Institution: University of York		
Unit of Assessment: 9 - Physics		
Title of case study: Atomic scale modelling of advanced magnetic materials and devices for industrial applications		
Period when the underpinning research was undertaken: 2008-2015		
Details of staff conducting the underpinning research from the submitting unit:		
Name(s):	**Role(s) (e.g. job title):**	**Period(s) employed by submitting HEI:**
Richard F L Evans Roy W Chantrell	Assistant Professor Professor	2008 - present 2004 - 2020
Period when the claimed impact occurred: 2016 - 2020		
Is this case study continued from a case study submitted in 2014? N		

1. Summary of the impact (indicative maximum 100 words)

Digital data storage is essential to modern life, storing exabytes of data including photos and videos that power cloud-based internet technologies such as Facebook and YouTube. Research at York has contributed to the development of next-generation storage technologies such as Heat-Assisted Magnetic Recording (HAMR) (Seagate), advanced media design (Advanced Storage Research Consortium), Magnetic Random Access Memory (MRAM) (Samsung Semiconductor, IMEC), and the development of new permanent magnetic materials (Toyota). This has been through the development of a new state-of-the-art software tool for simulating magnetic materials and devices at the atomic scale (VAMPIRE, https://vampire.york.ac.uk) and through research into magnetisation dynamics at elevated temperatures (HAMR). Partners state that York's contribution has been critical to the development of HAMR technology giving Seagate Technology a significant competitive advantage in a global market worth USD22 billion, and has led to savings in development time valued on the order of millions of Euro.

2. Underpinning research (indicative maximum 500 words)

Evans and Chantrell have developed atomistic and multiscale models of recording media and magnetic devices for the understanding of magnetisation structures and processes. Current magnetic recording technology is based on a scheme known as Perpendicular Magnetic Recording (PMR) due to the fact that information is stored with magnetisation perpendicular to the plane of the thin-film recording medium. The requirement for increasing storage density is to decrease the grain size of the recording medium whilst retaining thermal stability of written information. This is achieved by developing increasingly complex designs of recording medium on the nanoscale. HAMR is an entirely new technology based on the use of laser heating to temporarily lower the field required to reverse the magnetisation of the storage medium. This is an entirely new process of magnetic switching and a York atomistic model has been instrumental in developing an understanding of the underlying processes involved, including the discovery of a new and unexpected (so-called 'linear') reversal mechanism which plays a critical role.

Specifically in the underpinning research we:

1. Discovered the linear reversal mechanism [R1]. This is especially important since in linear reversal the magnetisation follows a path through zero, avoiding the slow precession over energy barriers. This is vital to reliable switching of the magnetisation when storing individual bits [R2].
2. Proved the necessity to heat through the Curie temperature for reliable recording [R2].
3. Explained the origin of dc noise – incorporated in the design of products shortly to come to market. [https://www.tomshardware.com/uk/news/seagate-20tb-hamr-hdd-2020]
4. Developed a theoretical model to drive the development of a susceptibility-based method to evaluate dispersions of Curie temperature (patented; [R3]).
5. Participated in the demonstration of 1.4 TBits/sq in with Invited paper at Intermag 2014 published as ref [R2], a new milestone in recording data density.
6. Carried out calculations using the kMC code to test magnet field profiles for fast and efficient demagnetisation of recording media [R4,R5], leading to optimised magnet design [R4].

The research is underpinned by the development of VAMPIRE [R6], a new state-of-the-art software package for atomistic modelling of magnetic materials. The package started development by Evans in 2009 and is a by-product of EU funded research

(ULTRAMAGNETRON and FEMTOSPIN). The package was the first massively parallel package of its kind enabling new kinds of simulations not previously possible. The initial version of the package was released as open source software in 2013 and has seen continual development over the years 2014-2020, evolving into the leading package of its kind in the world. The main VAMPIRE website has attracted over 210,000 page views since launch in 2013, and the user group has over 350 active members [E5]. The main methods paper [R6] has attracted over 425 citations (source: Google Scholar), and over 24,500 downloads (source: IOP) since publication in 2014. The technical capabilities of the VAMPIRE code focus on atomic scale modelling of high temperature magnetisation dynamics, material defects, interfaces and complex magnetic interactions such as 2-ion anisotropy and Dzyaloshinskii–Moriya interactions. These effects are critical to understanding the properties of nanoscale magnetic devices and the diversity and complexity of these devices has led to a rapid growth in the use of atomistic models.

