Modelling Atomic Ordering and Magnetocrystalline Anisotropy in $L1_0$ FeNi (Tetrataenite)

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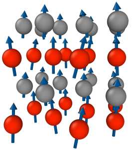
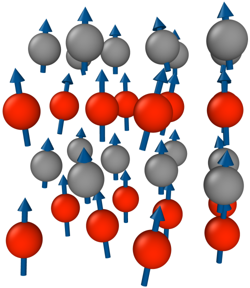


Talk Plan

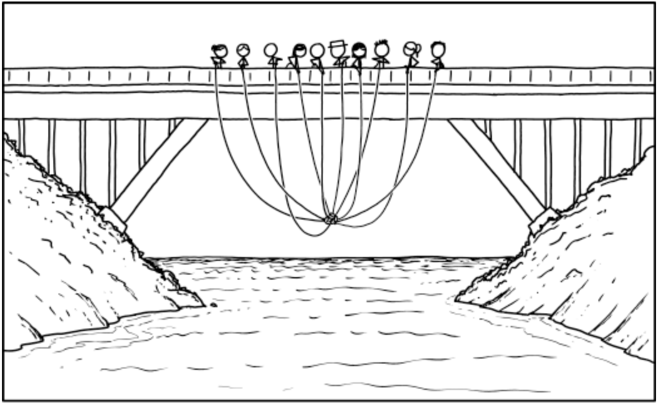
1. Context: Challenges and Opportunities.
2. Modelling Philosophy.
3. Results.
   - 3.1 Capturing existing experimental data[1,2].
   - 3.2 Modelling the influence of composition, strain, and applied field[3].
4. Conclusions.



[1] Woodgate, *et al.*, J. Appl. Phys. **134**, 163905 (2023).
[2] Woodgate, Lewis, Staunton, arXiv:2401.02809.
[3] Woodgate, Lewis, Staunton, in preparation.

Context: Challenges and Opportunities

Permanent Magnets: Myriad Applications



THE FIRST, AND LAST, WORLD MAGNET FISHING CHAMPIONSHIP

[0] https://xkcd.com/2944

Permanent Magnets: Myriad Applications

- 'Hard' permanent magnet: resists being demagnetised.
- Particularly important for 'green' technologies.
- Amount of NdFeB typically required[4] for:
  - Electric car drive motor: 1-3 kg.
  - Small, onshore wind turbine: 100-150 kg.
  - Large, offshore wind turbine: 2-4 t.

[4] Energy Policy **101**, 692 (2017).

Reliance on Rare-Earth Elements: Economic and Environmental Challenges

- Neodymium price[4]: \$11/kg in 2005, \$286/kg in 2011.
- Concerns around stability of global supply chain[5].
- Environmental issues.

[4] Energy Policy **101**, 692 (2017).
[5] European Commission, Joint Research Centre. doi:10.2760/303258

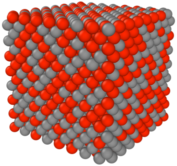
‘Gap’ in Performance Range of Permanent Magnets

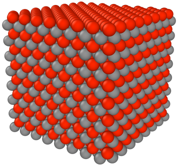
- Figure of merit: ‘maximum energy product’, $|BH|_{\text{max}}$
- Two key permanent magnets for commercial applications[6]:
  - $Nd_2Fe_{14}B$: $|BH|_{\text{max}}$ up to 470 kJm^{-3}
  - ‘Ferrites’ (*e.g.* $SrFe_{12}O_{19}$): $|BH|_{\text{max}}$ up to 38 kJm^{-3}
- NdFeB up to 25× price of ferrite!

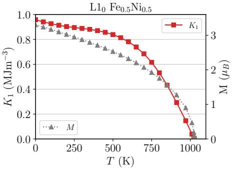
[6] Coey, Scripta Materialia **67** 524 (2012).

$L1_0$ FeNi: A Candidate to Fill the 'Gap'?

- Case for $L1_0$ FeNi (tetrataenite)[7]:
  - Theoretical $|BH|_{\max}$ of 335 $\mathrm{kJm^{-3}}$.
  - Good high-T performance[1]. Curie temperature $T_C > 830\ K$.
- BUT currently challenging to synthesise:
  - As cast, get disordered (A1) structure.
  - Need ordered $L1_0$ phase for hard magnetic properties.
- Can modelling help address this challenge?





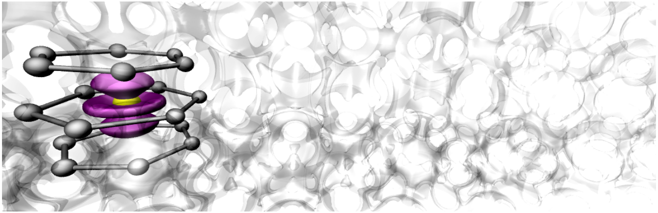


[1]Woodgate, *et al.*, J. Appl. Phys. **134**, 163905 (2023).
[7]Lewis *et al.*, J. Phys.: Condens. Matter **26** 064213 (2014).

