Mind the Gap: Developing $L1_0$ FeNi as a Permanent Magnet

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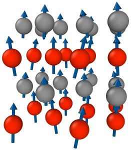
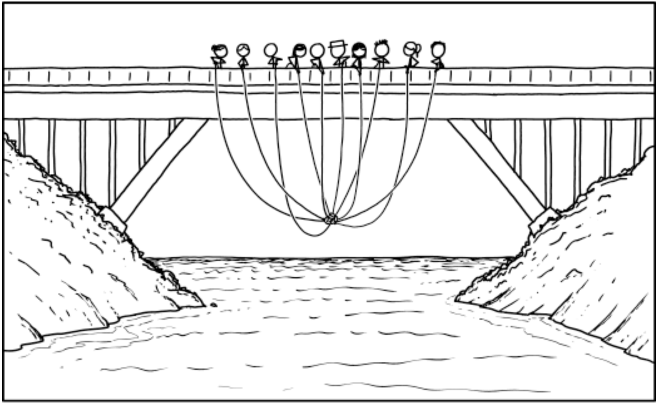


Permanent Magnets: Myriad Applications



THE FIRST, AND LAST, WORLD MAGNET FISHING CHAMPIONSHIP

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

Permanent Magnets: Myriad Applications

- Permanent magnet: magnetisation in absence of applied field.
- Particularly important for 'green' technologies.
- Amount of NdFeB typically required[1] for:
  - Electric car drive motor: 1-3 kg.
  - Small, onshore wind turbine: 100-150 kg.
  - Large, offshore wind turbine: 2-4 t.

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

Reliance on Rare-Earth Elements: Economic and Environmental Challenges

- Neodymium price[1]: \$11/kg in 2005, \$286/kg in 2011.
- China responsible for ∼70% of global RE supply[2].
- Environmental concerns.

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

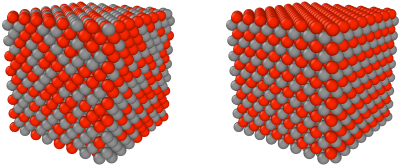
'Gap' in Performance Range of Permanent Magnets

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

[3] Scripta Materialia **67** 524 (2012).

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

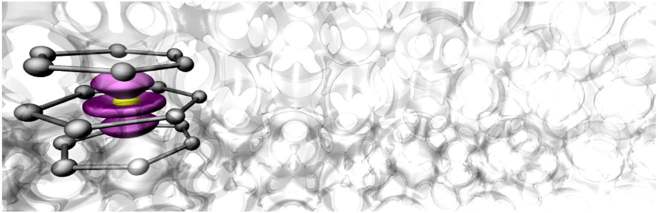
- Case for $L1_0$ FeNi (tetrataenite)[4]:
  - Theoretical $|BH|_{max}$ of 335 kJm^{-3}.
  - Good high-T performance. Curie temperature $T_C > 830$ K.
- BUT currently challenging to synthesise:
  - As cast, get disordered (A1) structure.
  - Need ordered $L1_0$ phase for hard magnetic properties.
- Can modelling help address this challenge?



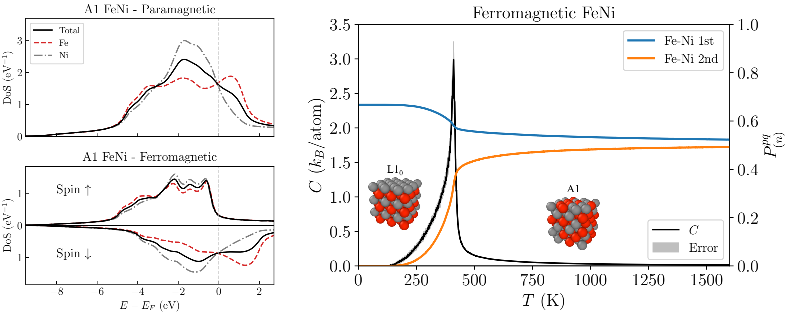
[4] Lewis *et al.*, J. Phys.: Condens. Matter **26** 064213 (2014).

