

## Diffusion Workshop Fall 03 Notes

Yali Li: Presented a MatLab version of Profiler

Morrall: Designing Oxidation Resistant Alloys: Criteria for Internal Oxidation (vital path)

Yang and Morrall: Horns

Wang: Phase Field

### Discussion

#### Experimental Issues

Isotope measurements are they needed, who is capable of still making the measurements?

Bulk metallic glasses

Hydrogen in metallic glass (Kirchheim) (J.Cahn)

#### Phase Field Methods

Crystal Phase Field (Ken Elder)

Action Item:  $\gamma/\beta$  w/  $\gamma$  precipitates

Try "effective" model in DICTRA

Morrall, Cahn and Boettinger also to pursue with Morrall's effective model.

Mobility of Stoichiometric phases: Can First Principles help????

Discussed possible optimization techniques for relating experimental data to mobility parameters. Presentations made by Campbell and Höglund demonstrated two methods of wrapping an optimizer around a DICTRA simulation.

### Wednesday morning Discussion

#### Action Items

1. Model (1-D diffusion) for multiphase layers that includes diffusion in both phases; e.g.,  $\gamma/\beta$  with  $\gamma$  precipitates (Cahn, Morrall, Wang)

2. Metastable end member (pure component) Self-Diffusion

a) Use alloy diffusion data from two binary systems with the same metastable end member to extract a consistent self diffusion coefficient for the metastable end member; e.g., fcc Ti from Ni-Ti and Cu-Ti. Is fcc Ti self diffusion coefficient the same? Choose systems with largest fcc region and best data). Pick a crystal structure and element that is mechanically stable or can be kept metastable by exterior constraints for b)

- b) Get a First Principles estimate for the above. (Yuri/Van de Walle)
3. Standard problems.
    - 1) Post Co-Ni data for exercise to extract concentration dependent interdiffusion coefficient.
    - 2) Post concentration profile for two layers for the same exercise.
  4. Find data showing measured diffusion path that goes through corner of three-phase tie-triangle; i.e.,  $\alpha > \beta + \gamma$ . (Morall). Note: from J. Morral reference is NASA Contractor Report 174852. The title is "A study of Interdiffusion in beta+gamma/gamma+gamma prime Ni-Cr-Al Alloys at 1200 C" by Lawrence A. Carol
  5. Post bibliography on web site
    - DICTRA references (math, applications, order diffusion model)
    - Experimental work Horns
  6. Multicomponent Optimization (CC LH)
    - Will choose a ternary system to try (Ni-Al-Cr)
    - Thompson, Morral, Romig Metall Trans. Vol 21A (1990) p 2679.
  7. Summarize experimental data on horns
  8. Find other things for phase field method to simulate (all).
  - 9 Full disclosure of DICTRA diffusion models; e.g., effective simplistic, etc.

#### Possible topics for next workshop

1. Measurements in multiphase couples (microprobe)
2. Geometry of diffusion paths/constraints
  - Summarize experimental data on horns
3. Diffusion in ordered phase (stoichiometric binary, sheet ternary phase, non-stoichiometric) DICTRA, other calculation methods, 1<sup>st</sup> Principles
3. Revisit inverse methods for extraction of D
4. Plastic deformation due to Kirkendall Effect
  - a. Papers by Baluffi and M. Cohen
5. What is the relation between the diffusion mobilities and creep activation energies?
6. Investigate whether crystal method of Ken Elder has any utility for our diffusion problems.
7. Diffusion in Bulk Metallic Glass