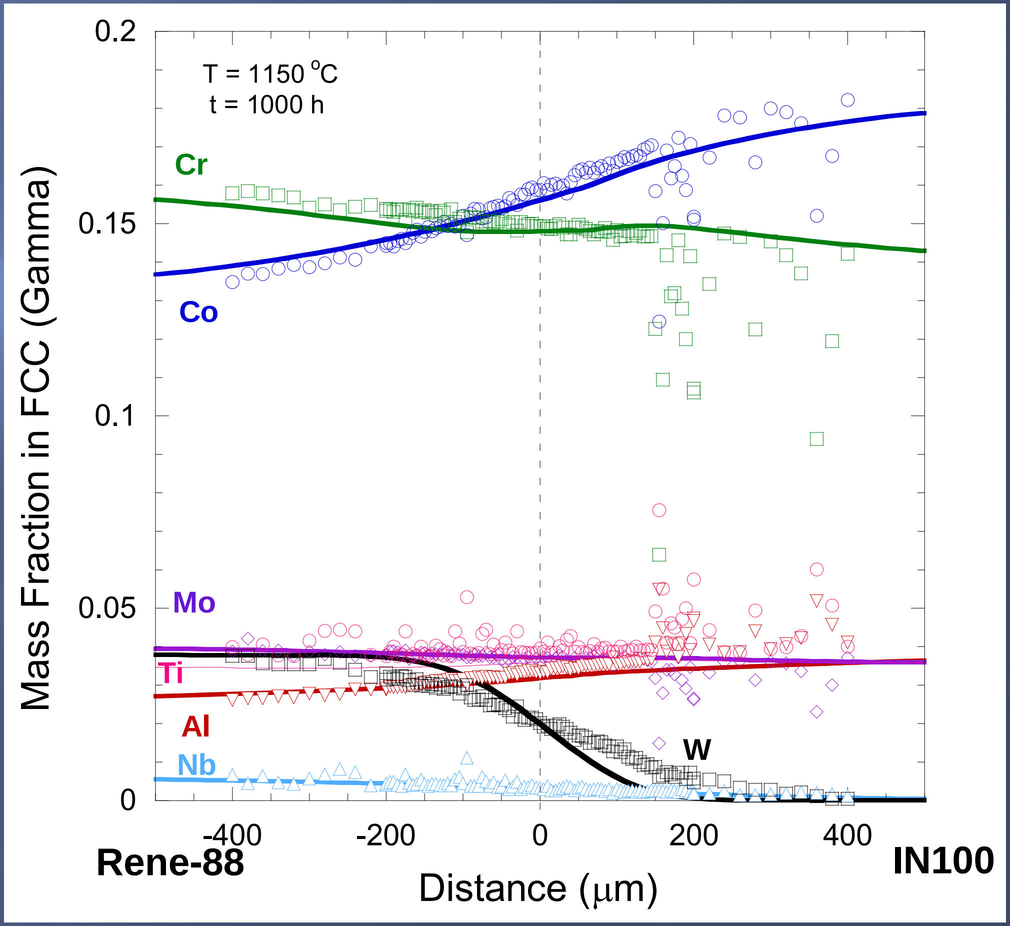
	Al	Co	Cr	Mo	Nb	Ta	Ti	W
Al	+119.5	+13.93	+34.83	+34.34	+42.43	+51.50	+49.51	+53.22
Co	−11.37	+17.00	−8.25	−5.67	−5.55	−1.83	−7.10	−9.69
Cr	−4.26	−5.37	+13.67	−3.21	+8.93	+9.91	+8.25	+2.49
Mo	−8.33	−0.280	−0.426	+7.57	−0.55	−0.36	−0.17	−0.45
Nb	+0.31	+0.25	+0.66	+0.27	+24.05	+0.74	+0.85	+0.31
Ta	−0.68	+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

