

## Spring 05 Workshop Notes:

### Action Items:

- Can we implement the Manning corrections into DICTRA and then compare simulation results with experimental work and Nagraj's results? (Just binary and ternary )
- Comparison of DICTRA and MultiDiflux results:
  - Couples to compare
    - Ni/Rene88 (single phase)
    - FeCrAl couples from Afina (single phase)
    - Ni/NiAl (GE Couple) (two phase) Carrie will post data
    - Sohn's NiAl/SA (superalloy) couples (multiphases)
  - Comparisons
    - D's calculated by both DICTRA and MultiDiflux for experimental data
    - Flux profiles (MultiDiflux based on experimental data; DICTRA based on simulations)
    - Composition profiles (DICTRA from fixed diffusion mobility database, MultiDiflux based on D's determined from experimental data)
- Develop standard problem for testing "Effective Diffusivity" models in multiphase structures. (Yuri, Day, Yunhzi)
  - Three possible cases:
    - Inert particles
    - Particles involved in diffusion process, but don't move
    - Particles grow and/or shrink
- Order diffusion: Clarify how the order diffusion model is implemented in DICTRA and how atomistic and first principles information can be used in other models.
- Decided on interest in ViewPoint Set and possible topics

### Topics for Future Discussion/Next Workshop

- Diffusion in order phases (Background and application)
- Ionic Diffusion (Oxides, Si) (Höglund)
- Interstitial diffusion and the Kirkendall effect
- 2-D diffusion: What's the best experimental geometry
- Diffusion paths
  - Non-equilibrium effects
  - "strange attractors"
  - Paths in binary systems with a temperature gradient
- Hipping

- Grain boundary diffusion
- Effects of thermal and electro migration on diffusion paths