Diffusion workshop Notes

Diffusion Barriers (John P.)

Ideal Properties (depending on application)

1. Material transport rate of A and B across X should be negligible.
2. Material transport rate of X into A and B should be negligible.
3. X should by be thermodynamically stable with respect to A and B
4. X should adhere to A and B
5. Specific contact resistance of A to X and X to B should be small
6. X should be homogeneous and of uniform thickness
7. X should be resistant to mechanical and thermal stress
8. X should be a good electrical and thermal conductor.

(from Nicolet, *Thin Solid Films*, 52 : 415 (1978).

Applications

Thin Films
Coatings
Permutation barrier

- food packaging
- gas lines (hydrogen economy)

Tian et al.: Measured resistance at barrier (interface)

Graff: When modeling barriers it is important to predict steady-state.

Role of defects important: defect spacing can increase diffusion length

What are the parameters of merit to characterize diffusion barriers?
Permeability= f(solubility, diffusion mobility) ?

Yongho – Application: Coating systems
Develop a reservoir

Dan Jossel: Diffusion Barriers for Superfill Applications

Morral: Horn Formation

- Double horns only found in DICTRA
- Differences between linear or parabolic composition dependent Ds

Larrson: Random-Walk Model solved in the lattice-fixed frame (alternate to current models used in DICTRA); no assumptions about the phase interface made.

Mishin Grain Boundary (GB) Diffusion

Fisher model

Topic 1) Impurity Diffusion along GB

- High temperature: triple product $s\delta D_b$; atoms leave the GB (case B)
- Low temperature : atoms don't leave GB, can calculate D_b (case C)
- Use B and C to calculate $s\delta$

Topic 2) GB diffusion to characterize GB structure and chemistry

Definition of pre-wetting; characterization between pre-wetting and wetting

Topic 3) Atomistic Mechanisms of GB

- Vacancies move through collective jumps
- At low temperatures: order grain boundary??
  - Closer to amorphous diffusion than lattice diffusion
  - Vacancies and interstitials are equally important

Agren (Onsager Relations: Are they Useful?)

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