3. References to the research (indicative maximum of six references) (York staff in bold)

[R1] Linear and elliptical magnetization reversal close to the Curie temperature, **N.Kazantseva, D. Hinzke, R. W. Chantrell** and **U. Nowak** Euro. Phys. Lett. 86 27006 (2009) (peer-reviewed publication), DOI: doi.org/10.1209/0295-5075/86/27006

[R2] High Density Heat-Assisted Magnetic Recording Media and Advanced Characterization—Progress and Challenges, Ganping Ju, *et al*, **Roy Chantrell**, and Jan-Ulrich Thiele, IEEE Trans. Mag., 51, 3201709 (2015) (peer-reviewed publication). DOI: doi.org/10.1109/TMAG.2015.2439690

[R3] Patent: US 9,103,729 B1 (2015), Method and apparatus for determining Curie temperature distribution of a sample of magnetic material. Ganping Ju, Jason L Pressesky, **Roy William Chantrell**, Xiaowei Wu, Xi Chen, Xiaobin Zhu and Yingguo Peng

[R4]. Hybrid design for advanced magnetic recording media: Combining exchange-coupled composite media with coupled granular continuous media. P. Chureemart, **R. F. L. Evans**, **R. W. Chantrell**, Pin-Wei Huang, Kangkang Wang, Ganping Ju, and J. Chureemart, Phys. Rev. Appl., 8, 024016 (2017) (peer-reviewed publication). DOI: doi.org/10.1103/PhysRevApplied.8.024016

[R5] First order reversal curves and intrinsic parameter determination for magnetic materials; limitations of hysteron-based approaches in correlated systems **Sergiu Ruta**, Ondrej Hovorka, Pin-Wei Huang, Kangkang Wang, Ganping Ju, and **Roy Chantrell**,
Sci. Rep., 7, 45218;DOI: 10.1038/srep45218 (2017) (peer-reviewed publication)

[R6] Atomistic spin model simulations of magnetic nanomaterials **R F L Evans, W J Fan, P Chureemart, T A Ostler, M O A Ellis and R W Chantrell** 2014 *J. Phys.: Condens. Matter* **26** 103202 (peer-reviewed publication, featured in JPCM Highlights of 2014). DOI: doi.org/10.1088/0953-8984/26/10/103202

4. Details of the impact (indicative maximum 750 words)

Prior to the York development of atomistic and multiscale modelling approaches, calculations of magnetisation structures and reversal mechanisms by industry invariably used a continuum formalism known as micromagnetics. The atomistic approach which we have developed is significantly more realistic in dealing with interfaces (for PMR media physics) and especially for spin dynamics at elevated temperatures (for HAMR physics) [R6]. The York VAMPIRE code has been adopted for device and materials design by several companies including Seagate Technology [E1], Western Digital, Samsung Semiconductor, Intel, and IMEC [E8], and has been integral in the development of the Advanced Storage Research Consortium, an industry consortium made up of key members of the magnetic storage sector. Its chairman writes: "Your contributions in the area of fundamental, first-principle magnetism, creating insight into the underlying atomistic and quantum mechanical origins of exchange, anisotropy, energy dissipation, spin polarization, thermally activated phenomena and much more, has been of the utmost benefit for us to be able to advance the understanding and deliver ever increasing capacity in our digital storage products." [E2]

Through a number of research projects with industry we identified a number of capability gaps in relating macroscopic magnetic properties to device performance. As part of these projects we developed new atomistic models of advanced magnetic materials (FePt multiscale atomistic and micromagnetic models, $Nd_2Fe_{14}B$, CoFeB/MgO) for application to industrial devices and technologies. To address these issues specifically we have included unique modelling capabilities into the code targeted for applications (HAMR simulations, spin transport, advanced materials) to enable industry-focussed research. This has enabled a new world-leading modelling capability that has contributed to the development of new technological devices such as digital data storage in hard disk drives, non-volatile memory technologies such as MRAM and new permanent magnets. Comments from a user survey on how the software has impacted their research include "*Vampire is important for my research. I use VAMPIRE for simulation of MTJs [Magnetic Tunnel Junctions] structure*" and "*In experiments we can only measure such things as the total magnetisation of our sample, and then we can theorize about how and why we get such a magnetisation. With VAMPIRE I can recreate the experiments and see exactly what is going on inside the system to confirm (or dismiss) our explanations. Furthermore, it is much easier to sweep parameters such as thickness or concentrations in Vampire than in experiments, which helps us to optimize our samples.*" [E6] User statistics for the VAMPIRE website [E6] indicates a significant reach, with over 200,000 unique page views in the period 1st Aug 2013-30th Dec 2020.

