End of 2nd year report: Timetable

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June 23, 2010

I have constructed a provisional plan for the content of the results chapters of my thesis, along with what needs to be done and (roughly) how long each part should take. I have ignored background theory etc. in this plan. Note that unless stated, the code is already written for the required computational simulations. The inhomogeneous disorder chapter may be split into two.

1. The correlated charge model *11 weeks*

   General analytical results Done a lot. Need to write. *2 weeks*

   Inclusion of all shells - analytical results Done a lot. Need to write and check is correct. *5 weeks*

   Links to other models Need a bit of investigation. Depending on significance of results this section may be larger. *4 weeks?*

2. Inhomogeneous disorder *21 weeks*

   (a) Surfaces *11 weeks*

   Analytical results for general concentration profile Done. Need to simplify what I've written. *2 week*

   Surface of homogeneous disordered alloy Done a lot (was included in a paper). Need to add discussion of screening to what is written. *2 week*

   Surface segregation Done a little (was included in a paper). Could explore parameter space more (more/less oscillations etc.). *4 weeks*

   Surface interfusion Done all sims (was subject of poster). Need to write (and relate to experimental results). *3 weeks*

   (b) Bulk *10 weeks*

   Analytical results for general concentration profile Done. Need to simplify what I've written. *1 week*

   Single thin-film Done alot. Need to write. *2 week*

   Periodic thin-film systems Done a lot. May have to do some isolated sims. Need to write up and compare analytic and computational to *an initio* results. *4 week.*

Single $A-B$ interface mixing Need to do some sims. and write. *3 weeks*

3. Multiple component CCM

   (a) Disordered alloys. *10 weeks*

   Analytical results Done all except Madelung energy for ¿1 shell. Written a little. I'd guess 2 weeks for the general Madelung energy formula, and 2 weeks to write. *4 weeks*

   Computational results Basically haven't done anything, not even written appropriate code. Planning to run simulations for ternary disordered alloys $A_xB_yC_z$ for different x, y and z. *6 weeks*

The times I have specified should be an upper limit. This totals 42 weeks, leaving about 18 weeks spare if I aim to finish by the end of my third year. This time would be spend writing the remainder of the thesis. If the above turns out to be an insufficient amount of content for my thesis, additional material from my first year could be added (none of which is mentioned above). Alternatively, I have ideas of other areas which could be investigated if required: such as the effects of short-range order.