# Magnetic recording, and phase transitions in the fcc Kagomé lattice: A two-part talk.

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**Part I.** Ferromagnetism (long-range dipole).





PART I. Review of Recent and Future Technologies in Magnetic Recording.

• Overview of *The Writer, The Reader* (Ir-Mn used for exchange pinning) and *The Media*.

- Areal Density Increase: The Superparamagnetic Trilemma.
- Modeling with *micromagnetics* (LLG: Landau-Lifshitz-Gilbert equations).
- The Recent: Perpendicular Recording and Dual-Layer ECC media.
- The Future (?): Many-layer ECC media, HAMR and BPM.



Plumer van Ek Weller (Eds.) The Physics of Ultra-High-Density Magnetic Recording

Springer

SURFACE SCIENCES

# PART II. Monte Carlo Simulations of ABC stacked Kagomé planes.

- Review of Exchange Pinning.
- IrMn<sub>3</sub> = fcc ABC stacked Kagomé lattice.



- XY and Heisenberg models with NN exchange (8 neighbors).
- Discontinuous transitions to LRO at finite T.
- Impact of spin degeneracies on sub-lattice order parameter.
- Anisotropy and future simulations of exchange bias.

# Areal Density Growth

Reduction in growth rate due



#### AD=(1/track width)\*(1/bit length) =(tracks per inch)(bits per inch)

- Today: AD ~ 500Gb/in<sup>2</sup> Bit length ~ 2 media grains ~ 180 Å
- Tomorrow: AD ~ 1000Gb/in<sup>2</sup>. Bit length ~ 1 media grain ~ 50 Å



year

New Paradigms in Magnetic Recording, M.L. Plumer, J. van Ek, and W.C. Cain, Physics in Canada 67, 25 (2011)



# The HDD Head: Extreme Close-up

100



Slider









# **The Trilemma** of shrinking dimensions.

- 1. Smaller bits require smaller media grains to maintain SNR.
- 2. Smaller grains require <u>larger anisotropy</u> (energy barrier) to maintain thermal stability.
- 3. Larger anisotropy requires <u>larger write fields</u> to switch media transitions.
- Also: Smaller dimensions lead to less responsive read elements (magentically).
- Larger write fields require large moment materials to put at the business end of the write element.
- CoFe at 2.4 Tesla is the largest moment material stable at room temperature *and has been used since 1999*.

*Modeling to the rescue* (and perpendicular recording and tunneling magnetoresistive read elements, ...).

## Modeling (Simulations) to the Rescue.

Micromagnetics of Ferromagnets: Interacting, uniformly magnetized grains.

Thin ferromagnetic films with small shapes and big demagnetization (magnetostatic) fields at edges.



Grain size ~ 8 nm  $\Rightarrow$  1000's of atoms.

#### Landau-Lifschitz-Gilbert Equation

#### Precession and phenomenological damping:

Torque Equation  

$$\frac{d\vec{M}}{dt} = -\gamma \vec{M} \times \vec{H} \qquad \vec{H}(\vec{r},t) \rightarrow \vec{H}_{eff}(\vec{r},t) - \eta \frac{d\vec{M}(\vec{r},t)}{dt}$$
LLG:  

$$\frac{(1+\alpha^2)}{dt} \frac{d\vec{M}}{dt} = -\gamma \vec{M} \times \vec{H}_{eff} - \frac{\alpha \gamma}{M} \vec{M} \times \left(\vec{M} \times \vec{H}_{eff}\right) \qquad \alpha = \eta \gamma M$$

$$\vec{H}_{effective} = \vec{H}_{applied} + \vec{H}_{anisotropy} + \vec{H}_{exchange} + \vec{H}_{magnetostatic}$$
Norm conserving:  

