Atomistic modeling of all-optical switchable magnetic materials

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PhD may follow: Yes

Summary :

The world of electronics is actively looking for smaller and compact components, which consume very little energy, capable of performing a huge number of operations. For the information storage and processing, magnetic materials based on rare earths and transition metals offer the possibility of manipulating information using laser pulses of a few femto seconds and thus aim at operating frequencies of the THz. This process of ultra-fast dynamics is the result of the combined action of several phenomena on magnetic moment carriers at the atomic scale. The purpose of the master proposal is to analyze by numerical modeling the process of the reversal of the magnetization according to the composition of the materials and their crystalline structure. For this, the Landau-Lifshitz-Gilbert equation that describes the dynamics of magnetic moments will be coupled to heat diffusion equations by involving electrons and phonons. This atomistic model will make it possible to understand the mechanisms of magnetic moment switching as well as to identify the most promising materials for their fabrication.

Full description :

The reversal of magnetization under the action of laser pulses was experimentally demonstrated in 2007 for amorphous thin layers of GdFeCo alloy [1]. Laser pulses circularly polarized of a few femto-seconds are sufficient to switch the magnetization of some rare-earth-transition metal compounds without the need to apply an additional magnetic field. The research activity around this remarkable property is very intense given the strong application potential targeting ultra-fast memory devices with very low consumption by integrating active parts all-optical switchable. The practical object is to combine a memory function (long-term information retention) with an ultra-fast write speed (~ THz). It is imperative to demonstrate that switching is deterministic and perfectly reproducible despite the multiple physical phenomena that are involved: exchange interaction, phono-electron coupling, photon-magnetization coupling. The success of the concept involves simultaneously experimental efforts and extensive modeling.

During this project, we propose to participate in the development of an adapted, efficient and powerful numerical model able to take into account several interactions to describe at the atomic scale the mechanisms of ultra-fast reversal of the magnetization. The formalism is based on the coupling between the dynamics of the magnetization and the ultra-fast heating induced by the laser pulse [2]. For each magnetic moment, composing the material, the phenomenological equation of Landau-Lifshitz-Gilbert motion will be numerically integrated taking into account the ultra-very fast variation of the local temperature during the duration of the laser pulse.

After a test / validation phase compared to the results reported in the literature, the model will be exploited for an in-depth analysis of the properties of new rare earth-transition metal compounds. The goal is twofold: to understand and master the mechanisms that drive the ultra-fast reversal in order to identify the best materials for the applications. The various material parameters necessary for a realistic modeling of a certain compound will be extracted from ab-initio calculations in connection with the theoretical team of Spintec. Confrontations with the experimental studies will be conducted in parallel with the MRAM team.

[1] C. Stanciu et al, Phys. Rev. Lett. 99, 047601 (2007).
[2] I. Radu et al., Nature 472, 205 (2011).

Requested skills :

condensed matter physics, nanosciences, basis in magnetism and programming