3.1 Publishable summary

3.1.1 Summary description

The FemtoSpin project has made rapid progress in a field of enormous scientific and technological importance. The scientific basis of the project is research in ultrafast magnetisation processes induced by the interaction of femtosecond laser light with magnetic materials. Experimentally, a light beam from a powerful-pulsed laser with a pulse width of around 50 femtoseconds is split into 2 beams. The first, high intensity (pump) beam is incident on the magnetic material, in the form of a thin film of thickness around 10nm, causing rapid heating. The second, low intensity (probe) beam is sent around a delay line, arriving at the sample with a controllable delay and used to measure the magnetisation of the film using a technique known as the Magneto-Optical Kerr or Faraday Effect. By means of such pump-probe experiments it has become possible to measure the magnetic response of a material on a timescale of tens of femtoseconds. This is a topic at the cutting edge of condensed matter and materials physics. In addition, for more detailed, element resolved, spin dynamics, similar experiments are done using femtosecond X-ray pulses that also give nanometer spatial resolution. FemtoSpin is predominantly aimed at developing models of the ultrafast magnetisation dynamics, but also has a core of leading experimental groups that provide validation as well as inspiration for the model development. The proven strong collaboration between the participants has led to a number of significant advances, including the explanation of the physical origin of a phenomenon known as Thermally Induced Magnetisation Switching (TIMS) in which magnetisation switching can be achieved by a heat pulse alone *in the absence of an applied field*. This astonishing result has triggered a major worldwide effort to provide a full understanding of the phenomenon and its translation into practical applications. The technical implications for information storage technology are extremely exciting, giving the possibility of increased data rates along with reduction of device complexity and power requirements.

The FemtoSpin project was carried out within a rapidly evolving industrial context. In terms of magnetic information storage, the drive to higher recording densities is based on Heat Assisted Magnetic Recording (HAMR), which uses laser pulses to heat the storage medium so as to allow reversal of the magnetisation. This relies on a combination of laser heating coupled with standard technology to generate a localised magnetic field to induce the magnetisation switching. Because of materials limitations, this field is limited in magnitude: a factor which will ultimately limit areal storage densities. Technologically, the complexity of manufacture of the write transducer is already slowing down the pace of development. The use of optical switching would remove the requirement for the inductive write transducer, significantly reducing both manufacturing costs and power requirements. At the same time, the field of spin electronics (or Spintronics), in which device functionality is dependent on the spin of the electron rather than simply the charge, is developing rapidly. Spintronics is a strong candidate to replace conventional electronics as this reaches its physical limitations. Again, optical reversal is a potential candidate for switching the magnetisation in spintronic devices.

3.1.2 Summary of objectives

- **Obtain fundamental knowledge of dynamic processes on the fs timescale;** this requires the development of new approaches to treat non-equilibrium electron dynamics, utilizing Density Functional Theory and applying these to understand the fundamental mechanisms underlying ultrafast spin dynamics.
- **Advanced atomistic models;** this includes spin models with equations of motion beyond Langevin dynamics; new approaches to induced spins and transport; integration of thermodynamic and quantum approaches

- **Mesoscopic model development**; this requires mesoscopic modelling using a generalised Landau-Lifshitz-Bloch (LLB) Equation; formulation for ferrimagnets and determination of LLB parameters from SDFT calculations and atomistic models.
- **Multiscale calculations and link to experiments**; verification of models against experiment; feedback from experiments to model development; material studies; large-scale calculations and device simulations.
- **Detailed materials studies;** candidate materials with especially promising properties on the femtosecond timescale will be investigated. This will encompass single-phase materials and alloys in addition to novel structured materials with engineered properties.

3.1.3 Work performed and major results achieved

The development of new technology based on opto-magnetic phenomena requires new models with a sufficiently strong physical basis. The models must be validated by comparison with state-of-the-art experiments. Within this background FemtoSpin has been highly successful, in particular in the following areas:

Multiscale model development. Optomagnetism is driven by the interaction between photons, conduction electrons, lattice vibrations and the atomic spins themselves. This is a complex problem involving the development and coupling of models on 3 fundamental lengthscales:
Electronic; theories of laser/spin interaction, predictions of important magnetic materials information. These have been investigated using Density Functional Theory (DFT) and analytical models, both for comparison with experiment and to link to atomistic models. Significant advances have been made in the understanding of the laser/spin interaction and in techniques for the determination of magnetic properties.
Atomistic models; using information from DFT, atomistic models introduce the thermodynamic aspects of the opto-magnetic phenomenon, allowing the heating effects of the laser pulse to be included.
Macrospin models; large scale simulations and device design rely on mesoscopic and continuum approaches based on macrospin models. Within FemtoSpin significant progress has been made in the development of macrospin models capable of simulating magnetic behaviour during the laser pulse. These models rely on input information from the atomistic approach to complete the multiscale formalism.
Model validation. The interaction between theoretical and experimental groups has been exemplary and has led to important model development and feedback to experiments.
Outputs

1. Calculations of specific materials design parameters enabling a Dutch patent (2008039). Patent process continuing in Europe (EP2795622 (A2)) and the United States (US2014368303).
2. Atomistic code (Vampire) on public release. Very good take-up by academia.
3. Preparing advanced optical and heat-assisted magnetic recording model (MARS) for public release.

