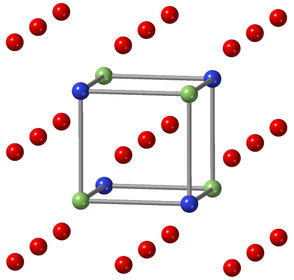
Physics of Magnets and the Arrangements of Atoms Comprising Them

Chris Woodgate
Supervisor: Julie Staunton

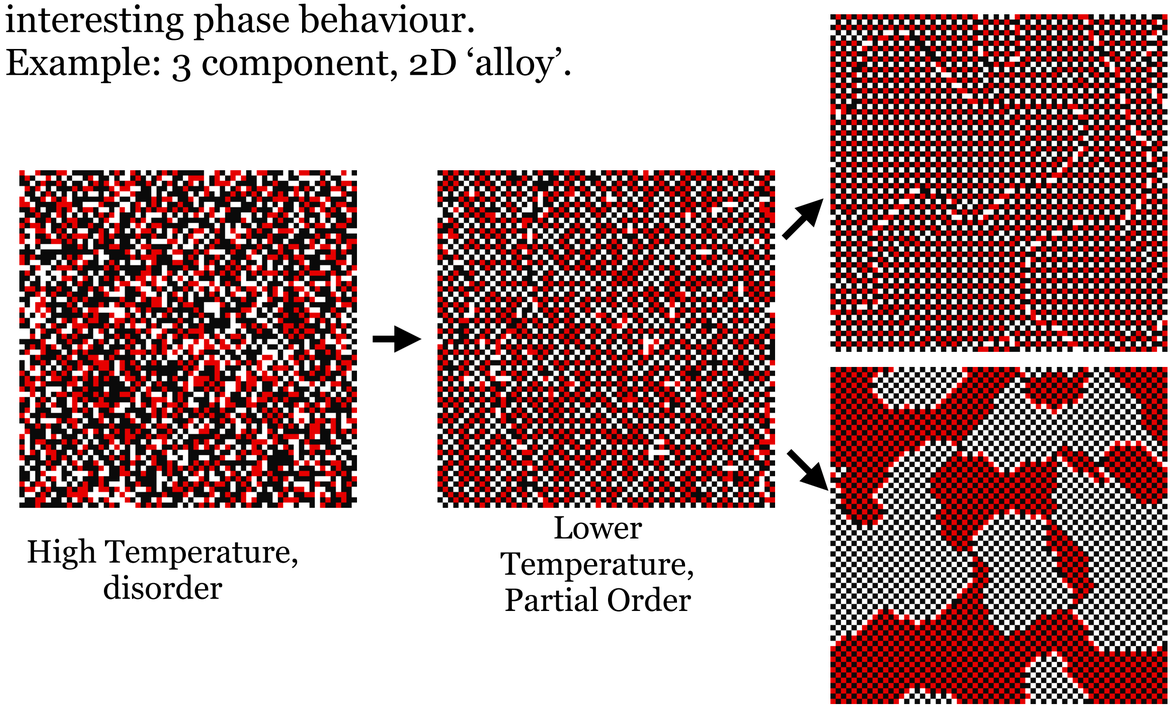
1. Motivation

- Magnetic materials find myriad applications.
- Would like to find candidates for new materials and fine tune the composition of existing ones.
- 'Good' permanent magnets are usually *alloys*.
- Currently studying Galfenol—peak in magnetostriction affected by composition [1].



2. Alloys—What's the Challenge?

- Alloys with three or more constituent metals can exhibit a variety of interesting phase behaviour.
- Example: 3 component, 2D 'alloy'.



High Temperature, disorder

Lower Temperature, Partial Order

Lowest Temperature

3. The Model

- Make use of a Landau-type theory of alloy formation and phase transitions—mean field approach.
- Use *ab initio* calculations to obtain quantities which describe nature of ordering.
- For example, can fit to a pairwise Hamiltonian based on site occupancies and interchange energies:

$$H(\{\xi_{i\alpha}\}) = \frac{1}{2}\sum_{\substack{i,j\\ \alpha,\beta}} V_{i\alpha;j\beta}\ \xi_{i\alpha}\,\xi_{j\beta} + \sum_{i\alpha}\mu_\alpha \xi_{i\alpha}$$

- Can feed average site occupancies back into *ab initio* calculations to study quantities of interest using the coherent potential approximation (KKR-CPA).

4. What Are We Currently Working On?

- Start simple—binary alloys!
- Galfenol ($Fe_{1-x}Ga_x$) has a peak in magnetostriction at x~0.2.
- Level of magnetostriction highly dependent on atomic arrangement.
- Working on a description of site occupancies as a function of Gallium

References:
[1] G. Marchant et al. Phys. Rev. B 99, 054415 (2019)
For more information see the Pretamag project: http://www.warwick.ac.uk/pretamag