René-N5 ($\times 10^{-14}$ 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

René-88/IN-100; 1000 h at 1150 °C





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

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

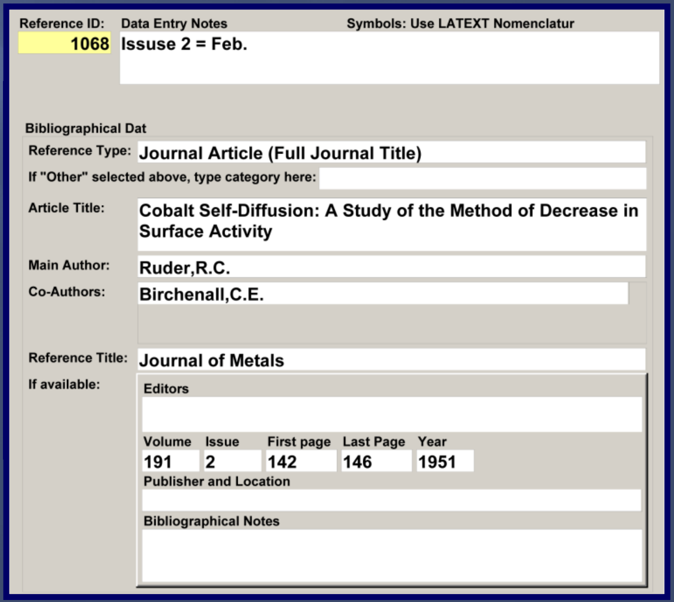
- Industrial and academic support: GE $5K initiation
- Center represents an unique collection summarizing the diffusion work between 1965-1980

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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Diffusion Database Center

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

Web site http://patapsco.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

Home | Mission | Research Programs | Publications | Personnel | Contact | Search

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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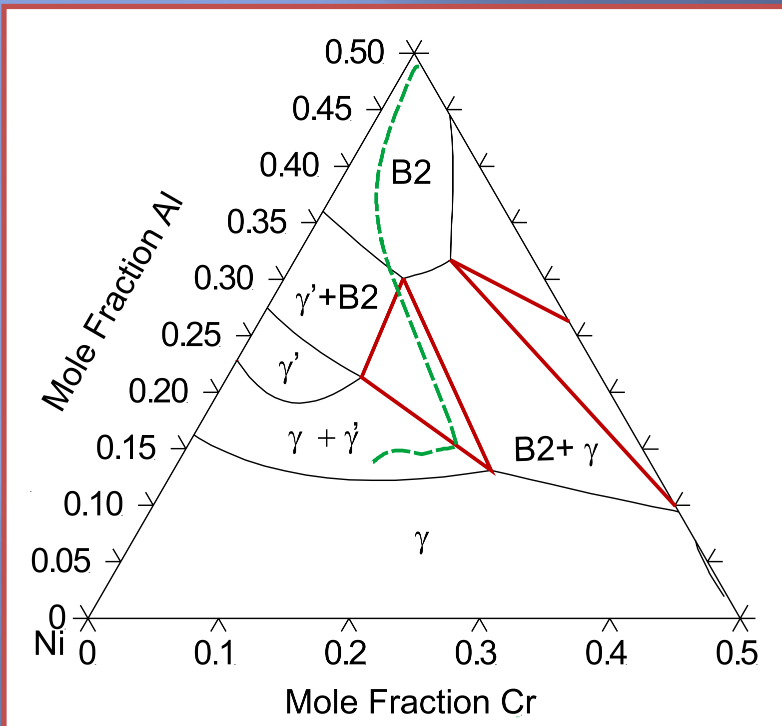
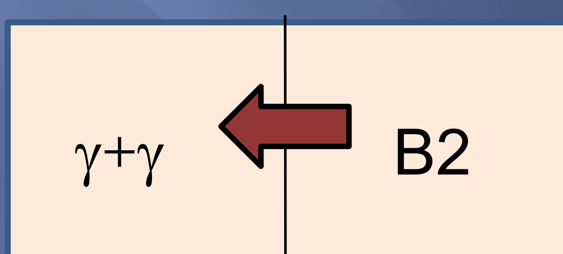
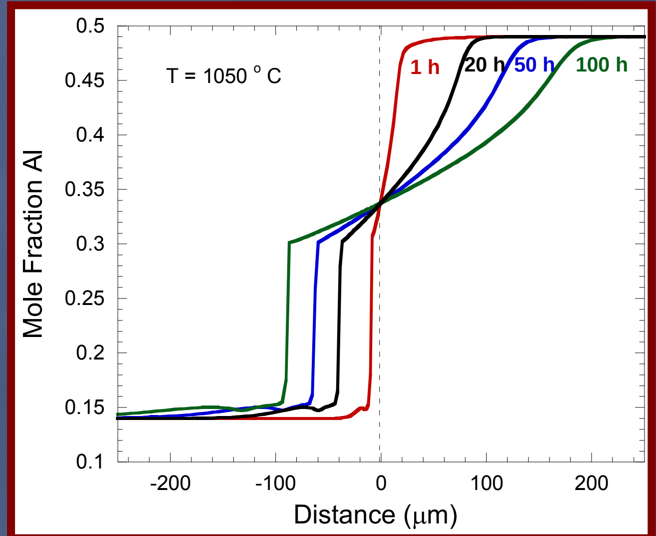
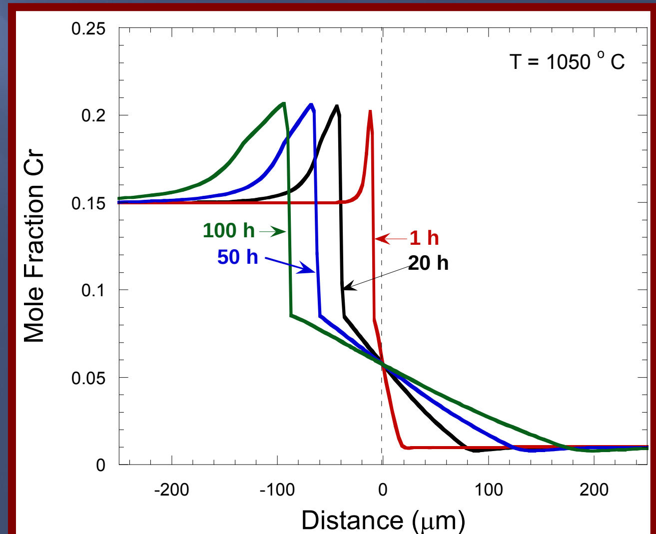
New Model in DICTRA: Homogenization Model*









