Experimental and Modeling Study of Thickness Dependence of Amorphous TbFeCo Magnetization

Xiaopu Li\textsuperscript{1}, Chung T. Ma\textsuperscript{1}, Dr. Howard Sheng\textsuperscript{2}, Dr. S. Joseph Poon\textsuperscript{1}

\textsuperscript{1}Department of Physics, University of Virginia
\textsuperscript{2}Department of Physics and Astronomy, George Mason University
Magnetic Materials and Applications

Compass “Si Nan”

Heat Assisted Magnetic Recording (Sánchez et al.)

Permanent magnet generator

Magnetic Random Access Memory

Electric Motor at Tesla Motors

Magnetic Skyrmion (Romming et al.)

11/11/2016
Ferrimagnetic Materials

- Multiple (Two) Sublattices
- Antiferromagnetic (AFM) Coupling
- Compensation \( (T_{\text{comp}}) \)
- Magnetic Oxides
  - e.g. ferrites \((\text{Fe}_3\text{O}_4)\) and garnets \((\text{YIG} = \text{Y}_3\text{Fe}_5\text{O}_{12})\)
- Magnetic Alloys
  - Rare-Earth Transition-Metal (RE-TM) alloys, e.g. GdFeCo, TbFeCo, TbSmFeCo
  - Compensated Heusler alloys, e.g. Mn\(_3\)Ga, MnPtGa

Ferrimagnetic RE-TM Alloys

- RE Sublattice: Gd, Tb, Sm
- TM Sublattice: Fe, Co
- AFM Coupling: RE-TM
- Features:
  - Tunable Compensation
  - Perpendicular Magnetic Anisotropy (PMA)
  - All-Optical Switching (AOS)
  - Skyrmion (GdFe, Lee et al.)

Experimental VSM Measurements of Saturation Magnetization ($M_S$) vs. Temperature of TbFeCo Thin Films

Thin films co-sputtered at 7 mtorr of Ar

- Tb at. 28%

Thin films single-sputtered at 1 mtorr of Ar

- Tb at. 26%
Classical Heisenberg Model

\[ \mathcal{H}(\mathbf{S}) = -\frac{1}{2} \sum_{i<j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i D_i (\mathbf{S}_i \cdot \mathbf{n}_i)^2 - \sum_i \mu_0 m_i \mathbf{S}_i \cdot \mathbf{H}_E - \frac{1}{2} \sum_{i \neq j} \frac{\mu_0 m_i m_j}{4 \pi R_{ij}^3} (3 (\mathbf{S}_i \cdot \mathbf{R}_{ij}) (\mathbf{S}_j \cdot \mathbf{R}_{ij}) - \mathbf{S}_i \cdot \mathbf{S}_j) \]

Amorphous Structure

a) Pseudo amorphous structure
b) Ab initio amorphous structure, e.g. from Prof. Sheng
Monte Carlo Metropolis Sampling and Parallel Tempering

1. Start with an arbitrary spin configuration $\alpha_k = \{S_1, S_2, ..., S_N\}$;
2. Generate a trial configuration $\alpha_{tr}$;
3. Calculate the energy $\mathcal{H}(\alpha_{tr})$ of the trial configuration;
4. If $\mathcal{H}(\alpha_{tr}) \leq \mathcal{H}(\alpha_k)$, accept by setting $\alpha_{k+1} = \alpha_{tr}$;
5. If $\mathcal{H}(\alpha_{tr}) > \mathcal{H}(\alpha_k)$, accept with relative probability
   \[ P = \exp\left( -\frac{\Delta\mathcal{H}}{k_BT} \right) \]
   Choose a uniform random number $r_j$ where $0 \leq r_j \leq 1$
   \[ \alpha_{k+1} = \begin{cases} 
   \alpha_{tr}, & \text{if } P \geq r_j \text{ (accept)} \\
   \alpha_k, & \text{if } P < r_j \text{ (reject)} 
   \end{cases} \]

For each Monte Carlo sweep (MCSWP), the steps from 1 to 5 are repeated for $N$ times, where $N$ is the total number of spins in the system.

Parallel tempering

\[ P[ (E_i, T_i) \rightarrow (E_{i+1}, T_{i+1}) ] = \min\left\{ 1, \exp\left[ \frac{(E_{i+1} - E_i)}{k_B} \left( \frac{1}{T_{i+1}} - \frac{1}{T_i} \right) \right] \right\} \]
Parallel Tempering for $M_S$ vs. $T$ of RE-TM

Ostler et al. PHYSICAL REVIEW B 84, 024407 (2011)
Atomistic Structure with Depth Profile of Tb-Fe Pair Ratio

Corresponds to thin films co-sputtered at 7 mtorr of Ar
Atomistic Structure with Depth Profile of Tb-Fe Pair Ratio

Corresponds to thin films single-sputtered at 1 mtorr of Ar
Modeling Thin Films of Different Thicknesses

Corresponds to thin films co-sputtered at 7 mtorr of Ar

Corresponds to thin films single-sputtered at 1 mtorr of Ar
Thickness Dependence of Compensation Temperature

Corresponds to thin films co-sputtered at 7 mtorr of Ar

Corresponds to thin films single-sputtered at 1 mtorr of Ar

11/11/2016
Summary

• Thickness dependence of ferrimagnetic compensation temperature has been shown experimentally by VSM measurements.

• Amorphous structure with depth profile of Tb-Fe pair ratio has been used in atomistic modeling. The simulation results are consistent to both sets of the samples prepared at different conditions.