Micromagnetic Modelling of Multicrystalline Parallelepiped-Based Bionized Nanoferrite (BNF) Nanoparticles

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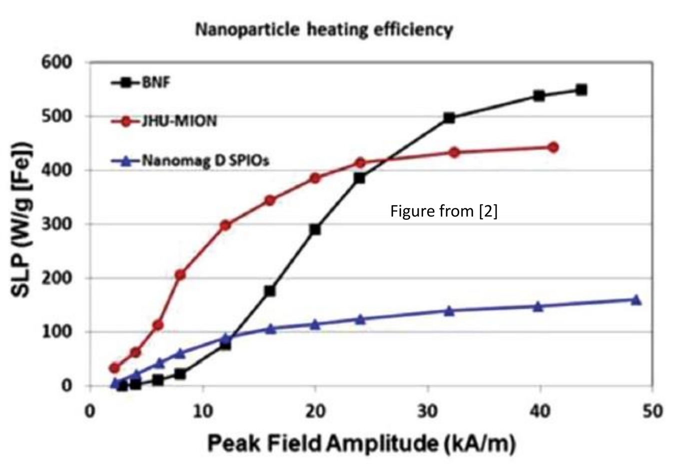
Introduction

Magnetic Nanoparticle Hyperthermia

- Magnetic nanoparticle hyperthermia is an up-and-coming cancer treatment [4]
- Magnetic nanoparticles are injected into the tumor, and an alternating magnetic field is applied. This causes the particles to release heat, which destroys the tumor



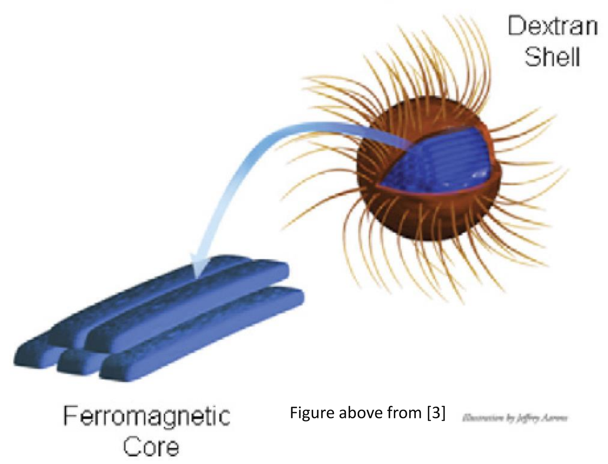
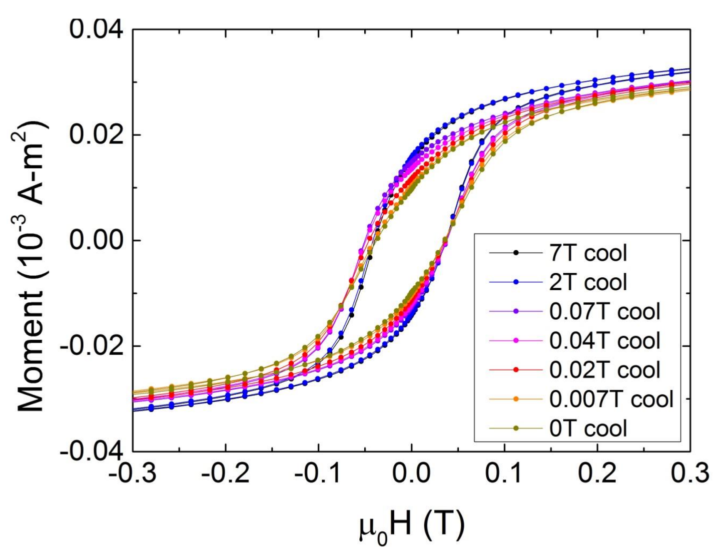


Figure above from [3]



Experimental hysteresis loops for BNF particles cooled in different fields, from [1]

