A major driver of the global economy has been the continuous scaling of electronic devices to ever smaller dimensions. The microelectronics industry has used Moore's law for decades to provide new generations of faster and cheaper electronics to consumers (e.g. computers, cell phones, handheld devices). However, this push to smaller dimensions is now hitting key physical barriers that threaten to halt this progress. DRAM and SRAM memories face major challenges related to power dissipation and energy consumption, which grow worse at smaller scales. The continued scaling of Flash memory is also encountering significant barriers due to charge loss and fluctuation at small dimensions. The 2013 ITRS report notes that with float-gate devices, "there is a fundamental issue of non-scalability of tunnel oxide and interpoly dielectric" and that "this geometric limitation will severely challenge scaling far below 20 nm half pitch". These scaling problems have led several companies (Samsung, Toshiba, SanDisk, Intel- Micron, Hynix) to abandon further Flash device level scaling and instead focus on constructing 3D memory cell architectures.

To address these challenges the goal of the NVM conference was to bring together an international community of researchers from academia, government labs, and industry to discuss how atomistic simulations can help advance non-volatile memory research, and to help build greater bonds between industry and academia to inspire future research collaborations.

Programme:

The conference opened with a session entitled 'Current Memory Technology' which provided a broad overview and context for the following three days. The key note speaker, Rahul Sud traced the current challenges faced in the field of semi-conductor memory via the birth, evolution and impact of the semiconductor industry. He was followed Marco Bernasconi and Silvia Picozzi who addressed by key themes which would be discussed in more detail over the course of the three days - Phase Change Memory and Relativistic Ferroelectrics.

The second session examined Phase Change Memory, with talks from Riccardo Mazzarello, Tao Wang, and Riccardo Bertacco. The end of day one, and start of day two (sessions 3 and 4), looked at Resistive RAM with 13 presentations. This was the largest thematic cohort, and provided an indication of the breath and complexity of this field.

At the end of day one, the poster session which saw input from 13 participants, including PhD students from 9 different institutions across 4 countries. This provided space for reflection and deliberation on future research and the day's discussions. The final two sessions (sessions 4 and 5) addressed NRAM across 12 talks and covering novel NRAM properties, and range of papers addressing spin transfer torque RAM and perpendicular magnetic anisotropy.

To view the conference programme and abstract book please click here.

Conclusion:

The three-day workshop brought into clear focus the current challenges faced with traditional memory technologies (DRAM, SRAM, Flash) and the need for research to address these challenges; research that was highlighted throughout the three day conference. By bringing together international experts across academia cutting edge research to address future non-volatile memory were identified, examined and discussed, Including Resistive RAM (Oxide based RAM, Conductive Bridge, and Selector Technology), Phase Change Memory (A likely candidate for Intel-Micron's 3D

XPoint Technology) and Magnetic RAM (Spin Transfer Torque, Spin Orbit Torque), to positive responses from the participants. Evaluation of conference participants views on their expectations for the conference and aspects of the conference that they found most important indicated that networking and exchange of ideas was a key outcome. Also participants commended the range of topics, but also noted that there was sufficient specificity in particular areas to support depth of discussion, and provide impetus for future research. Importantly, all respondents said that they would recommend this conference to others in the field. The quotes below are indicative of the general sense of satisfaction amongst respondents to the evaluation:

It was beneficial to “meet professionals in our research area to exchange experience and exchange innovative ideas”; “the seminars were of very high level and I had the opportunity to discuss with colleagues on several topics of interest for my research activity”; “the quality of invited speakers was excellent”; “It helped me to get a broad perspective on the subject and to increase my knowledge on the matter. It also helped me to meet colleagues working on the same field.”

The NVM conference brought fifty researchers from academia and industry together for three days to discuss innovations in this fast moving field to very positive effect.

Plenary Session

Revolution in Semiconductor Memories --- and the radical transformation of semiconductor business models as Moore's Law ends

Rahul Sud
Silicon Capital

Invited Speakers

Atomistic Simulations of Phase Change Materials for Data Storage

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Chalcogenide compounds such as GeTe and GeSbTe alloys are attracting an increasing interest for their application in Phase Change Memories (PCM). This novel type of electronic non-volatile memory rests on a fast and reversible transformation between the crystalline and amorphous phase of a chalcogenide film due to Joule heating. The two phases corresponding to the two states of the memory can be discriminated because of their large difference in electronic conductivity.