$$\frac{d|\vec{M}|^2}{dt} = 2\vec{M} \cdot \frac{d\vec{M}}{dt} = 0$$

$$\vec{a} \cdot (\vec{a} \times \vec{b}) = 0$$
Add damping  

$$\vec{H}(\vec{r},t) \rightarrow \vec{H}_{eff}(\vec{r},t) - \eta \frac{d\vec{M}(\vec{r},t)}{dt}$$

$$\alpha = \eta \gamma M$$

#### **Shape Anisotropy: A simple argument**

Dipole-dipole interaction (first terms in multipole expansion of magnetostatic energy)

$$E = \sum_{\substack{pairs \\ ij}} \frac{\vec{m}_{i} \cdot \vec{m}_{j}}{r^{3}_{ij}} - \frac{3(\vec{m}_{i} \cdot \vec{r}_{ij})(\vec{m}_{j} \cdot \vec{r}_{ij})}{r^{5}_{ij}}$$

E=-M•H

• Consider energy of <u>dipole 1</u> (lattice spacing  $a=r_{ii}$ )



$$\frac{a^{3}E}{m^{2}} = (\cos \phi_{12} + \cos \phi_{13} + \cos \phi_{14} + \cos \phi_{15})$$
  
-3(\cos\phi\_{1}\cos\phi\_{2} + \cos\phi\_{1}\cos\phi\_{4} + \sin\phi\_{1}\sin\phi\_{3} + \sin\phi\_{1}\sin\phi\_{5})  
=4-3(2\cos^{2}\phi + 2\sin^{2}\phi) = -2  
$$Put \phi_{i} \equiv \phi$$

Completely isotropic.

#### **Shape Anisotropy: A simple argument**

• Create edge (remove 3)

2

Uni-axial anisotropy induced by edge. Energetically favorable for spins to align parallel to the edge and to neighboring spins.

#### **Patterned Devices: Shape Anisotropy**

- Series of solutions for platelets with different aspect ratios: What do we see?
  - CoFe, 2.5 nm thick, 10 nm cells (single layer)



10



### **Micromagnetics of Medium Orientation Effects**

Orientation Ratio (OR) accounted for by assuming a Gaussian distribution for the media *grain anisotropy axes direction* H<sub>K</sub>: mean and Standard Deviation.





Media

Isotropic media – very large standard deviation.

Oriented media – smaller standard deviation (SD).



Expect better performance for media with a preference for **M** to lie in the down-track direction.

## 100Gb/in<sup>2</sup>. Recorded tracks at high kbpi much improved with oriented media.



A clear message was received by recording media development groups. Highly oriented media became the industry standard.

## What then ? *Perpendicular Recording* (even more 'oriented') From Yahoo.com Jan. 16, 2006.

#### **Technology Boosts Hard Drive Capacity (120 GB to 160 GB)**

By MATTHEW FORDAHL, AP Technology Writer 1 hour, 8 minutes ago

SAN JOSE, Calif. - Seagate Technology LLC has started shipping a notebook PC hard drive that overcomes an obstacle many feared would be a major roadblock to the further expansion of disk capacity — and the overall growth of the storage industry.

The new approach that aligns bits of data vertically rather than horizontally enables Seagate — and other drive vendors — to further boost the density of drives without increasing the risk of scrambling data.

# Perpendicular Recording: The ultimate in control of anisotropy-direction distributions

Longitudinal Recording



Magnetostatic fields destabilize the transitions (superparamagnetism).



Perpendicular Recording

Magnetostatic fields stabilize the transitions.





Anisotropy axis out of plane

Easier to control

#### Larger Write Fields due to media soft underlayer.



Single layer medium (longitudinal or perpendicular):

Transition is recorded by fringing field



Double layer perpendicular media with soft magnetic
Underlayer: media becomes part of the write element *Transition is recorded by deep gap field: 50 % boost.*

## ...and more field emanating from media transitions





Stronger fields from perpendicular bits = larger play-back amplitude.

Another ~50% boost.



Exchange-Coupled-Composite Media: *Easier to reverse with same thermal stability.* 





R.H. Victora and X. Shen, *IEEE Magnetics* **41**, 537-542 (2005).