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* Larsson and Engtröm, 2006

Previous topics

- Optimization of mobility parameters
- Diffusion in ordered phases (Ni-Al)
- Diffusion Barriers
- Kirkendall Effect and Stress
- Measurement of Multicomponent Diffusion Coefficients

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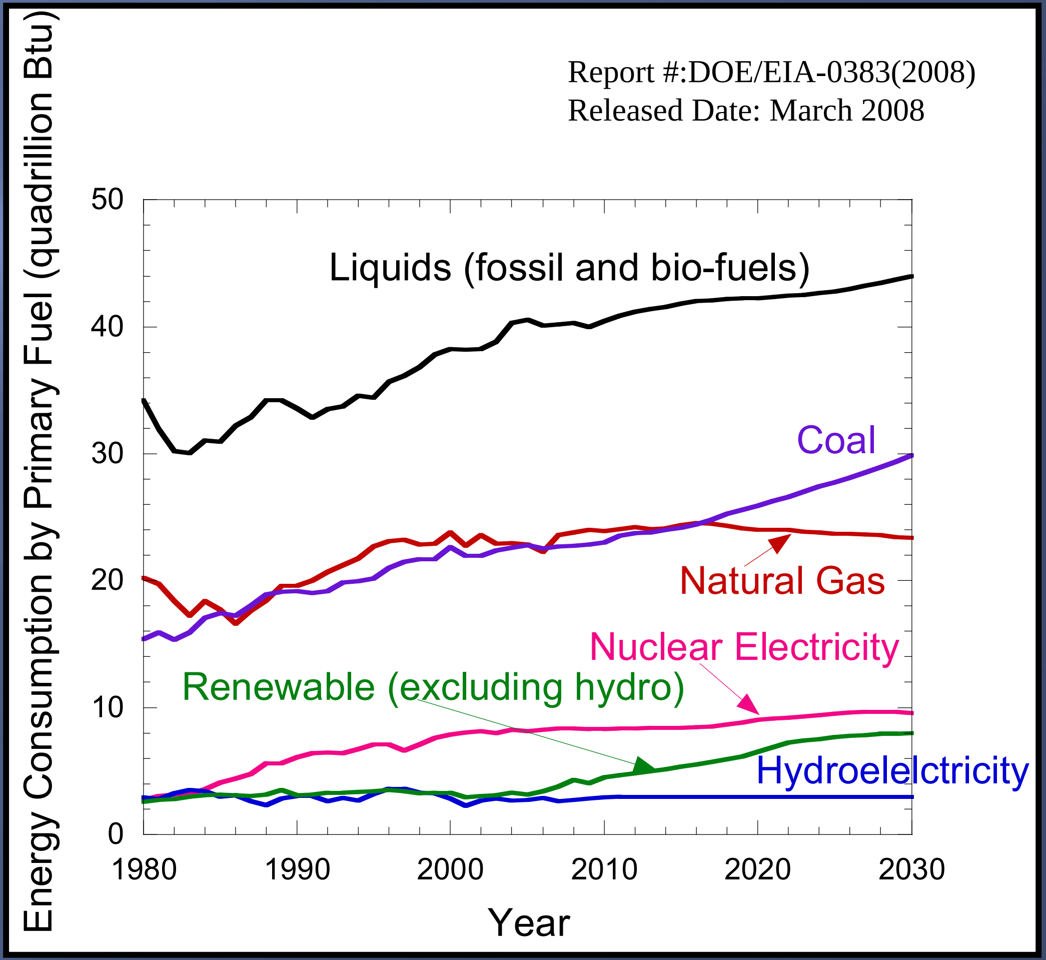
Why Sustainable Energy

