Simulation of Magnetization Dynamics in Materials

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Outline

• Motivation
• Introduction to magnetization dynamics
• Method - Atomistic Spin Dynamics
• Case studies
  – Exchange-accelerated switching
  – Inertia-like switching scenarios
• Conclusions
Motivation

How can the storage density of magnetic media be increased further?

Can spin replace charge for more power efficient computing?
Magnetic data storage

Information stored by the magnetic configuration.

Bits are written by switching the magnetization

Controllable and local switching:
Stable magnetic configurations - Magnetic anisotropy
Spin based computing - Magnonics

Use magnetic excitations to store and process data
Spin currents without charge currents

Two types of non-equilibrium spin currents in solids.

- Conduction-electron spin current
- Spin-wave spin current
- Inverse spin-Hall effect

Y Kajiwara et al. *Nature* 464, 262

C. W. Sandweg et al., *PRL* 106, 216601 (2011)

Graphics: Alan Stonebraker
Important quantities

**Magnetic exchange energy:**
The cost in energy connected to changing the angle between magnetic moments.

**Magnetic anisotropy energy:**
The cost in energy related to rotating the magnetization.

Can have several different origins, and strengths:

- **Magnetocrystalline** anisotropy from the spin-orbit interaction (crystal and electronic structure)
- **Shape** anisotropy from electrostatic dipole-dipole interactions
- **Exchange bias** due to strong coupling between ferromagnetic and antiferromagnetic materials
The theoretical foundation

Density Functional Theory has proven to be a reliable tool for calculating materials properties. From the electron density, the total energy and related quantities can be calculated without experimental input.

\[ -\frac{\hbar^2}{2m} \nabla^2 + V_s(\vec{r}) \phi_i(\vec{r}) = \epsilon_i \phi_i(\vec{r}) \]

\[ n(\vec{r}) = \sum_{i}^{N} |\phi_i(\vec{r})|^2 \]

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Nobel prize in Chemistry - Walter Kohn 1998

Good description of the magnetic properties

What about dynamics and finite temperatures?
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Magnetization dynamics

Magnetic processes are present at a large variation of time scales

Current technologies are approaching the nano-regime
Scales of magnetization dynamics

**Device/Domain level**
Magnetization as \( m(r) \)
Above nanoseconds
Micromagnetic simulations

**Individual atomic moments**
Discrete moments
Nano - picoseconds
Atomistic spin dynamics

**Electronic level**
Magnetization as \( m(r) \)
Femtoseconds
Time Dependent DFT
Atomistic magnetization dynamics

Originally formulated for magnetization densities (continuous), the equation of motion for discrete magnetic moments can be described by the Landau-Lifshitz-Gilbert, LLG, equation:

\[
\frac{d\mathbf{m}_i}{dt} = -\gamma \mathbf{m}_i \times \mathbf{B}_i - \alpha \frac{\gamma}{m_i} \mathbf{m}_i \times (\mathbf{m}_i \times \mathbf{B}_i)
\]

Precession  Damping

\(\gamma\) gyromagnetic ratio
\(\alpha\) damping parameter
\(\mathbf{B}_i\) effective field (internal+external)

The switching time depends on the damping and the magnitude of the effective field!

\(\alpha\) is materials specific and typically small \(0.1 < \alpha < 0.001\)
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Atomistic spin dynamics method

Temperature can be included by means of Langevin dynamics: Add stochastic temperature dependent field $b_i$.

$$\frac{dm_i}{dt} = -\gamma m_i \times (B_i + b_i(T)) - \alpha \frac{\gamma}{m_i} m_i \times (m_i \times (B_i + b_i(T)))$$

The effective field can be calculated from the spin model $B_i = -\frac{\partial H}{\partial m_i}$

$$H_{iex} = -\frac{1}{2} \sum_{i \neq j} J_{ij} m_i \cdot m_j$$  
Heisenberg exchange

$$H_{DM} = -\frac{1}{2} \sum_{i \neq j} D_{ij} \cdot m_i \times m_j$$  
Dzyaloshinskii-Moriya exchange

$$H_{ani} = K \sum_i (m_i \cdot e_{ani})^2$$  
Uniaxial anisotropy

$$H_{ext} = -B_{ext} \cdot \sum_i m_i$$  
Applied magnetic field

$$H_{dd} = -\frac{1}{2} \sum_{i \neq j} Q_{ij}^{\mu\nu} m_i^\mu m_j^\nu$$  
Dipolar interactions (Long ranged!!)
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\mathcal{H}_{ani} &= K \sum_i \left( m_i \cdot e_{ani} \right)^2 & \text{Uniaxial anisotropy} \\
\mathcal{H}_{ext} &= -B_{ext} \cdot \sum_i m_i & \text{Applied magnetic field} \\
\mathcal{H}_{dd} &= -\frac{1}{2} \sum_{i \neq j} Q_{ij}^{\mu \nu} m_i^\mu m_j^\nu & \text{Dipolar interactions (Long ranged!!)}
\end{align*}
\]
Atomistic Spin Dynamics in action

Sample simulation:
Magnetization switching of a 400 nm Fe film with holes.

