Connecting atomic ordering with magnetic properties in FeNi alloys

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Why Are We Interested?

Permanent Magnets: Applications

– Growing demand in renewable energy sector.

– 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.

Moving Away from Rare-Earth Elements

Permanent magnet marked is dominated by materials based on rare-earth elements, *e.g.* Nd, Sm, Pr. These are a highly constrained resource. It is desirable to find alternative materials.

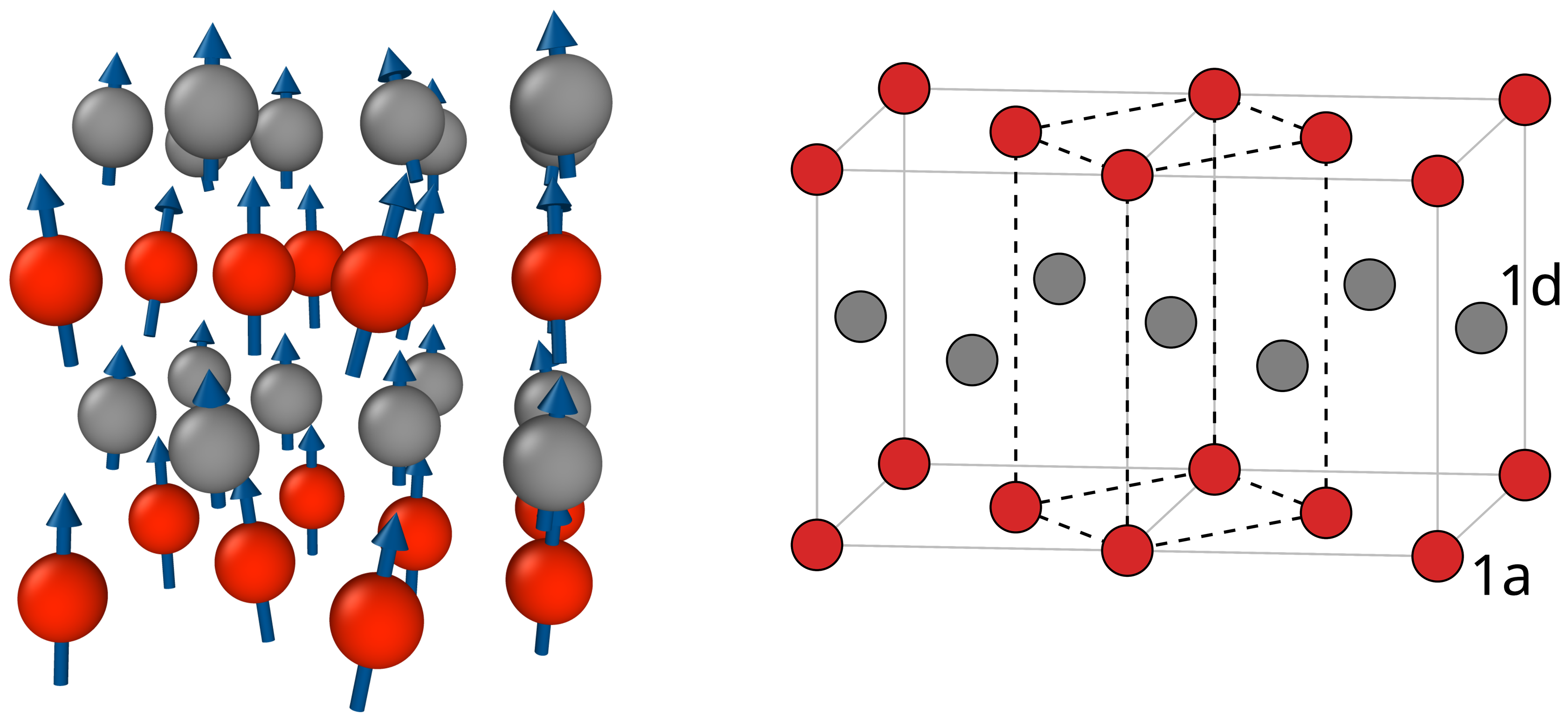
'Gap' Magnets

Rare-earth supermagnets (*e.g.* $Nd_2Fe_{14}B$) are more than an order of magnitude stronger than oxide ferrites (*e.g.* $SrFe_{12}O_{19}$). Need a material to fill this 'gap' in intermediate capabilities at intermediate cost (2).