PCMs are emerging as a leading contender for the realization of the so-called storage class memories that are sought to fill the performance gap between volatile DRAM and non-volatile Flash memories. Storage class memories are believed to usher in seminal changes in the memory and storage hierarchy for all computing platforms ranging up to high-performance computing.

In the last decade, atomistic simulations based on density functional theory (DFT) have provided useful insights on the properties of chalcogenide alloys of interest for PCMs [1]. Still, large simulation cells and long simulation times beyond the reach of DFT simulations are needed to address several key issues of relevance for PCM operation. To overcome these limitations, we have developed an interatomic potential for the prototypical phase change compound GeTe by fitting a large DFT database with a neural network (NN) scheme. Large scale (10^4 atoms) NN simulations allowed us to get insights on the thermal transport and on microscopic origin of the high crystallization speed of these materials [2].

In this talk, I will present the results of NN simulations on the kinetics of homogeneous and heterogeneous crystallization of GeTe and on the structural relaxations leading to the aging of the amorphous phase and to a drift in the electronic resistance [3] which is a particularly critical issue for PCM operation.

REFERENCES

[1] S. Caravati, M. Bernasconi, M. Krack, T. Kuehne, M. Parrinello, Appl. Phys. Lett. 91, 171906 (2007); Lencer et al., Adv. Mat. 23, 2030 (2011).

[2] G. C. Sosso, G. Miceli, S. Caravati, J. Behler, M. Bernasconi, J. Phys. Chem. Lett. 4, 4241 (2013); J. Phys. Chem. C 119, 6428 (2015); J. Phys. Chem. B 118, 13621 (2014); Phys. Rev. B 86, 104301 (2012); ibidem 85, 174103 (2012); Physica Status Solidi **A** 213, 329 (2016).

[3] S. Gabardi, S. Caravati, G.C. Sosso, J. Behler, and M. Bernasconi, Phys. Rev. B 92, 054201 (2015).

Relativistic Ferroelectrics: a novel class of multifunctional materials

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The discovery of novel properties, effects or microscopic mechanisms in modern materials science is often driven by the quest for the coexistence and/or coupling of several functional properties into a single compound. Within this framework, by exploiting the interplay between spin and dipolar degrees of freedom via spin-orbit coupling in ferroelectric semiconductors, I will focus on the tight link between k-dependent spin-splitting in the electronic structure, spin-texture and electric polarization. Based on density functional simulations, I will show our theoretical predictions of a giant Rashba spin-splitting in "bulk" crystalline GeTe[1], prototype of novel multifunctional materials - labeled as Ferro-Electric Rashba Semi-Conductors (FERSC)[2] - where the chirality of the spin texture is one-to-one linked to polarization. As the latter can be induced/controlled/switched via an electric field in a non-volatile way, the integration of spin-orbitronics with ferroelectricity is envisaged.

REFERENCES

[1] D. Di Sante, P. Barone, R. Bertacco and S. Picozzi, *Electric Control of the Giant Rashba Effect in bulk GeTe*, Adv. Mater. **25**, 509 (2013); M. Liebmann et al, *Giant Rashba-type Spin Splitting in Ferroelectric GeTe(111)*, Adv. Mater. **28**, 560 (2016)

[2] S. Picozzi, *Ferroelectric Rashba Semiconductors: a novel class of multifunctional materials,* Front. Physics **2**, 10 (2014)

Simulation and Modelling of the Switching Dynamics in Electrochemical Metallization and Valence Change Memory Cells

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Resistive switching devices based on the valence change mechanism (VCM) or the electrochemical mechanism (ECM) have attracted great attention due to their potential use in future non-volatile memories. Both types of cells exhibit a bipolar operation principle: The cells can be set from a high resistive state (HRS) to a low resistive state (LRS) with one voltage polarity and reset back to the HRS by applying the opposite voltage polarity. To understand the dynamics of these devices and identify the relevant processes on the atomic scale, device modelling on the continuum and atomic scale is required. Continuum methods are applied to simulate the dynamic device behaviour, whereas atomic models give further insight into specific processes on the atomic scale and can thus serve as input for the continuum models. In this contribution, continuum and atomistic models for resistive switching will be presented.