Simulation time: 1 ns.
Small simulation made on desktop machine.

B. Skubic, J. Hellsvik, L. Nordstrom, and O. Eriksson

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Computational efficiency

The Hamiltonian is localized. ~100 interactions / spin
Solving the stochastic LLG equations is computationally quite cheap. But the time steps are small. ~0.1 fs

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Parallelization performance

Test simulation: FeCo system with realistic interactions from DFT

Can get close to micrometer range for bulk systems!
Summary - so far

- Magnetization dynamics is of technological importance and offers many theoretical challenges.
- Data storage applications. Building on existing techniques.
- Possibility of using spin currents without charge currents. New paradigms for low energy computing.
- Atomistic spin dynamics is a viable tool for these studies.
- Efficient parallelization and supercomputers make bridging to experimental length scales possible.
- Method very useful for smaller systems as well.
Improving on switching times

Two apparent approaches

I) Change the applied field
   Perpendicular fields => precessional switching
   Currents instead of fields: Spin transfer torque

II) Use the internal fields

   Normally $B_{\text{int}} \gg B_{\text{appl}}$
   Take advantage of $B_{xc}, B_{ani}$.

Tailor the internal exchange fields:
   Artificial antiferromagnet
   Antiferromagnetically coupled spin valve.
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Artificial antiferromagnets

Magnetic heterostructures can have oscillatory interlayer exchange couplings. RKKY exchange

Well known example: \textbf{Fe/Cr/Fe}

Fe layers couple ferro or antiferromagnetically depending on Cr thickness

Most known for
Spin-dependent transport: \textbf{GMR}


Fert and Grünberg Nobel Prize 2007 for the GMR effect!
Exchange accelerated switching

Switch the two Fe layers simultaneously. Opposed field on each Fe layer, from applied current.

Seemingly "traditional" switching, i.e. applied field enters through the damping torques.

However, due to the antiferromagnetic interlayer couplings, internal field affects the dynamics.
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ASD simulations for 0 K.
Exchange parameters from DFT.
Applied field of 0.1T antiparallel to starting state.

Fe/Cr/Fe:

The switching is determined by the damping torque of the applied field and the \textit{precessional} torque from the \textit{internal} field.

Order of magnitude faster switching!

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Compare with bulk Fe:

Inertia-like switching dynamics

In the LLG equation, no acceleration term is present: **Lack of inertia.**

But an optically generated magnetic field pulse has been showed to switch the magnetic state of the canted antiferromagnetic compound HoFeO₃.

**Inertia-driven spin switching in antiferromagnets**

A. V. Kimel*, B. A. Ivanov², R. V. Pisarev³, P. A. Usachev³, A. Kirilyuk¹ and Th. Rasing¹

The explanation was that the antiferromagnetic order vector does have inertia.


Can this phenomenon be seen for other systems?
Is there an alternative explanation?

Time to revisit the artificial antiferromagnet Fe/Cr/Fe!
Inertia-like switching dynamics

Applied fields with varying time, strength, and direction was simulated for the Fe/Cr/Fe trilayer.

Now with added shape anisotropy (easy plane $K \sim 0.06$ mRy)

Response from a 5 picosecond pulse with $B=(3, 0, 5)$ T

The system evolves long after the pulse has stopped.
Inertia-like switching dynamics

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![Graph showing the response from a 5 picosecond pulse with $B = (3, 0, 5) T$.]

The system evolves long after the pulse has stopped.
Inertia-like switching dynamics

Why do the time evolution go on after the pulse?

The simplest explanation: **Redistribution of energy**
The pulse tilts the moments, increasing the internal exchange and anisotropy energies.
After the pulse, the system relaxes back to a low energy state.

**But the magnetization can switch.**
Inertia-like switching dynamics

The increased internal energy can be seen as the angle between the antiferromagnetic sublattices.

And what about ferromagnetic systems?

Considering a decoupled Fe layer with anisotropy.

Even here, a clear time evolution of the magnetization after the pulse is seen.

Conclusions

• Theory can help predicting and explaining novel magnetization switching processes

• In artificial antiferromagnets, like Fe/Cr/Fe trilayers, the antiferromagnetic exchange interactions can improve the switching speeds by an order of magnitude.

• Energy transfer and competing interactions can cause inertia-like behaviour of the magnetization in artificial antiferromagnets.
  – Possibility of switching even in the absence of the applied pulse.

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