Modelling Philosophy

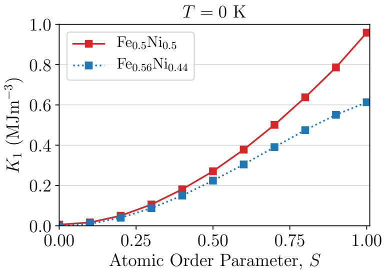
Modelling Philosophy

- Permanent magnetism is an inherently *quantum* phenomenon.
- Model at the level of ions and electrons to capture:
  - Chemical bonds, atomic ordering.
  - Magnetic moments, magnetic anisotropy, Curie temperatures.
- Tool to do this: DFT (LDA, KKR-CPA, DLM Picture).
- Focus on intrinsic physical quantities: magnetocrystalline anisotropy energy, magnetisation, Curie temperature.



Results

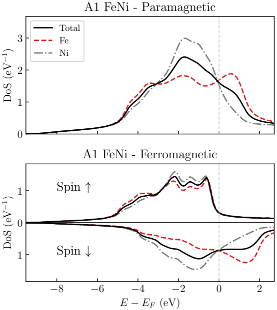
Magnetic Properties are Best for Pristine $L1_0$ Structure

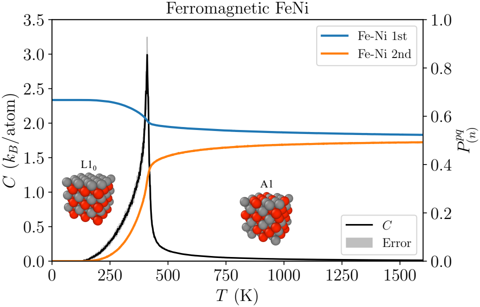


- Hard magnetic properties maximised when maximal atomic ordering achieved[1].
- Thermal fluctuations are important[1].

[1] Woodgate, *et al.*, J. Appl. Phys. **134**, 163905 (2023).

Magnetic Ordering *Drives* Atomic $L1_0$ Ordering

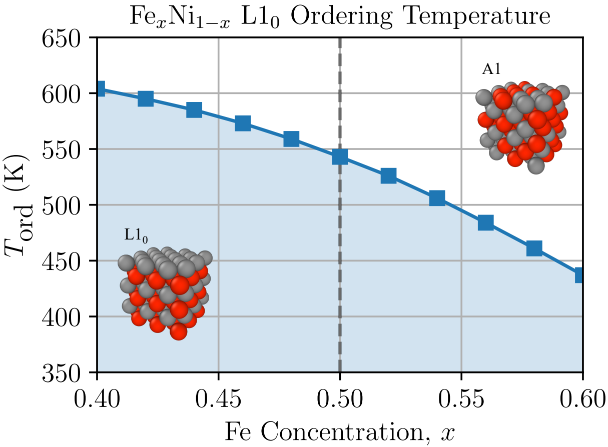




- Ferromagnetic order *crucial* to formation of $L1_0$ phase[2].
- Alloying additions could also help[2].

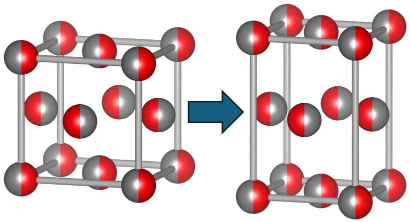
[2] Woodgate, Lewis, Staunton, arXiv:2401.02809.

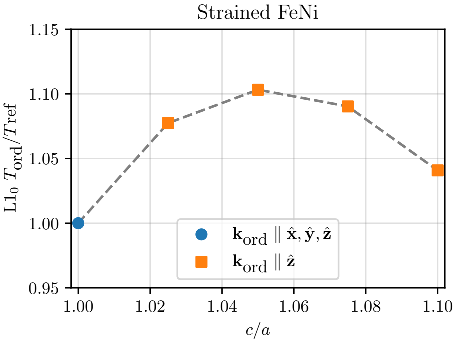
Composition Controls Atomic Ordering Temperature



[3] Woodgate, Lewis, Staunton, in preparation.

Strain Accelerates A1 → $L1_0$ Transformation





- Applied magnetic field also selects a single $L1_0$ variant[1,3,8].

[1] Woodgate, *et al.*, J. Appl. Phys. **134**, 163905 (2023).
[3] Woodgate, Lewis, Staunton, in preparation.
[8] Lewis, Stamenov, Adv. Sci. **11** 2302696 (2024).

Conclusions

Take-Homes

FeNi: Candidate Rare-Earth-Free ‘Gap’ Magnet

Theoretical maximum energy product between that of NdFeB and oxide ferrites. Good finite-temperature performance. *But* bulk synthesis remains challenging.

Varying Composition Controls Atomic Ordering Temperature

Modelling suggests that moving off-stoichiometry towards Ni-rich compositions increases atomic ordering temperature.

Strain and Magnetic Field Accelerates Transition

DFT-predicted atomic ordering temperature is increased and (moreover) a single $L1_0$ variant is selected.

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