From materials to circuits: Multiscale modeling of nano-magnetic switches

Avik Ghosh
ECE, Physics

Virginia NanOComputing (VINO)
http://www.ece.virginia.edu/vino

Y. Xie, J. Ma, K. Munira
W. Butler (UA), M. Stemanova, I. Rungger, S. Sanvito (Dublin)

DARPA / IBM / NSF-Genome / UVa Emerging Fund
Spin Torque market needs to navigate a complex phase space

- \( E_{	ext{diss}} \approx 1 \text{pJ} \)
- \( \tau \approx 100 \text{ ps} \)
- \( \text{WER} \approx 10^{-9} \)
- \( \Delta \approx 60 \)

- \( \text{TMR} \approx 200\% \)

- Material
- Device
- Ckt codesign

Retention failure (unintended flip) → increase \( \Delta \)
Write failure (failure to flip) → increase \( I \)
Decision failure (failure to read) → increase \( I \)
Read disturb (flip during read) → increase TMR

http://www.ief.u-psud.fr/~zhao/papers/2012/microreliable.pdf
Integrated Simulation Platform (NanoTCAD)

**Bandstructure Module**
- Atomistic DFT
- Semi-empirical tight-binding
- Continuum Effective Mass

**Transport Module**
- Non-equilibrium Green's function
- Modified Simmons equation

**Micromagnetic Module**
- LLG for single-domain magnets
- OOOMF/M3 multidomain solvers
- Langevin/Fokker Planck for WERs
Energy-delay-error codesign

\[ E_{\text{diss}} = IV\tau \]

\[ i = \frac{I}{I_c} \]

Error Curve (WER, \( \tau \))

Stochastic Model

Macrospin Model

Transport Model

Munira, Ghosh, Butler, IEEE TED 2012
Physics based compact models

1D Fokker Planck solution (Butler)

\[ I_c = \frac{(4qk_B T/\hbar)\alpha \Delta}{\eta(V)} \]

\[ \Delta = (H_K M_S - 4\pi M_S^2)\Omega \mu_0 / 2k_B T \]

\[ i = I/I_c \]

LLG (JZ Sun)

Modified Simmons model (Munira, Ghosh)

\[ WER = 1 - \exp \left[ \frac{-\pi^2 \Delta (i-1)/4}{ie^{2\alpha \gamma H_k (i-1)/(1+\alpha^2)} - 1} \right] \]

\[ J_0(V) = \left( \frac{q^2}{4\pi^2 \hbar d^2} \right) \left[ (\varphi - qV/2)e^{-2\sqrt{2m(\varphi - qV/2)d^2/\hbar^2}} - (\varphi + qV/2)e^{-2\sqrt{2m(\varphi + qV/2)d^2/\hbar^2}} \right] \]

\[ J_\sigma = \frac{16k_0 \beta^2}{(\beta^2 + k_0^2)} \left[ \frac{k_0^+ \cos^2(\theta/2)}{\beta^2 + k_0^+} + \frac{k_0^- \sin^2(\theta/2)}{\beta^2 + k_0^-} \right] \]

\[ J(V, \theta) = [J_{\uparrow}(V, \theta) + J_{\downarrow}(V, \theta)]J_0(V) \]

Munira, Ghosh, Butler, IEEE TED 2012
Compact Models for tradeoffs

(a) AP to P switching

(b) P to AP switching

Device to Device variations

Beyond simple models: DFT Atoms to Circuits

Geometry (DFT)

Transport (DFT/NEGF)

I-V
TMR

Switching

Torque

Write Error
(Stochastic LLG/Fokker Planck)

Write Error

SPICE

Fe/MgO/Fe

Xie, Munira, Rungger, Stemanova, Sanvito, Ghosh – Wiley 2016
Magnetic Contacts:
High-throughput materials Genome for Heuslers

Full Heusler L2₁ \((X₂YZ)\)

Half Heusler C\(_{1b}\) \((XYZ)\)

Inverse Heusler XA \((XYZ)\)

Tendency to form half-metals

Heusler Survey
- 576 L\(_2\)₁ (full) Heusler \(X₂YZ\).
- 405 XA (inverse) Heusler \(XXYZ\).
- 378 C\(_{1b}\) (half) Heusler XYZ
- \textbf{http://heusleralloys.mint.ua.edu} (DOS, bands, spin polarization, \(M_S\), Formation energy \(E_f\), …)

Co\(_2\)MnSi

Energy (eV)

DOS (/eV)
Select X and Y from transitional metals and Z from group III, IV or V

For each alloy, calculate $E(a)$ for multiple initial moment configurations (Ferro vs Ferri, e.g.)

Check against other binary and ternary phases to calculate hull distance energy

www.oqmd.org

Relaxation: Check for tetragonal distortion

Find minimum energy configuration

Calculate Magnetic moment Formation energy DOS, bands, etc.