Modelling Heat Release

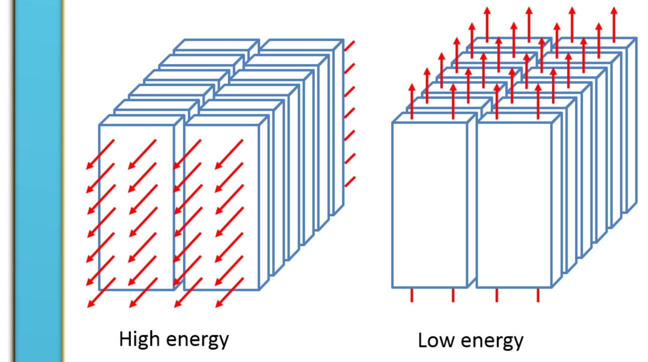
- The heat energy released by the particles in one cycle of the magnetic field is equal to the area enclosed by the hysteresis loop
- The heat depends on a number of factors, including temperature and orientation

Bionized Nanoferrite (BNF) Particles

- BNF particles are a promising candidate for magnetic nanoparticle hyperthermia
- They are composed of stacks of parallelepiped-shaped crystals
- They produce large amounts of heat at high magnetic fields

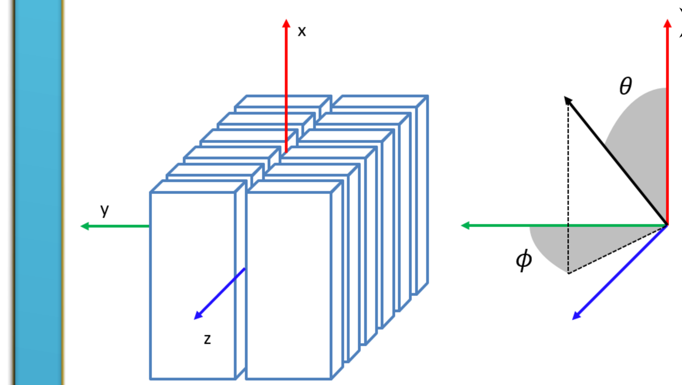
The objective of my research was to accurately characterize the behavior of BNF nanoparticles in a magnetic field

Anisotropy Results

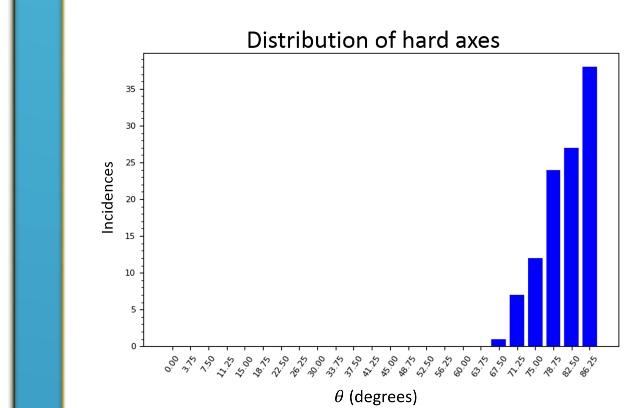


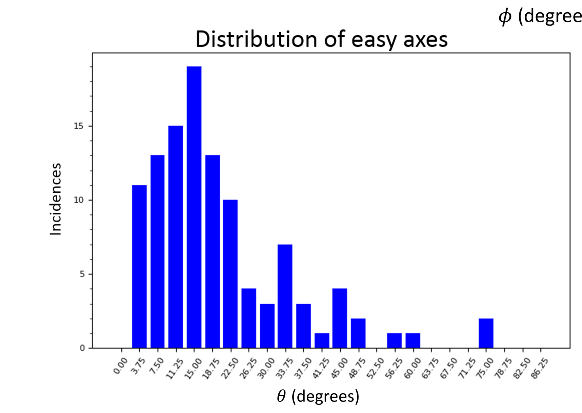
Magnetic Anisotropy

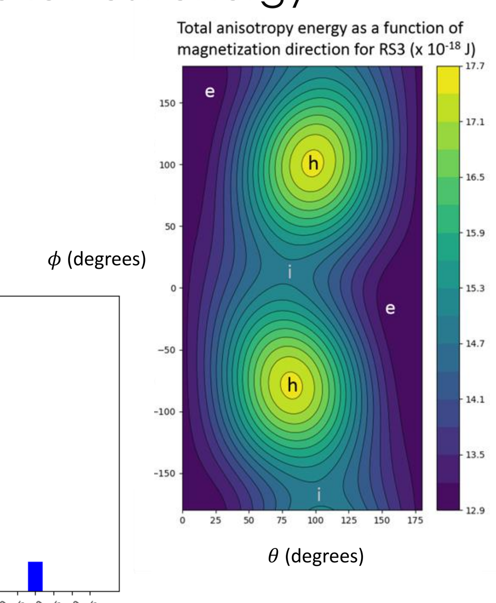
- Magnetic anisotropy is the directional dependence of magnetic properties
- Energy of the particle can be higher or lower, depending on magnetization direction
- An important characteristic is the "easy axis" – the magnetization direction with the lowest energy