$L1_0$ FeNi: A Rare-Earth-Free 'Gap' Magnet?

Opportunities

– Near-equiatomic FeNi is known to crystallise in the tetragonal $L1_0$ structure.



– Theoretical maximum energy product (3), $|BH|_{\max}$, of 335 kJm^{-3}. (Close to NdFeB but without use of rare-earths.)

– High Curie temperature → suitable for elevated temperature applications.

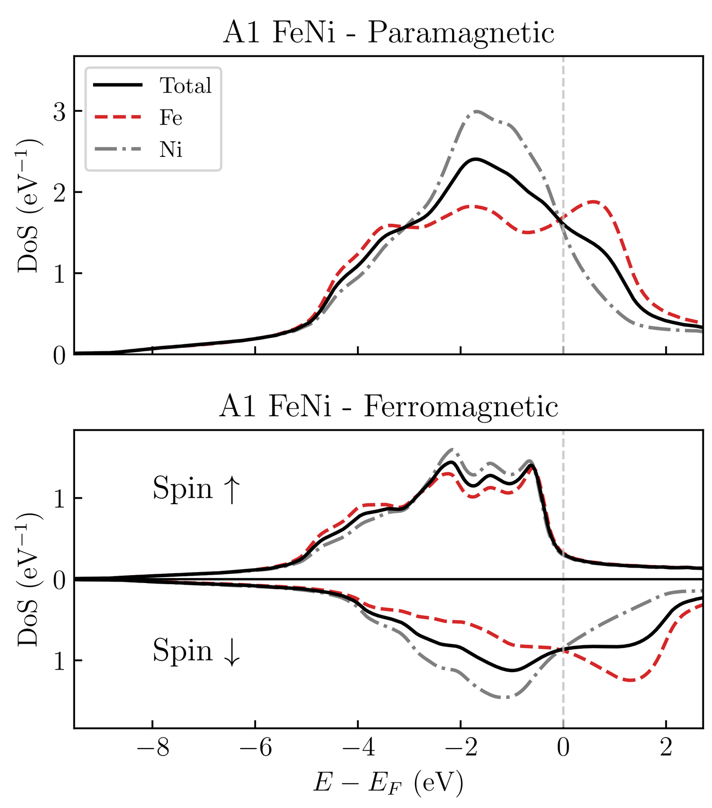
Challenges

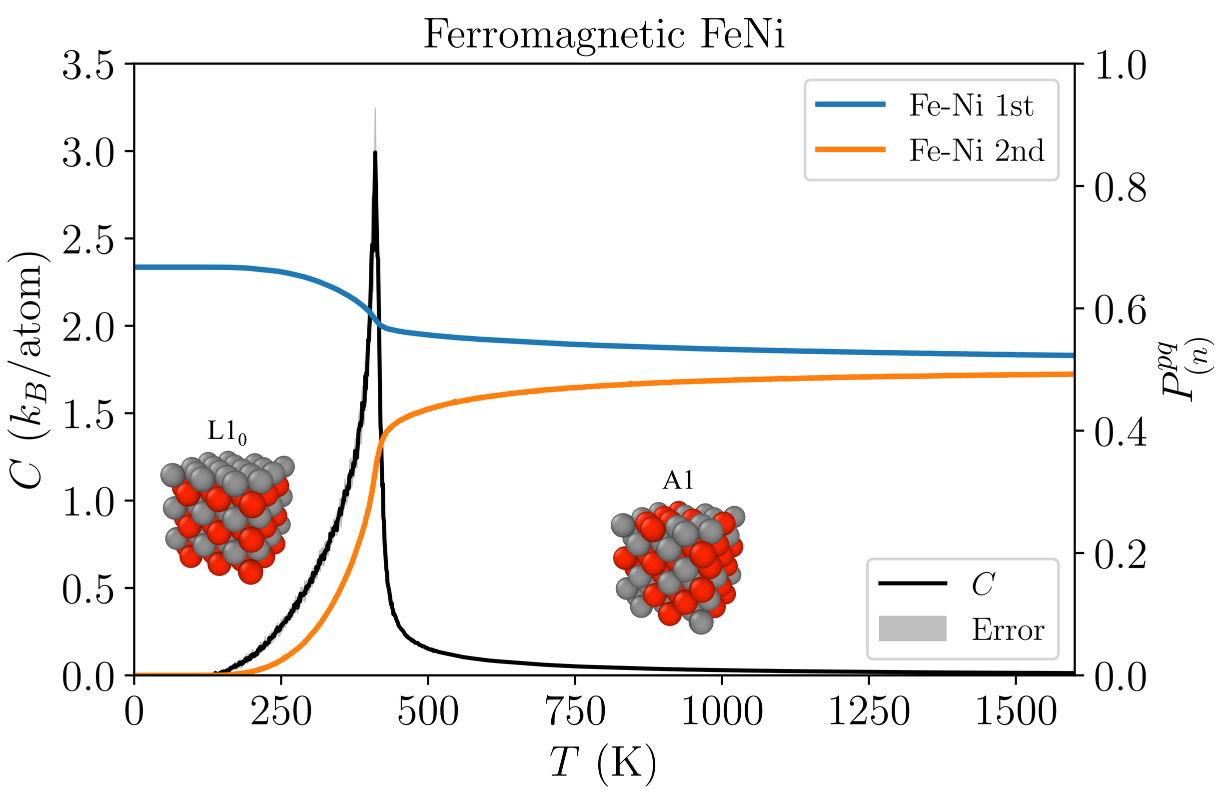
– As-cast, get atomically disordered A1 phase → cubic symmetry, magnetically soft.

– Low atomic ordering temperature results in sluggish kinetics → near-impossible to synthesise in bulk using conventional processing techniques.