The software tools are used in-house for the design of proprietary materials and devices, and an indication of the impact is given by the European Materials Modelling Council: '*The ability to model recording head reliability is estimated to have saved 6 months in the development time of new HAMR technology and tens of millions of Euro in development costs.'* [E4] The VAMPIRE code was instrumental in providing fundamental understanding of these processes; for example Seagate have used the VAMPIRE code to model the recording process and to guide media design [E1]. Seagate's Senior Engineering Director comments: "The close collaboration with the York Computational Magnetism Group with our engineering team at Seagate has enabled us to gain a significant competitive advantage and we expect to be the first company in the world to release a HAMR product, expected in 2021" [E1]. Seagate expect to ship their first commercial HAMR drives in 2020: "We remain on track to begin shipping our first commercially available HAMR drives in late 2020 on 20TB capacities. HAMR technology will be the industry's path to achieving drive capacities of 30, 40, 50 terabytes and even higher", CEO, Seagate Technology" [E7]. HAMR hard disk drives will enable new growth of storage capacities over the next 10-20 years well above those achievable with the current perpendicular recording technology.

Magnetic Random Access Memory, or MRAM, is a new non-volatile memory technology which will significantly reduce energy usage in a huge range of computing and personal devices such as smartphones and tablets. The device scale is in the 5 – 30 nm size range and relies on an understanding of the fundamental device properties at the atomic level, including complex interfacial properties and defects. The VAMPIRE code is being used by SAMSUNG Semiconductor, IMEC [E8] and Intel to provide input to device modelling and design to accelerate the commercialisation of this technology. This development is dependent on ongoing research led by the York group in collaboration with industry into the fundamental thermodynamic properties of nanoscale MRAM devices.

Through a joint research project with Toyota Motor Corporation, we have developed atomistic models of permanent magnet materials. These models have guided the development of new reduced rare-earth content magnets that are to be commercialised in the next generation of hybrid cars built by Toyota. The York group is a key member of an industry-funded research consortium "Development of Magnetic Material Technology for High-efficiency Motors for Next-Generation Automobiles" that contributed to the development of advanced permanent magnets with reduced reliance on critical rare earth metals [E3].

The extensive modelling developments led by the York Computational Magnetism group, including the ongoing capability enhancement of the VAMPIRE code, are having a broad impact on the development of new magnetic technologies worldwide. "*The technical and scientific contributions of the York Computational Magnetism group have been instrumental in the design and optimisation of advanced recording media at Seagate, in particular for next generation heat assisted magnetic recording (HAMR) technology*" [E1] and the VAMPIRE package has been embedded in the R&D process of major MRAM device manufacturers "*The VAMPIRE software package has enabled a world leading and unique capability to model the properties of MRAM devices at the atomic level embedded into our research and development process*" [E8]. As part of the simulation team, we provide state-of-the-art models contributing to fundamental understanding that enables Toyota to develop next generation high performance permanent magnets, with worldwide applications in next-generation electric vehicles, motors and wind turbines [E3].

5. Sources to corroborate the impact (indicative maximum of 10 references)

[E1] Letter, Senior Engineering Director, Seagate Technology, USA
[E2] Letter, Advanced Storage Research Consortium (ASRC) Steering Committee Chair
[E3] Letter, Grand Master. Toyota Motor Corporation, Japan
[E4] Case study of the European Materials Modelling council. https://emmc.info/wp-content/uploads/2017/10/2016-02-12-Integrated-Recording-Model-for-Heat-Assisted-Magnetic-Recording-HAMR-seagate.pdf
[E5] User statistics for VAMPIRE package, collected from Google Analytics Web Data, 2021
[E6] User survey for VAMPIRE package, collected by R Evans, 2020
[E7] https://www.techradar.com/news/seagate-ships-18tb-hdds-but-breakthrough-hard-drives-will-arrive-later-this-year
[E8] Letter, Program Director, IMEC