First, I will discuss the dynamics of the switching in ECM cells on the continuum scale. Using compact models it will be shown that the switching kinetics are limited by electron-transfer reactions, ion migration and electro-crystallization [1, 2]. The RESET process is also influenced by the nature of the electronic contact in the LRS. This can be either a tunneling gap or a galvanic contact, which is characterized by quantized conduction effects [3]. In the case of a galvanic contact, the RESET process is rather gradual and can be best explained by thermally-assisted self-dissolution of the conductive filament [4]. Furthermore, atomistic kinetic Monte-Carlo simulations will be presented that demonstrate how mechanical stress influences the filamentary growth [5].

In the second part, I will focus on the switching dynamics of VCM devices. The typical *I-V* characteristics will be discussed, including the nature of the abrupt SET and gradual RESET behaviour [6]. The switching relies on the redistribution of mobile donors such as oxygen vacancies or cation interstitials. The SET process is characterized by an abrupt current increase, which is caused by a positive feedback between current increase, Joule heating and acceleration of the ion motion. In contrast, the RESET process is rather gradual. This behaviour is explained in terms of ionic drift and diffusion processes approaching equilibrium [7]. Furthermore, the opportunities of atomic scale modelling with respect of ion hopping transport [8], electron conduction mechanism and redox reactions will be discussed.

REFERENCES

. [1] S. Menzel, S. Tappertzhofen, R. Waser, and I. Valov, “Switching Kinetics of Electrochemical Metallization Memory Cells,” *PCCP*, vol. 15, pp. 6945-6952, 2013.

. [2] J. van den Hurk, S. Menzel, R. Waser, and I. Valov, “Processes and Limitations during Filament Formation and Dissolution in GeSx-based ReRAM memory cells,” *J. Phys. Chem. C*, vol. 119, pp. 18678-18685, 2015.

. [3] S. Tappertzhofen, E. Linn, S. Menzel, A. J. Kenyon, R. Waser, and I. Valov, “Modeling of Quantized Conductance Effects in Electrochemical Metallization Cells,” *IEEE Trans. Nanotechnol.*, vol. 14, pp. 505-512, 2015.

. [4] S. Menzel, N. Adler, J. van den Hurk, S. Tappertzhofen, I. Valov, and R. Waser, “Simulation of polarity independent RESET in electrochemical metallization memory cells,” *2013 5th Ieee International Memory Workshop (imw)*, vol., pp. 92-95, 2013.

Atomic disorder - intrinsic source of variability in RRAM materials

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Resistive RAM devices can be scaled down below 10 nm [1], meaning that the discrete nature of atomic structure of the materials may already be observed in device operation properties. Based on First-principles Density Functional Theory simulations of RRAM materials for solid electrolyte or selector function, we show that atomic disorder of amorphous state (state of the filament) can exhibit large variability in terms of defect stability and kinetic barriers.[2] These have a great impact on filament resistance evolution in time – during forming the filament, shortly after (filament relaxation) or long time retention of the filament resistance.

REFERENCES

[1] B. Govoreanu et al., Ext. Abstr. SSDM Conf.,Nagoya, Japan, 1005 (2011)

[2] S. Clima et al., Electron Device Lett 36, 769 (2015)

First principles simulations of doping effects on RRAM forming and switching characteristics

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Simulating Oxygen Vacancies in TMOs for Resistive Switching Applications