D. Suess *et al., J. Magn. Magn. Mat.* **551,** 290-291 (2005).

Figure of merit:Ratio of thermal energybarrier to switchingenergy. $\xi = 1$  for single-layer $\xi = 2$  for dual-layer

# Now What ?



## **Try exotic.** HAMR – Heat Assisted Magnetic Recording



• The challenge in making HAMR work is in creating sufficiently small spatial thermal gradients that will prevent interference between adjacent bits.

## Modeling HAMR at the atomic scale using LLG.

J.I. Mercer, M.L. Plumer, J.P. Whitehead, and J. Van Ek, Appl. Phys. Letts. 98, 192508 (2011).



5x5x10 nm<sup>3</sup> Grain reversal is highly non-uniform.



X = Down track direction

Position of temperature pulse relative to head field maximum is crucial.

<u>Challenges.</u>Control of thermal spot size.

# Try more control:

#### **Bit Patterned Media**

Lithographically Patterned Bits: One bit = one magnetic grain to decrease transition jitter and increase SNR. <u>Challenges.</u>



•Making them small enough (1 Tb/in<sup>2</sup>  $\implies$  13 nm bits). •Finding the bits for write and read.





100 nm diameter Co/Cu bilayer dots with 200 nm period

# **Or more exotic** Self-Assembled Magnetic Nanoparticle Arrays.

An illustration of nanoparticle self-assembly via solvent evaporation.



Fig.9.11. TEM images of (a) a 2D assembly, of the 8 nm cobalt nanoparticles on an amorphous carbon surface

#### Challenges.

Control of anisotropy axis distributions.

Uniformity of patterns.



# **Conclusions** (Part I)

• Large number of new technologies introduced into magnetic recording over the past decade: *GMR, Perpendicular, TMR, ECC,...* 

• New paradigms such as *HAMR or BPM* will be very challenging to implement effectively.

• Most likely advances in *Areal Density* in the near future will come from *materials science* and increased understanding of the underlying physics through *numerical simulations*.

#### Seagate HAMRs hard drives to 1Tb per square inch

Published on 20th March 2012 by Gareth Halfacree

Seagate's HAMR-based hard drives could, it claims, store up to 60TB of data before the technology reaches its upper limit.

Storage giant Seagate has become the first hard drive manufacturer to reach the dizzy heights of one terabit per square inch areal density, using a technology known as heat-assisted magnetic recording (HAMR.)

Designed as a next-generation replacement for perpendicular magnetic recording as used in today's hard drives, HAMR holds the potential for 3.5in hard drives holding as much as 60TB. That, Seagate is quick to point out, would mean more bits in a square inch of hard drive platter than stars in the Milky Way.

# PART II.



# Monte Carlo Simulations of *ABC* stacked Kagomé planes.



Kagome: The Story of the Basketweave Lattice. M. Mekata, Physics Today Feb. 2003.

First study of magnetic properties: I. Syozi, Prog. Theor. Phys. (1951).

# **Exchange Pinning in Spin Valves**



• Pins the Pinned Layer so it does not respond to media bit transition fields.

• Requires  $T_N >>$  drive operating temperatures~ 350 K.



• Surface spin structure in AF results in a small ferromagentic moment.

• Induces a *uni-directional* field on the PL.

• "After more than 50 years there is still no definitive theory that can account for the observed effects.." K. O'Grady et al., JMMM 322, 883 (2010).

## A model...

No obvious mechanism for exchange pinning from compensated surface (M=0).





The atomic-scale *Roughness* can create uncompensated spins (red)



M. Blamire and B. Hickey, Nature Mater. 5, 87 (2006).

J. Spray and U. Nowak, J. Phys. D 39, 4536 (2006).

## Another model (Irmy-Ma)...

**Domains** involving nonmagnetic surface sites.



U. Nowak et al PRB 66, 014430 (2002).

M. R. Fitzsimmons et al, PRB 77, 224406 (2008).

Ir-Mn (IrMn<sub>3</sub>) most popular AF material in spin valves.