- EIA predicts US energy consumption to increase by 19% between 2006 and 2030 (from 99.5 quadrillion Btu to 118 quadrillion Btu)

- Global demand for electricity is expected to increase by 160% by 2050.



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Hydrogen

- Production of hydrogen
  - Fossil fuel
  - Renewable energy source
  - Nuclear
- Conversion to energy
  - Traditional combustion methods
  - Electrochemical processes in fuel cells.

1998 Ford P2000 FCV Mid-size/Full-size

How does hydrogen diffuse in a wide range of media ?

- Membranes
- Metal hydrides
- Pipelines
- Others

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Photovoltaics

Production of terrestrial solar modules has grown at a rate of about 30% to 50% per year for the last 8 years.

- Primarily silicon based wafers (84% in 2005), but limited by supply issues with silicon
- Alternative to silicon: thin film technologies :
  - α-$CuInSe_2$ (CIS)
    - Lower manufacturing costs
    - a high absorption coefficient (~ $10^5 cm^{-1}$),
    - excellent radiation resistance,
    - direct band gap
    - wide range of stoichiometry

To make cost effective need to reduce processing time from ~ 30 min to < 3 min.

Nuclear

Material degradation is the primary cause of unplanned outages.

In 2006, the United States Department of Energy summarized materials research needs for advanced nuclear systems as follows:

"The fundamental challenge is to understand and control chemical and physical phenomena in multi-component systems from femto-seconds to millennia, at temperatures to 1,000°C, and for radiation doses to hundreds of displacements per atom (dpa)."[10]

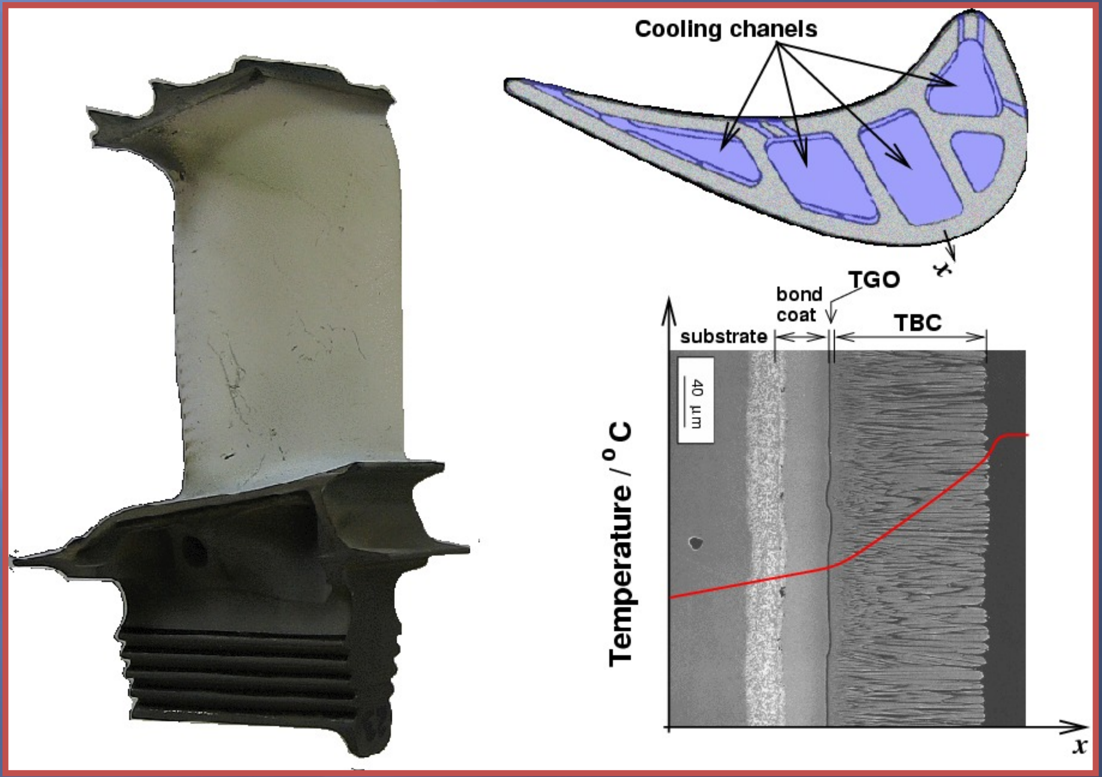
Materials Issues for Advance Fuel cycles