These are the direction conventions used. θ is the angle measured from the x axis, and ϕ is the angle measured from the y axis in the y-z plane.





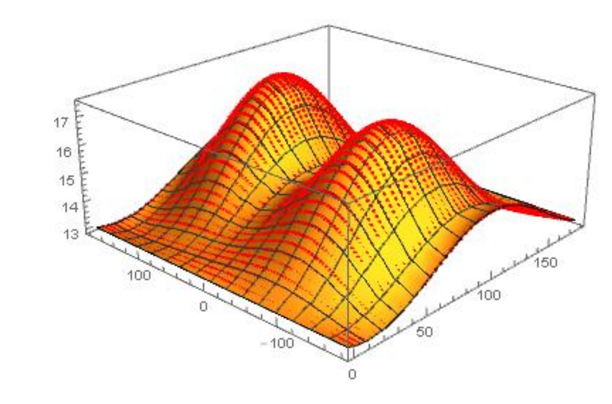


Model Fitting

- Fitted a model to the simulation data
- Triaxial anisotropy: particle has one easy axis, one hard axis, and an intermediate axis
- All axes should be ~90˚ apart, which is what is observed

$$E = K_a V \alpha^2 + K_b V \beta^2$$

This is the energy data for one the of the simulated particles, RS3. Only the magnetocrystalline anisotropy energy and shape anisotropy energy are shown here. The white e's mark the easy axis, the grey i's designate the intermediate axis, and the black h's represent the hard axis.