Identify promising candidates to experimentalist
Materials Genome and Machine Learning

Hull distance for stability

47 HH with $\Delta E_{HD} < 0.1$ eV/atom

Competing Phases

Visualize formation energy

Charge Density Plot

Machine Learning/Classification Algos
New Half-metals discovered

1359 full, $\frac{1}{2}$ and inverse Heuslers studied.
50 HH stable (e.g. RhTiP, RuVAs, NiScAs)
Zero moment half-metals (e.g. MnCrAs)

$$M_{tot} = N_V - 18$$
Layered Heuslers: \( \frac{1}{2} \) metal + MA

\[ \text{Co}_2\text{MnAl} \quad \text{Co}_2\text{FeSi} \quad \text{Co}_2\text{MnAl-Co}_2\text{FeSi layered [111]} \]

21 with layering in [001], [110] and 8 layered in [111]

Multiple ways of layering, \(~50\%\) have PMA to defeat thin film demag
e.g. [111] \( \text{Co}_2\text{MnSi-CoTiSi} \) has \( H_k \sim 48 \text{ kOe} \)
Materials to Transport
Materials to transport with NEGF
Spin Symmetry filtering

\[ TMR \sim 2000\% \text{ (SIESTA)} \]
Oxygen vacancies reduce TMR

$s$ symmetry ($\Delta_1$ band)
Spin unpolarized
defect state at midgap

Depolarizes $\Delta_1$ band
at vacancy site

If vacancy near interface,
TMR plummets

Rungger/Sanvito
From read (TMR) to write (STT) with NEGF

Fe | MgO | Fe:

Co | MgO | Co:

FeCo | MgO | CoFe:

CoFe | MgO | FeCo:

Xie, Munira, Stemanova, Rungger, Sanvito, Ghosh 2014
Switching in $\text{Co}_{60}\text{Fe}_{20}\text{B}_{20}/\text{MgO}/\text{Co}_{60}\text{Fe}_{20}\text{B}_{20}$

For a pulse width of 10ns

(in-plane 70 nm x 250 nm x 2nm)

Switching from $\uparrow \downarrow$ to $\uparrow \uparrow$

Switching from $\uparrow \uparrow$ to $\uparrow \downarrow$

Munira/Ghosh/Soffa, Nanoel Dev Handbook 2013
Micromagnetism with LLG equation

\[ \mathbf{I} = 2\text{MA/cm}^2, \quad HK = 2000 \text{ Oe}, \quad MS = 500\text{emu/cc} \quad \alpha = 0.01 \]

\[ \mathbf{I} = 2\text{MA/cm}^2, \quad HK = 20000 \text{ Oe}, \quad MS = 500\text{emu/cc} \quad \alpha = 0.01 \]
Thermal Fluctuation (TF): blessing or curse?

- Curse for static thermal stability, $\Delta(=E/K_BT) > 60$ at room temperature

- Blessing for STT $\rightarrow$ TF kicks magnetization out of stagnation point (initial angle distribution)

- Torque $\sim \sin \Theta$
  $\uparrow$ temperature

- Sub-Volume Excitations

- Backflow

E. Chen, Intermag, 2010

- ↑ temperature
- ↑ static error

Munira/Ghosh
Fast numerical solution of error rates with FPE

\[
\frac{\partial \rho}{\partial t} = -\nabla \cdot (L \rho) + D \nabla^2 \rho
\]

\[L = L_{\text{prec}} + L_{\text{damp}} + L_{\text{STT}}\]

\[D : \text{diffusion coefficient}\]
STT switching error rate from FPE simulation

Fokker-Planck equation can simulate the thermal fluctuation and is computationally more efficient than solving stochastic equation.

Fokker-Planck and stochastic LLG gives the same result.

Near critical current switching in MTJ

Gajek, et al. APL 2012

Xie, Ghosh (unpublished)
STT switching for given WER in diff regions

\[ P = \exp \left\{ -\frac{\tau}{\tau_0} \exp[-\Delta(1 - i)^\beta] \right\} \]

\[ \tau_0 = \frac{1 + \alpha^2}{\alpha' \mu_0 H_K} \]

\( \beta \): geometry dependent, 2 for P-MTJ

No analytical solutions for \( i < 1 \). For \( i > 1 \), one can fit the exp data with \( i \gg 1 \) formula

\[ P = 1 - \exp \left[ -\frac{\pi^2}{4} \Delta \exp \left( -\frac{2\tau}{\tau_0} (i - 1) \right) \right] \]

Sun's approx

\[ P = 1 - \exp \left[ -\frac{\pi^2}{i} \Delta (i - 1) \exp \left( 2\tau \frac{i}{\tau_0} (i - 1) \right) - 1 \right] \]

Analytical 1D FPE


STT switching for given WER in diff regions
Summary

✓ Unified tool for materials to circuits
✓ Energy-delay-reliability co-design
✓ $\frac{1}{2}$ metals and layered $\frac{1}{2}$ metals for high performance contacts
✓ First principles torques, TMR including morphology
✓ Fast FPE solvers for error rates

Spicefy !!

Beyond STT: GSHE (Bi2Se3), Straintronics (Ni/PZT), VCMA, Domain Wall

Incoherent switching
This book is aimed at senior undergraduates, graduate students and researchers interested in quantitative understanding and modeling of nanomaterial and device physics. With the rapid slow-down of semiconductor scaling that drove information technology for decades, there is a pressing need to understand and model electron flow at its fundamental molecular limits. The purpose of this book is to enable such a deconstruction needed to design the next generation memory, logic, sensor and communication elements. Through numerous case studies and topical examples relating to emerging technology, this book connects 'top down' classical device physics taught in electrical engineering classes with 'bottom up' quantum and many-body transport physics taught in physics and chemistry. The book assumes no more than a nodding acquaintance with quantum mechanics, in addition to knowledge of freshman level mathematics. Segments of this book are useful as a textbook for a course in nano-electronics.

Avik Ghosh is Professor of Electrical and Computer Engineering and Professor of Physics at the University of Virginia. He is a Fellow of the Institute of Physics (IOP), senior member of the IEEE, and has received the IBM Faculty Award, the NSF CAREER Award, a best paper award from the Army Research Office, and UVA's All University Teaching Award.