March 2003 Workshop Notes:

Introduction: NIST motivation

Diffusion review:
        Need to clarify notation
        J-C Zhao presented work on diffusion multi-poles
        Additional web resource: Defect and Diffusion Forum

 http://www.scientific.net/default.cfm?pg=1&issn=1012-0386&isbn=3-908450-75-6

Presentations on Profiler and DICTRA
        Need for tool to calculate planar layer solutions

Other effects & Darken approach
        Is Darken analysis good enough? No
        When is it good enough?   Need to clarify limitations
        Modified Darken (Manning) is probably good enough

        Non-equilibrium vacancies
        Composition dependent molar volume
        Vacancy wind
                (Day. Did ternary analysis; need marker locations to determine a
                        makes 5% contribution (possibly up to 15%)

                References: Manning, J. R., Metall. Trans. **1** (1970) 499.
                                    Carlson, P. T. et al., Metall. Trans. **6A** (1975) 1245.

        Deformation and Diffusion
                No conservation of lattice sites
                Surface deformation in diffusion zone
                Creep law is coupled with diffusion

MultiDiflux:
        Currently single phase, 3 components, interdiffusion coefficients
        Execution line **mdf.exe datainput**filename
        Assume similarity solutions; check 2 time for validation of similarity solution

Inverse Methods: J. Morral: Butterfly effect (Ni-Cr-Al β-NiAl Thesis)

ACTION ITEM: Use Mulitdiflux error analysis and propagation and try J. Morral
example

Teaching Item: Determine diffusion coefficient as a function of composition (from experimental data) and then re-calculate diffusion profile using determined D f(composition).

Next meeting items:

New people
        Funding agencies ???
        Academia:
        National Labs:
        International:

More specific goals

Suggestions for topics
        Multiphase problems/Microstructural evolution
        Quality of Data/ Experimental Practices/ Data Smoothing Functions
        Diffusion in ordered phases
        Nano-Effects
        Diffusivity in amorphous glasses
        Grain boundary Diffusion

ACTION ITEMS

- Roadmap report ???

- Best Practice Guide for Diffusion Experiments

- Zhao to distribute experimental data (JZ)

- Make MultiDiflux available (MD)

- Update Profiler/ Mathematica code like Profiler (JM)

- Make Howmet data available (CC)

- Program multiphase planar layer (NP)

- Web site include: attendance, slides, bibliography (CC)

- Other suggestions: Viewpoint set for Scripta Mat.

- Teaching tools: Afina, Nick, Philibert