Other Outputs

4. Publications; 70 papers in high impact journals including Nature journals (7) and Physical Review Letters (2) and Scientific Reports (3).
5. 68 invited papers at International conferences
6. Organisation of a summer school in Nijmegen
7. Initiation of the Ultrafast Magnetism Conference (Rasing, Chantrell with Bigot and Huebner; first edition in Strasbourg in 2013 and second in Nijmegen in 2015)

FemtoSpin has made a large impact in terms of generating the understanding of optomagnetic processes. The model development at all lengthscales has led to the production of a multiscale model chain taking magnetic parameters from ab-initio calculations into atomistic models which then provide parameterised information for macroscopic calculations. This process leads to macroscopic models with a strong physical basis for use in materials and device design. At the atomistic level we have developed the first approach taking into account the distinction between internal moments in Gd metal and studied the effects on the ultrafast dynamics. Atomistic model calculations also demonstrated the origin of the thermally assisted magnetisation reversal in the excitation of specific magnetic spin waves which transfer angular momentum between the transition metal and rare-earth sublattices leading to a transient ferromagnetic-like state which initiates the magnetisation reversal. This led to the prediction of a set of design rules for TIMS and the prediction of TIMS in synthetic ferrimagnets.

Scientific highlights

- Development of an ab-initio code for the calculation of the opto-magnetic field (i.e. the magnetization induced by circularly polarized laser light), on the basis of the derived quantum theory for the opto-magnetic field.
- A theoretical framework has been derived for demagnetization due to transfer of the spin of hot (laser-excited) electrons to the phonon system and the resulting demagnetization rates were ab-initio computed for 3d ferromagnets.
- Ultrafast demagnetization due to spin transport has been investigated and was shown to give rise to emission of THz radiation
- Understanding the TIMS phenomenon and its prediction in structured media
- Atomistic/ab-initio model of Gd – beyond the fixed spin model and successful validation by comparison with experiments.
- Studies of differential spin dynamics on FeNi. Full multi-scale modeling of the material and comparison with experiment.

Multiscaling and collaborative code development

- ab-initio determination of magnetic properties and parameterization of atomistic spin Hamiltonians (Budapest, Uppsala, Konstanz, York); automatic generation of spin model parameters for the Vampire atomistic code is almost complete.
- Macrospin simulations and atomistic testing/ parameterization (ICMM, Konstanz, York). This collaboration has produced a suite of models optimized for continuous and granular media. This collaboration has also developed a ferrimagnetic LLB equation for macrospin simulation.
- (ICMM, RU, York); atomistic and macrospin approaches have been combined to produce understanding of the dynamic behavior of ferrimagnetic materials during the thermally induced magnetization switching process.

Femtospin code development: public code release

- York atomistic code (Visual Atomistic Massively Parallel IntegRation Engine; VAMPIRE). On public release, Details available from vampire.york.ac.uk. Described in invited topical review; R. F. L. Evans, et. al., J. Phys.: Condens. Matter, 26, 103202 (2014) (23pp) *(selected as one of the highlights of 2014 in J. Phys.: Condens. Matter).* Code in trial use in industry

- MAgnetic Recording Simulator; MARS. Developed for advanced simulations of all-optical recording and HAMR in collaboration with Seagate/WD.

Future industrial prospects

Although technical difficulties remain to be overcome, Heat Assisted Magnetic Recording (HAMR) is closing in on providing the next generation of ultrahigh density recording systems. In May 2014 Seagate announced a 1.4Tbit/in^2 areal density demonstration (the first to exceed conventional recording demonstrations) having previously shown 1000 hours of continuous write (the benchmark requirement). However, HAMR densities will be limited by the available write field (around 1Tesla) using inductive technology, due to the requirement of avoiding errors due to thermally induced back switching. Due to the physical and technical understanding within the FemtoSpin project, all-optical recording must be considered a realistic candidate for progress beyond HAMR. Here it must be noted that all candidate technologies face similar problems of writing and stability at extreme densities, and the large effective fields involved in all-optical technology could give it a strong advantage. Equally important could be the removal of inductive technology from the writing process in magnetic recording, leading to very significant design and process simplifications with important implications for cost reductions and reduced environmental impacts; that latter also enhanced by significantly reduced energy cost per bit in the write process. This represents an important potential advance for European industrial potential, supporting the major production centre of Seagate in Northern Ireland which produces around 25% of the world-wide total output (around 1 billion p.a.) of recording heads; an important European industrial resource.

3.1.5 The address of the project public website

http://femtospin.eu/