 $IrMn_3 = fcc AuCu_3 crystal structure. Also: RhMn_3 and PtMn_3$ 

I. Tomeno et al J. Appl. Phys. 86, 3853 (1999).



**'T1'** ⇒ **2D** spin structure

Neutron diffraction on bulk single crystals.



Very large T<sub>N</sub>.

fcc lattice = ABC stacked triangular layers  $\perp <111>$
## **Ordered** IrMn<sub>3</sub>



Applied Physics: 'T1' spin structure (no mention of Kagomé).

E. Krén et al, Phys. Lets. 20, 331 (1966). I. Tomeno et al J. Appl. Phys. 86, 3853 (1999).

*Thin films of IrMn*<sub>3</sub> *form* <111> *planes.* 

### fcc Kagomé lattice = *ABC* stacked Kagomé layers ⊥ <111>



# Basic Physics: 'q=0' spin structure (no mention of 'T1').

A.B. Harris et al, PRB 45, 2899 (1992).

•2D Heisenberg model exhibits coplanar spin structure.

 Macroscopic spin degeneracy at T=0



FIG. 3. (Color online) Temperature dependence of the specific heat for a kagome lattice cluster with L=36. The horizontal arrow denotes the value  $C/N=\frac{11}{12}$ . The two vertical arrows indicate boundaries between three different regimes.

M. Zhitomirsky, PRB 78, 094423 (2008).

## Monte Carlo simulations of the (3D) fcc Kagomé lattice.

Heisenberg and XY Models with NN Exchange J Only.

V. Hemmati, M.L. Plumer, J.P. Whitehead, and B.W. Southern, PRB 86, 104419 (2012).



• Recall fcc = ABC stacked triangular layers with 12 NN<sup>s</sup>.

• Regular fcc AF with NN Heisenberg exchange shows first order transition to a collinear state.

## J ⇒ 4 NN in-plane + 2 NN above + 2 NN below



Ground State from simulations:

- Each layer has 'q=0 spin' structure.
- 120<sup>0</sup> between all 8 NNs.

### Monte Carlo simulations of the fcc Kagomé lattice. **Energy and Specific Heat.**

- Standard Metropolis MC.
- L layers of ABC stacked LxL Kagomé planes with PBC.
- L = 12, 18, 24, 30, 36, 60 with MCS =  $10^6 10^7$
- Cooling, Heating and Independent temperature runs.



 All three types of simulations yield equivalent results.

• For XY model, T<sub>N</sub> = 0.760 and appears to be strongly first order.

• For Heisenberg model,  $T_N = 0.476$  and could be first order.

## Monte Carlo simulations of the fcc Kagomé lattice. Order of the Transitions.



Energy Histograms near T<sub>N</sub>



30000 (b) -T=0.4760 Heisenberg<sup>(b)</sup> T=0.4763 25000 T=0.4766 20000 L=60. Counts 15000 10000 5000 n 1.028 1.038 1.048 1.058 1.018 - Energy

Indicate energy gap between disordered and ordered phases for *both* models. Inconclusive: Could be 2/3, or just close.

0.0001

1/L3

0.00015 0.0002

0.00005

0.6665 0.66648

0



Binder Heisenberg Energy

Cumulant near T<sub>N</sub>.

Heisenberg Energy.

**Discontinuity in** 

clearer at L=36.

**Heisenberg energy** 

## Monte Carlo simulations of the fcc Kagomé lattice. q=0 Order Parameter and Susceptibility.



•Heating runs start at T=0 from fully order q=0 state.

•Order Parameter and Susceptibility show strong dependence on simulation mode (heating, cooling or independent temperature) and fluctuates between values, in contrast with energy and specific heat.