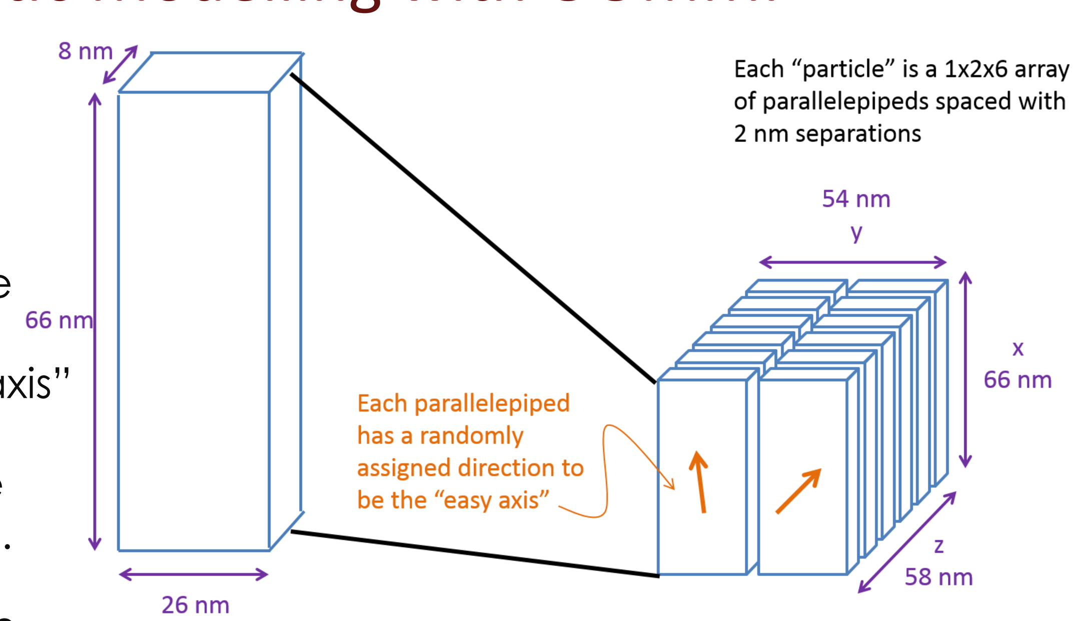


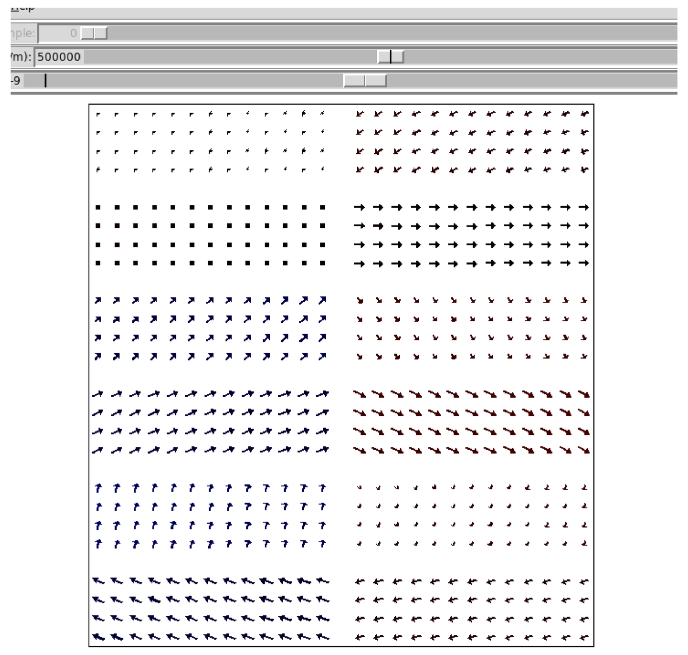
The data in red, with the fitted model in orange

Micromagnetic Modelling with OOMMF

OOMMF Simulations

- Particles were modelled as 12 parallelepiped "crystals"
- Each particle is different because the component crystals have random directions assigned to be the "easy axis"
  - Determined by "RandomSeed" (RS) value
- Particles named by their RS value (i.e. RS1, RS2, etc.)
- The magnetization is discretized into 2nm x 2nm x 2nm cells
- The program applies a magnetic field to the particle, and records how the particle responds

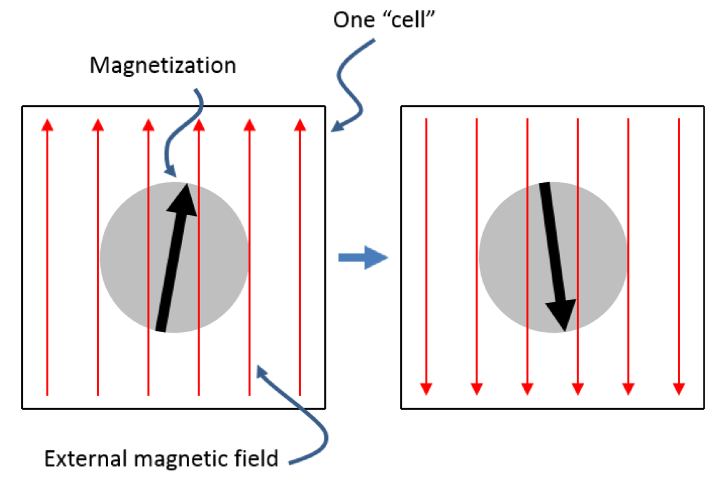




A visualization of OOMMF simulating a particle. This is a top-down view. The little arrows represent magnetization of the "cells".

2 Types of Simulation

- To investigate the anisotropy energy of the particle
- To construct hysteresis loops for the particle in various orientations



The magnetization changes depending on the direction of the external magnetic field

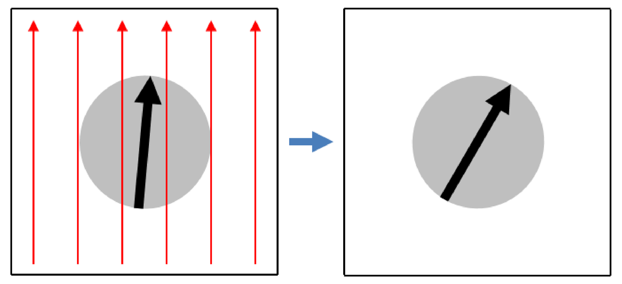
Hysteresis Results

Magnetic Hysteresis

- Most of the magnetization is retained after the external field has been removed – it has become magnetized
- An applied field in the opposite direction is required to demagnetize the material