- spent nuclear fuel reprocessing
- improved fuels for light water reactors
- high temperature gas-cooled reactors and liquid metal fast burner reactors
- coolants for heat transfer and transport
- waste form development

Todd Osman, JOM, Jan 2008, 10-13

Materials for Power Generation

- Improved coatings for high temperature performance
- Improved microstructure control; improve stability -> longer service life



After T. Sourmail, www.thomas-sourmail.org, 2004

Agenda

Monday May 12, 2008

8:30-9:00 Introductions and Welcome

9:00-9:15 Brief review of previous workshops (C. Campbell)

Diffusion Challenges for Developing Materials for Sustainable Energy Applications

9:15-9:45 "H Diffusion in Pd and Pd Alloy Membranes. The Role of Non-ideality" (T. Flanagan, U. Vermont)

9:45-10:15 "Hydrogen Diffusion in Steels" (Z. Feng and L. Anovitz, ORNL)

10:15-10:45 Diffusion in CIGS (α-$CuIn_xGa_{1-x}Se_2$) Photovoltaics (W. Kim, Institute of Energy Conversion, U. Delaware)

10:45-11:15 Discussion/ Break

11:15-11:45 "U-Mo/Al Alloys Diffusion Couples : Fuel/Cladding Interactions" (Y.Sohn, UCF)

11:45-12:15 "Uncertainties in Multicomponent Diffusivities and the Determination of Long-Term Diffusivities at Low Temperatures" (J. LaCombe, U. Nevada-Reno)

Lunch 12:30-1:30

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Agenda

Monday May 12, 2008

First –Principles

1:30-2:00 " Diffusion of Transition Metal Solutes in Nickel" (R. Reed, U. Birmingham, UK)

2:00-2:30 "First-Principles Calculations of Diffusion Coefficients in fcc, bcc and hcp" (Z. Liu, Penn State)

2:30-3:00 "Diffusion coefficients from first principles: from intercalation compounds to complex alloys" (A. van der Ven, U. Michigan)

3:00-3:30 "Diffusion of Substitutional Impurities in bcc Fe: First-Principles Modeling" (M. Asta, U. California – Davis)

3:30-3:45 "Atomistic Simulations in Industrial Research: Workshop Summary" (C. Becker, NIST)

3:45-4:00 Break

Modeling Applications

4:00-4:30 "Modeling of Diffusion-induced transformations in Ni superalloys (A. Mirsa, QuesTek)

4:30-5:00 "Apply Phase Field Modeling to Real Systems by Integrating with PanEngine" (K. Wu, CompuTherm)

5:00-5:30 "TC-PRISMA" (P. Mason, Thermo-Calc AB)

6:30 Dinner

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Agenda

Tuesday, May 15

8:45-9:00 Welcome

9:00-9:30 “Update on Diffusion Mobilities in Oxide Systems” (J. Ågren, KTH)

9:30-9:45 “Diffusion Mobilities in the Cu-In-Se system” (C. Campbell, NIST)

9:45-10:15 Discussion/ Break

10:15-10:45 Single-Phase Layer Formation in Two-Phase Diffusion Couples (J. Morral, OSU)

10:45-11:15 “Phase field Simulation of Thermotransport” (Sohn, UCF)

11:15-11:45 “Singularities in Diffusion Paths” (J. Li, U. Penn, OSU)

11:45-12:30 Discussion/Action Items

12:30 Adjourn/Lunch

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