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Resistive Switching of transition metal oxides relies on the re-orientation of oxygen vacancies within the metal-oxide. The behavior of these oxides can be simulated by various finite element techniques and compact modeling that allow to gain further insights into the fundamental processes that determine the resistive switching effect.
In order to realize and design new memory devices the industry relies on behavioural models of the memory cell. Key aspects to describe these memory cells are still debated. For example, a comprehensive charge transport expression that correlates defect density and conductivity is still missing (1), (2). The models for setting and resetting the cell are largely dependent on migration of anionic defects or anions as well as thermal effects (3), (4) as well as charge trapping effects (5).
While the nature of the oxygen vacancy migration can be described very well by utilizing Nernst-Planck equations and treating the vacancy as an ion; the question remains, how can a void in an ionic solid depict the properties of an actual ion. For this case, DFT simulations should enable to take a closer look at the properties of oxygen vacancies.
In this presentation I'm going to present some the modelling techniques used by the industry to predict the cell behaviour and their short comings as well as important aspects that still need to be addressed to make this technology a candidate for future memory applications. Moreover, I will show some results from DFT calculations to characterize the properties of the oxygen vacancy in the metal oxide to shed some light on the nature of the migration of the vacancy in an electric field.

REFERENCES

1. Chiu, F.-C. A Review on Conduction Mechanisms in Dielectric Films. *Adv. Mater. Sci. Eng.* **2014,** 1–18 (2014).
2. Park, S., Magyari-köpe, B. & Nishi, Y. Impact of Oxygen Vacancy Ordering on the Formation of a Conductive Filament in TiO 2 for Resistive Switching Memory. **32,** 2010–2012 (2011).
3. Waser, R., Dittmann, R., Staikov, G. & Szot, K. Redox-Based Resistive Switching Memories - Nanoionic Mechanisms, Prospects, and Challenges. *Adv. Mater.* **21,** 2632–2663 (2009).
4. Larentis, S. *et al.* Resistive Switching by Voltage-Driven Ion Migration in Bipolar RRAM — Part II : Modeling. **59,** 2468–2475 (2012).
5. Yang, M. Y. *et al.* Charge-dependent oxygen vacancy diffusion in Al2O3-based resistive-random-access-memories. *Appl. Phys. Lett.* **103,** 093504 (2013).

Non-equilibrium transport theory from single molecules to nanoelectronics devices: examples of non-volatile memory cells

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Non-equilibrium transport theory has been most well developed and tested in the community for the precise measurement science. The self-consistent theory for electric and phonon currents including the coupling between them describes local heating, heat generation and heat dissipation phenomena accompanying electric conduction [1]. Scanning tunneling microscope (STM) break junction measurements testified that the self-consistent theory is accurately working. While the first principle non-equilibrium Green's function (NEGF) method is capable to make quantitative prediction of the electric conductance and the thermopower for small molecule in the ballistic regime [2], the theory explains the temperature dependences of them for long molecules in the hopping region qualitatively, [3,4] thanks to the improved low energy physics description. Recently, the theory has been extended for the problem of the current noise [5] and the group of ETH applied the theory to the heating problem of the gate-all-around field effect transistor [6]. In some cases of non-volatile memories such like the resistive random access memory (ReRAM) and the interfacial phase change memory (iPCM), the memory switch ON/OFF is associated with the current induced atomic move [7, 8]. In this workshop, we will focus our attention to this problem in the context of our project for the incorporation of the theory into the first principle order-N method based NEGF [9] that is capable to handle devices up to the μm channel length. Especially, we will put our focus on our present application results on the ReRAM.

REFERENCES

[1] Y. Asai, *Theory of local heating in single molecular bridge junctions*, Phys. Rev. B 84, 085436 (2011).

[2] S. K. Lee, M. Bürkle, R. Yamada, Y. Asai and H. Tada, *Thermoelectricity at the molecular scale: a large Seebeck effect in endohedral metallofullerenes*, Nanoscale, 7, 20497 (2015).

[3] S. K. Lee, R. Yamada, S. Tanaka, G. S. Chang, Y. Asai, and H. Tada, *Universal Temperature Crossover Behavior of Electrical Conductance in a Single Oligothiophene Molecular Wire*, ACS Nano, 6, 5078-5082 (2012).

[4] Y. Li, L. Xiang, J. L. Palma, Y. Asai and N. J. Tao, *Thermoelectric effect and its dependence on molecular length and sequence in single DNA molecules*, Nature Communications, 7, 11294 (2016).