Modelling Approach

- Permanent magnetism is an inherently *quantum* phenomenon.
- Model at the level of ions and electrons to capture:
  - Chemical bonding.
  - Magnetic moments.
- Tool to do this: Density Functional Theory (DFT).
- Focus on intrinsic physical quantities: magnetocrystalline anisotropy energy, magnetisation, Curie temperature.



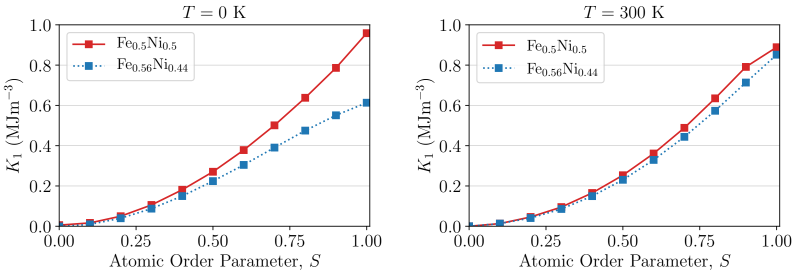
Capturing Structural Transition



- Ferromagnetic order *crucial* to formation of $\mathrm{L1_0}$ phase[5].
- Alloying additions could also help[5].

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

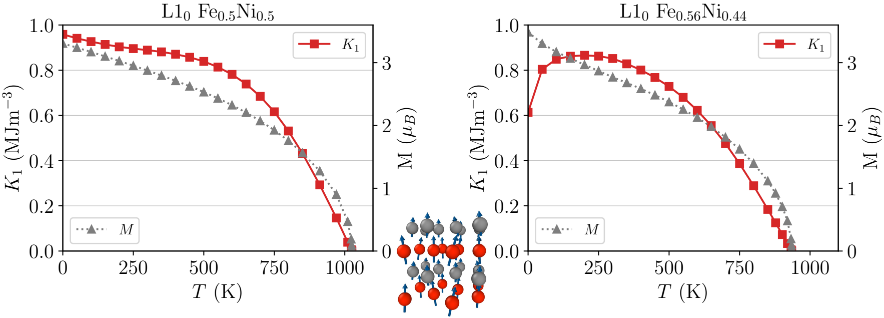
Impact of Composition and Atomic Order on Hard Magnetic Properties



- Hard magnetic properties maximised when maximal atomic ordering achieved[6].
- Thermal fluctuations are important[6].

[6] Woodgate, Patrick, Lewis, Staunton, J. Appl. Phys. **134**, 163905 (2023).

Including Thermal Fluctuations

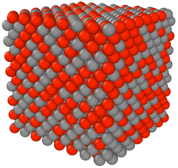


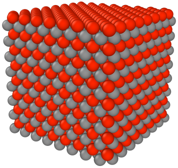
- Capture temperature dependence of magnetisation and anisotropy energy[6].
- Verify robust finite-T performance.

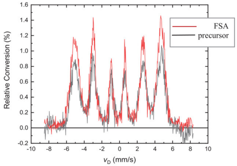
[6] Woodgate, Patrick, Lewis, Staunton, J. Appl. Phys. **134**, 163905 (2023).

Accelerating Ordering—Applying Stress and Magnetic Field?

- Recent experimental work shows applied strain and magnetic field during annealing accelerate transformation[7].







- Preliminary modelling results verify this and (further) suggest that a single $L1_0$ variant is selected during ordering[8].

[7] Lewis, Stamenov, Adv. Sci. **11** 2302696 (2024).
[8] Woodgate, Lewis, Staunton, in preparation.

Take-Homes

FeNi: Candidate Rare-Earth-Free 'Gap' Magnet

Theoretical maximum energy product between that of NdFeB and oxide ferrites.

Synthesis of $L1_0$ Phase In Bulk Remains Challenging

Applied magnetic field and/or mechanical stress appear to accelerate atomic ordering.

Computational Modelling Provides Unique Insight

Can understand why existing materials behave how they do, and suggest routes to manufacture new ones.

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