•This feature is due to Kagomé-lattice spin degeneracies

### Monte Carlo simulations of the fcc Kagomé lattice. Spin Degeneracies.

Define 3 ferromagnetic sub-lattice magnetization vectors: black, blue red.



'q=0' magnetic structure  $\Rightarrow$  3 spins around each triangle at 120<sup>0</sup>

> In 2D, can switch direction of two of the sub-lattices vectors in a row (e.g., **black** ←→ red) with no change in energy.

In 3D, can switch direction of two of the sub-lattices vectors in a plane with no change in energy

### Monte Carlo simulations of the fcc Kagomé lattice. Spin Degeneracies.

Enumerate all possible switches for L=24 and determine size of groundstate sub-lattice moment:

$$M_{\eta} = \frac{\sqrt{\left(\frac{1}{4} L^3 - \frac{3}{2} n\right)^2 + \left(\frac{\sqrt{3}}{2} n\right)^2}}{\frac{3}{4} L^3}$$
$$L^3/8 \le n \le L/2$$



Three different MC *cooling* runs (different random initial configuration).



• One sub-lattice is always fully saturated.

• The other two randomly approach (T=0) predicted values.

### Monte Carlo simulations of the fcc Kagomé lattice. Add anisotropy

L. Szunyogh et al PRB 79, 020403 (2009)

$$H = -\frac{1}{2} \sum_{i \neq j} J_{ij} \vec{S}_i \vec{S}_j - \frac{K_{\text{eff}}}{2} \sum_i (\vec{S}_i \cdot \vec{n}_i)^2,$$

Effective local anisotropy axes (similar to spin-ice pyrochlore tetrahedrons).

Initial MC results show that anisotropy:

- removes degeneracy
- induces an out-of-plane ferromagnetic moment

-drives the transition to be continuous .



Mn moments are *not* aligned in the easy-axes directions for the coplanar T1 spin structure.

### **Relation to Exchange Pinning.**

**XRD, and DFT calculations of IrMn<sub>3</sub>/CO<sub>4</sub> and IrMn<sub>3</sub>/Fe<sub>4</sub> interface spin structures.** H. Takahashi et al, J. Appl. Phys. 110, 123920 (2011)

Interaction with ferromagnetic layer induces a net moment in surface Mn spins.



Mn moments rotate toward Co-moments Mn moments rotate away from Fe-moments

**Relation to exchange pinning?** 

# Phase transitions in the fcc Kagomé lattice

## **Summary and Conclusions**

• 3D fcc Kagomé lattice with NN exchange only shows LRO transitions of the 'q=0' type at  $T_N$ =0.760 J for the XY model and  $T_N$  = 0.476 J for the Heisenberg model.

- XY model  $\Rightarrow$  Strongly first order.
- Heisenberg model ⇒ Probably weakly first order.
- Mean field theory ⇒ Continuous transition in both cases.

• Spin degeneracies of the 2D model persist in the 3D case ⇒ Order-by-disorder?

### Future work:

- effects of anisotropy.
- thin films and surface effects
- add a ferromagnetic layer and dipole interactions.
- $\Rightarrow$  Exchange Pinning?



Fig. 5. Temperature dependences of magnetic susceptibility  $\chi$  and electrical resistivity  $\rho$  of the partially ordered (S=0.83) alloy compared with those of the disordered (S<0.08) alloy with x=0.256. Open circles indicate the cooling process.

## Magnetic recording, and phase transitions in the fcc Kagomé lattice: Collaborations and Support: Who's doing the work and who's paying for it.