Insights from DFT-based Modelling

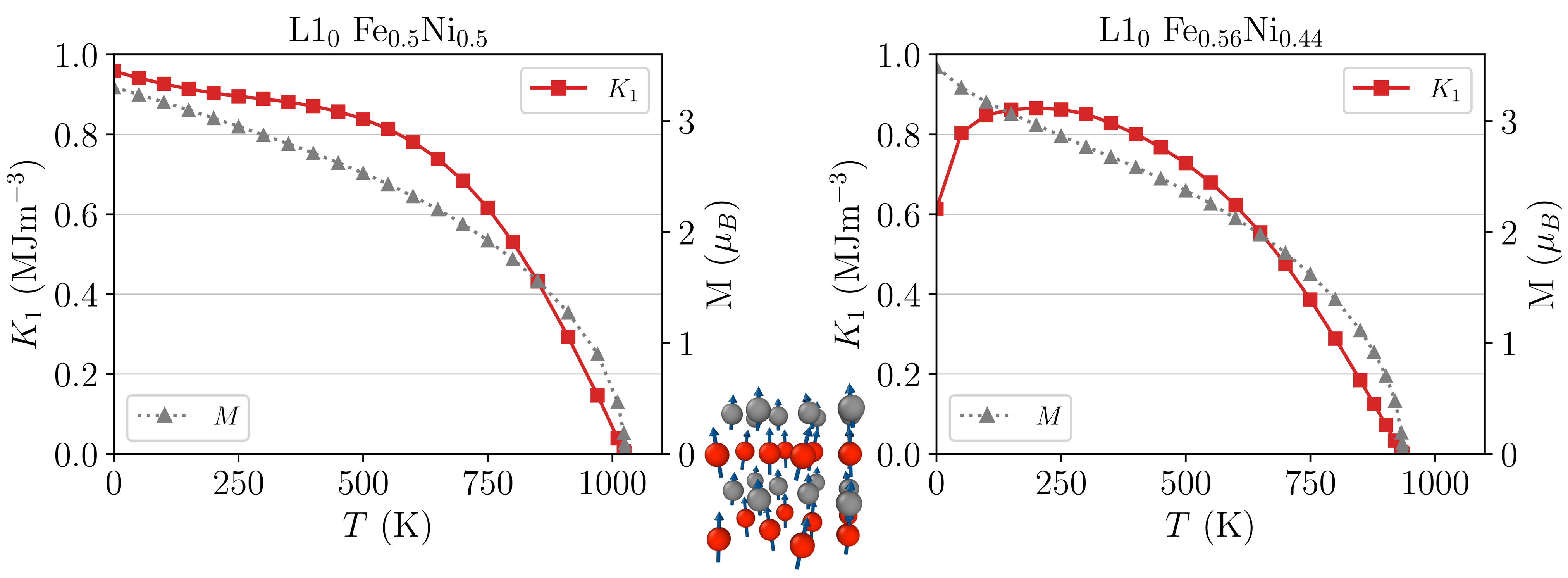
A1 → $L1_0$ Atomic Ordering





– $L1_0$ ordering only predicted when material simulated in *ferromagnetic* state (5).
⟹ processing must take place below Curie temperature.

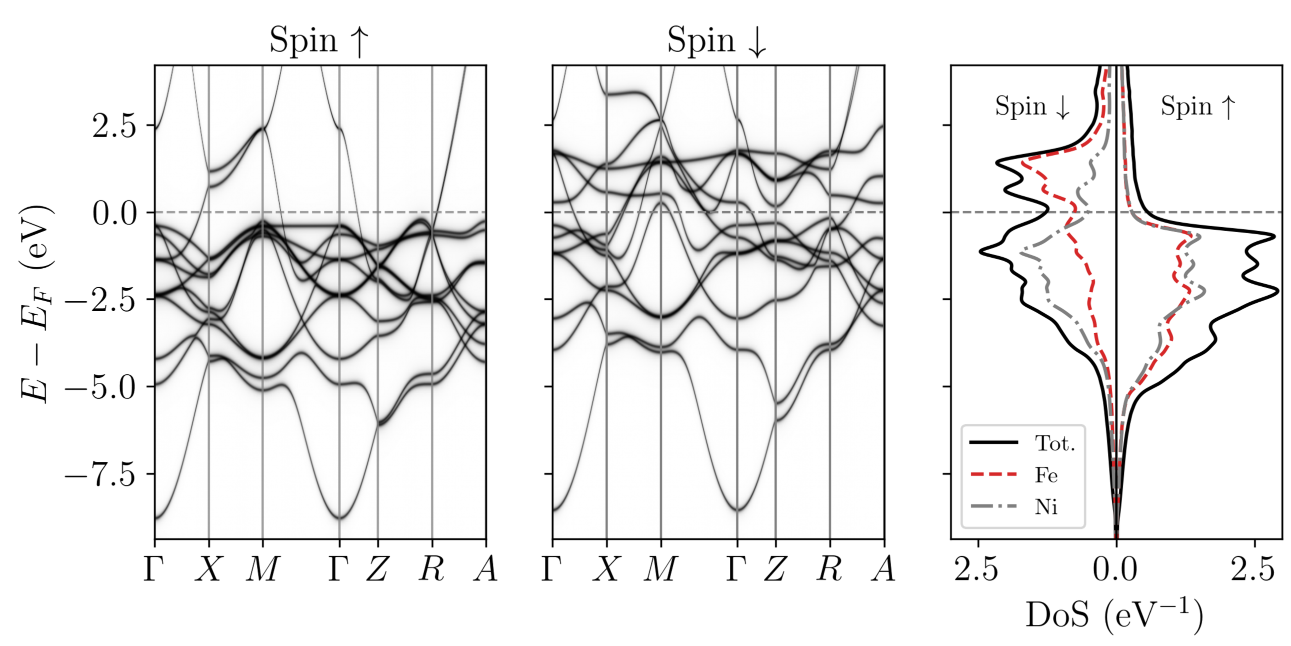
Magnetic Properties at Finite Temperature



– Can use the 'disordered local moment' picture to describe the temperature dependence of uniaxial magnetocrystalline anisotropy coefficient, K_1, as well as the magnetisation of the material as a function of temperature (4).

– Verify robust finite temperature performance across a range of stoichiometries.

$L1_0$ FeNi: Bandstructure



Conclusions

– DFT-based modelling captures key physics of FeNi including chemical ordering and magnetic properties.

– Need to explore less conventional processing techniques: application of magnetic field, stress?

Acknowledgements

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