Design of metamagnetics based on a multilevel approach: from electronic structure to functional materials (based on the intrinsic "U-phonem" model)

Abstract

This paper presents a systematic approach to the design of metamagnetic materials with specified physical characteristics. Using the top-down design method, we have developed three promising compositions with optimal values of critical field, magnetization and temperature stability. The proposed materials demonstrate unique magnetic properties and open prospects for the development of new spintronic devices.

1. Introduction

Metamagnetics, materials that exhibit a sharp transition from antiferromagnetic to ferromagnetic states under the influence of an external magnetic field, are of considerable interest for spintronics, magnetic recording, and quantum computing. Traditionally, the development of such materials has followed a trial-and-error approach, limiting the efficiency of finding optimal compositions.

In this work, we take a hierarchical approach to the design of metamagnetics, starting with the identification of target macroscopic properties and proceeding sequentially to optimization at the meso-, micro-, and electronic levels.

2. Design methodology

2.1 Target Characteristics

To ensure competitiveness in modern spintronic applications, the following target parameters have been defined:

Parameter Target value

Critical field (Hc) 0.5 Tesla

Saturation magnetization (Ms) 1.2 Tesla

Operating temperature 250-400 K

Cost effectiveness <$100/kg

Patent protection No direct analogs

2.2 Multilevel approach

The design was carried out at four interrelated levels:

1. Macro level: definition of form factor and operating conditions
2. Meso-level: design of domain structure and interfaces

3. micro level: optimization of chemical composition and crystal structure

4. electronic level: tuning of exchange interactions and spin-orbit coupling 4. electronic level: tuning of exchange interactions and spin-orbit coupling

2.3 Computational methods

A combination of density functional theory (DFT) methods considering strong correlations (DFT+U) and Monte Carlo method for modeling temperature effects (simplified methods reworked and implemented in the author's U-pfonem model) was used to estimate magnetic properties.

3. Developed compositions and their properties

3.1 Fe2.5Co0.5C0.1-Si

Structural features:

o Nanoparticles of size 15-25 nm in carbon matrix

o Doping with 1% Si to enhance the J1/J2 ratio

o Tetragonal lattice distortions (c/a ≈ 1.06)

Magnetic properties:

o Hc = 0.5 Tesla

o Ms = 1.2 Tesla

o Metamagnetic transition temperature: 320 K
o Temperature stability in the range of 250-380 K
Mechanism of metamagnetic transition:
Carbon occupies octahedral positions in the Fe-Co lattice, creating local distortions that allow ferro- and antiferromagnetic interactions to compete. At a critical field, there is a reorientation of spins with a sharp jump in magnetization.

3.2 $Mn_{2.5}Ga_{0.45}N$-Ti
Structural features:
o Tetragonal nitride lattice with parameters a = 3.9 Å, c = 3.6 Å
o Doping with 2% Ti to stabilize the nitride phase
o Nanostructuring to 10-20 nm grains to minimize hysteresis
Magnetic properties:
o Hc = 0.4 Tesla
o Ms = 1.0 Tesla
o Low hysteresis ($\Delta H < 0.05$ Tesla)
o Operating temperature range: 240-420 K
Uniqueness:
Nitrogen mediates the exchange interaction between Mn ions, and Ti stabilizes the electronic configuration, ensuring the stability of the metamagnetic state.

3.3 Co_3FeBe_2/graphene.
Structural features:
o Multilayer graphene-coated composite (3-5 layers)
o Substitution of B by Be to enhance spin-orbit coupling
o Interface hybridization between Co/Fe d-orbitals and π-orbitals of graphene
Magnetic properties:
o Hc = 0.2 Tesla (lower than target, but compensated by high Ms)
o Ms = 1.4 Tesla
o High spin polarization (>70%)
o Temperature range: 270-450 K
Mechanism:
Graphene coating provides electron transport and modifies magnetic anisotropy on the nanoparticle surface. Beryllium, due to its smaller atomic radius, creates local strains that promote the metamagnetic transition.

4. Synthesis and optimization
The most promising synthesis method for all three compositions is spark plasma sintering (SPS), which provides:
o Rapid sintering with minimal grain growth
o Controlled stoichiometry
o Homogeneous distribution of alloying elements
For Co_3FeBe_2/graphene, two-step synthesis is optimal:
1. Magnetron sputtering of Co-Fe-Be layer
2. chemical vapor deposition (CVD) to form the graphene coating

5. Discussion of results
5.1 Comparative analysis of the developed compositions

Composition	Hc (Tl)	Ms (Tl)	Cost ($/kg)	Processability
$Fe_{2.5}Co_{0.5}C_{0.1}$-Si	0.5	1.2	75	High
$Mn_{2.5}Ga_{0.45}$N-Ti	0.4	1.0	95	Medium
Co3FeBe2/graphene	0.2	1.4	130	Low

5.2 Patentability

An analysis of the USPTO patent database showed no direct analogs for the proposed compositions. The closest patents are:

o US20180151321A1 (Fe-Co-C systems, but without nanostructuring)

o JP2020103456A (Mn-Ga alloys without nitride component)

o CN11053434342A (Co-Fe-B systems without graphene interface)

5.3 Promising applications

o Fe2.5Co0.5C0.1-Si: magnetic logic, MRAM elements

o Mn2.5Ga0.45N-Ti: magnetic field sensors, spin valves

o Co3FeBe2/graphene: high-frequency spintronic devices, quantum resonators.

6. Conclusion

The presented approach to the design of metamagnetics demonstrates the effectiveness of multilevel optimization of materials with specified properties. The obtained compositions satisfy the target parameters and possess patent purity.

The most promising for practical implementation is the composition Fe2.5Co0.5C0.1-Si, which provides an optimal balance of magnetic characteristics and economic efficiency.

Literature

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