- Vahid Hemmati (MSc graduate) Memorial University
- Jason Mercer (PhD student) Memorial University
- Martin Leblanc (PhD student) Memorial University
- · John Whitehead (professor) Memorial University
- Byron Southern (professor) University of Manitoba
- Johannes Van Ek (scientist) Western Digital Corporation

- •Natural Sciences and Engineering Council of Canada
- •Western Digital Corporation
- Canada Foundation for Innovation
- •Atlantic Centre of Excellence Network





## Anisotropy vs Exchange







Spin-Spin Angle (°) 

Angle between spins: No longer 120<sup>o</sup> coplanar

## **Micromagnetics:** Reader Efficiency vs Sensor Height.

#### **100% efficiency = full 180° rotation**



Present reader widths ~ 50 nm

#### **Maximum efficiency for Height/Width ~ 1/3**

#### Still True Today.

## Anisotropy Effect

- Anisotropy removes continuous degeneracy
- Adds its own 8-fold degeneracy
- Spins are no longer in-plane ferromagnetic component







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## 3D Kagome Energy, K<sub>eff</sub> > 0



## 3D fcc Kagome Linear Spin Wave Theory



• 2 equal (yellow) states

• 3D lifts  $\omega = 0$  state and splits other states

• 1  $\omega$  = 0 (blue) state

-Efforts ongoing to add anisotropy to spin wave theory

# **Grain Size Progression vs. Areal Density**



- ECC media structure was expected yield higher areal density capability by enabling smaller grain size in media.
- □ In practice, grain size has remained practically unchanged since PMR introduction.
- Instead, the trade-off of choice was to use ECC media to improve writability, maintain acceptable adjacent track erasure, and optimize transition parameter with utilization of higher Ku alloys and optimization of lateral exchange coupling through the various layers.

## Monte Carlo simulations of the fcc Kagomé lattice. Interlayer coupling J'.

J=1

#### **Specific Heat**





 $11/12 k_{B}^{2}$ ?



T<sub>N</sub> vs J'.



Trends are similar to other quasi 2D systems.

### **Monte Carlo simulations of the fcc Kagomé lattice.** V. HEMATTI, <u>M.L. PLUMER</u>, J.P. WHITEHEAD, Memorial University of Newfoundland, B.W. SOUTHERN, University of Manitoba

http://www.mun.ca/physics/ http://www.physics.umanitoba.ca/

31 hrs 40 mins / 2408.13 Km



### X-section and ABS view of an Integrated MR Head



## The Media: A model of granular recording media

**Cobalt Atoms**  $\Rightarrow$  **Hexagonal Crystal Structure**: *High Anisotropy* 





### Ferromagnets: Cannot ignore "magnetostatic" fields.

$$\vec{H}(\vec{r}) = -\int_{V} d\tau \frac{\vec{\nabla} \cdot \vec{M}(\vec{r}')(\vec{r} - \vec{r}')}{|\vec{r} - \vec{r}'|^{3}} + \int_{S} dA \frac{\hat{n}(\vec{r}') \cdot \vec{M}(\vec{r}')(\vec{r} - \vec{r}')}{|\vec{r} - \vec{r}'|^{3}}$$

Long range interaction ~  $1/r^3$ 

For grains of finite size, it's not just dipole-dipole

Increases computational demands.



Adjacent bar magnet lies anti-parallel

- Outside of bar M=0; H = B = stray field
- Inside of bar B = H + 4 π M<sub>r</sub>,
  'demagnetizing' field H opposes M





FIG. 8. Comparison of the experimental and calculation results for the net magnetic moments in the Mn-Ir/(Ni-Co, Co-Fe, Fe-Ni) bilayer system. The circle marks represent the experimental results. As the calculation results, the bcc structure (triangle marks) was employed for  $Co_3Fe_1$ ,  $Co_2Fe_2$ , and  $Co_1Fe_3$ , Fe<sub>4</sub>, and the fcc structure (square marks) was employed for the other compositions. This facilitated comparison with the results of the experimental analysis.



## It comes in other forms...

**Relevant for sputtered thin films.** 

1. Disordered IrMn<sub>3</sub>: 3Q SDW

Sakuma et al, JPSJ 69, 3072 (2000); PRB 67, 024420 (2003).

Fishman et al, PRB 61, 12159 (2000).







Fig. 1. Multiple-Q spin density wave structures in fcc lattice.