[5] Y. Asai, *Vibronic spectroscopy using current noise*, Phys. Rev. B 91, 161402 (R) (2015).

[6] R. Rhyner and M. Luisier, *Minimizing Self-heating and heat dissipation in ultrascaled nanowire transistors*, Nano Letters, 16, 1022 (2016).

[7] X. Zhong, I. Rungger, P. Zapol, H. Nakamura, Y. Asai and O. Heinonen, *The effect of a Ta oxygen scavenger layer on HfO2-based resistive switching behavior: thermodynamic stability, electronic structure, and low-bias transport*, Phys. Chem. Chem. Phys. 18, 7502 (2016).

[8] H. Nakamura and Y. Asai, *Competitive effects of oxygen vacancy formation and interfacial oxidation on an ultra-thin HfO2-based resistive switching memory: beyond filament and charge hopping models*, Phys. Chem. Chem. Phys. 18, 8820 (2016).

[9] M. Bürkle and Y. Asai, poster presentation in this NVM Psi-k workshop.

Forming processes of OxRRAMs

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Electron Injection Facilitated Defect Creation in Amorphous Oxides

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Electroforming in resistive random access memory (RRAM) cells employing amorphous silica and hafnia films results from application of high bias and is often accompanied by electron injection. In these systems, the nature of electron trapping sites is important for understanding the mechanisms of electrical breakdown and resistance switching. Extra electrons are usually trapped at defect sites, such as oxygen vacancies and impurities. Our DFT calculations performed using CP2K show that intrinsic precursor sites in amorphous network also can accommodate up to two extra electrons due to polaronic relaxation [1,2]. Trapped electrons are shown to weaken the corresponding Me-O bonds resulting in an efficient bond breaking pathway for producing neutral O vacancies and charged O interstitials characterized by low activation energies [1,2]. Newly generated O ions are shown to migrate rapidly through the oxide with a barrier of about 0.3 eV to the positive electrode while O vacancies remain behind [3]. Finally, we discuss how the defect creation is related to the concentration of pre-existing vacancies in the system. Our results rule out simple vacancy diffusion and spontaneous Si-O bond breaking as the source of Frenkel defects in pristine, neutral a-SiO_2 as the activation energies required for these processes are very high (3-4 eV). Combining these findings we propose a mechanism for electron injection facilitated defect formation in a-SiO_2 and HfO_2. These results are discussed in the context of experimental data on time to dielectric breakdown and conductive filament formation in RRAM devices.

REFERENCES

[1] S. R. Bradley, A. L. Shluger, and G. Bersuker, *Electron-Injection-Assisted Generation of Oxygen Vacancies in Monoclinic HfO_2*, Phys. Rev. Applied **4**, 064008 (2015).

[2] D. Z.Gao, A.-M. El-Sayed, and A. L. Shluger, *Mechanism of creation of Frenkel defects facilitated by electron injection in amorphous SiO_2,* (Submitted).

[3] A. Mehonic, M. Buckwell, L. Montesi, M. S. Munde, D. Z. Gao, S. Hudziak, R. J. Chater, S. Fearn, D. McPhail, M. Bosman, A. L. Shluger, and A. J. Kenyon, *Nanoscale transformations in metastable amorphous silicon-rich silica*, Advanced Materials (Accepted)

Multiscale modeling of electron-ion interactions for engineering novel electronic devices and materials

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In this work we will present a multiscale simulation platform modeling the microscopic interactions and chemical reactions (e.g. bond breaking) between electrons and atomic species (ions, vacancies, dangling bonds). The simulation platform connects the microscopic properties of materials (including atomic defects and interfaces) to the electrical behavior of the device, representing a virtual space for the design of novel electron device concepts purposely exploiting the atom-electron interactions.
Among the wide number of applications that can be potentially targeted, in this presentation we will show how to use this simulation-platform to design ReRAM devices and selectors based on binary/ternary oxides (HfO_2, Al_2O_3, TiO_2, ..).