Important Characteristics

- Remanance – the magnetization remaining at zero field
- Coercive field – the field required to reduce the magnetization to zero
- Area enclosed – the area within the loop, represents the energy lost over one cycle of the field

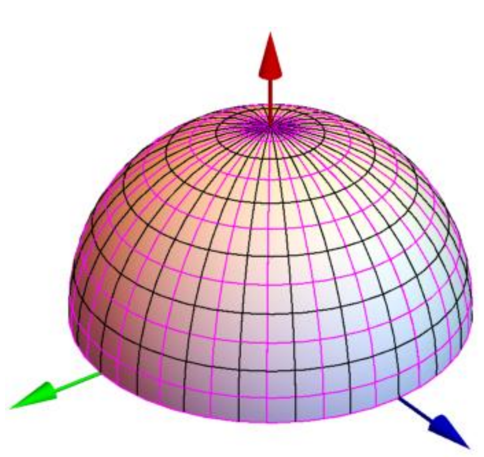


The magnetization stays in the same general direction when the field is removed

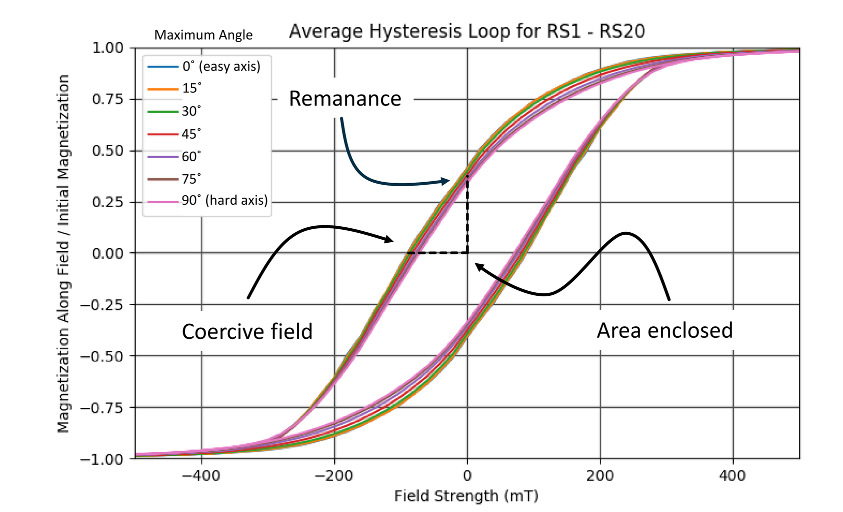
Hysteresis Loops in Different Orientations

- Hysteresis loops were constructed with the applied field in different directions relative to the particle, to emulate their orientations in a magnetic field
- The loops were weighted by solid angle and averaged
- They were averaged based on the max angle from the easy axis to the field direction, i.e. the first loop is just the easy axis, the second is the easy axis and the first "latitude" line, etc.

The red arrow designates the easy axis. Each intersection of the black lines represents a direction for the applied field. The areas enclosed by the purple lines mark the solid angle "surrounding" each direction. Each black "latitude" line is 15˚ apart, as well as each black "longitude" line.



All the average hysteresis loops (from RS1 to RS20) on one plot. The loops are colored based on their max angle from the easy axis.



Conclusions

Anisotropy

- The easy axes were found to be clustered close to the long axis of the crystals, averaging about 20˚ away
- The hard axes were much more concentrated, averaging around 80˚ from the long axis of the crystals
- The easy, hard, and intermediate axes were all roughly 90˚ apart, which is what is expected by triaxial anisotropy

Hysteresis

- The magnitude of the remanance, coercive field, and area enclosed tended to decrease with increasing maximum angle
- This makes sense, because it is expected that the easy axis has higher values for these characteristics, and that directions further away have lower values

References

[1] Dennis, Boekelheide, Gruettner, to be published (2017)
[2] Dennis, Boekelheide, Gruettner, *Advanced Functional Materials* (2015)
[3] Dennis, Boekelheide, Gruettner, *Nanotechnology*(2009)
[4] Jordan, Wust, Fähling, John, Hinz, Felix, *International Journal of Hyperthermia* (1993)