Ab-initio Insight into Vacancy Formation and Diffusion in Resistive RAM Oxides

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Extended horizons: true atomistic simulations of junctions, interfaces and surfaces

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Ferroelectric tunnel junctions: Mechanisms for the tunneling electroresistance effect

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Ferroelectric materials are characterized by a spontaneous electric polarization switchable by an applied electric field, which makes them attractive for application in non-volatile memory devices. Recent developments in thin-film ferroelectricity have demonstrated the possibility of achieving a stable and switchable ferroelectric polarization in nanometer-thick films. This discovery opened up the possibility of using thin-film ferroelectrics as barriers in tunnel junctions, where a bi-stable ferroelectric polarization allows toggling the amplitude of the tunneling current across the junction [1,2]. Contrary to ferroelectric capacitors where leakage currents are detrimental to the device performance, the conductance of a ferroelectric tunnel junction (FTJ) is the functional characteristic of the device, thus providing a conceptually new approach for non-volatile memories based on ferroelectrics [3]. The signature property of a FTJ is the tunneling electroresistance (TER) effect – a sizable change in resistance of the junction upon the reversal of the electric polarization of the ferroelectric barrier. Large values of TER are favorable for device application of FTJs, and thus understanding the physical mechanisms responsible for TER is critical.

This talk will review our current understanding of the mechanisms controlling the tunneling electroresistance effect in ferroelectric tunnel junctions [4]. Starting from simple models for TER based on modulation of barrier height [5], we will address more intricate physical mechanisms responsible for this behavior, as revealed from density-functional calculations of the electronic, magnetic and transport properties of FTJs [4]. In particular, we will discuss the effects of interface termination [6], the Schottky barrier and barrier metallization producing TER [7]. For FTJs with magnetic electrodes we show that the interplay between ferroelectricity and magnetism can lead to a switchable magnetic phase transition at the interface resulting in a large TER effect [8]. We will discuss these mechanisms in some detail providing links between theoretical modeling and experimental results where appropriate.

REFERENCES

1. E. Y. Tsymbal and H. Kohlstedt, *Tunneling across a ferroelectric*, Science **313**, 181 (2006).
2. E. Y. Tsymbal, A. Gruverman, V. Garcia, M. Bibes and A. Barthélémy, *Ferroelectric and multiferroic tunnel junctions*, MRS Bulletin **37**, 138 (2012).
3. E. Y. Tsymbal and A. Gruverman, *Ferroelectric tunnel junctions: Beyond the barrier*, Nature Materials **12**, 602 (2013).
4. J. P. Velev, J. D. Burton, M. Y. Zhuravlev and E. Y. Tsymbal, *Predictive modeling of ferroelectric tunnel junctions*, npj Computational Materials (2016), in press.
5. M. Y. Zhuravlev, R. F. Sabirianov, S. S. Jaswal, and E. Y. Tsymbal, *Giant electroresistance in ferroelectric tunnel junctions*, Physical Review Letters **94**, 246802 (2005).
6. J. P. Velev, C.-G. Duan, J. D. Burton, A. Smogunov, M.K. Niranjan, E. Tosatti, S. S. Jaswal and E. Y. Tsymbal, *Magnetic tunnel junctions with ferroelectric barriers: Prediction of four resistance states from first-principles*, Nano Letters **9**, 427 (2009).
7. X. Liu, J. D. Burton and E. Y. Tsymbal, *Enhanced tunneling electroresistance in ferroelectric tunnel junctions due to reversible metallization of barrier*, Physical Review Letters **116**, 197602 (2016).
8. J. D. Burton and E. Y. Tsymbal, *A giant tunneling electroresistance effect driven by electrically controlled spin valve at a complex oxide interface*, Physical Review Letters **106**, 157203 (2011).

Contributions of impurities and surfaces to the device design

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The development of novel materials for the design of memory storage devices shows an enormously large number of degrees of freedom. In my talk I will focus on the spin-dependent transport properties of systems influenced by impurities and surfaces. The main mechanism I will discuss is the spin Hall effect enabling the creation of pure spin currents in nominally non magnetic materials.

In the first part I will introduce the mechanisms leading to the effect driven by spin-orbit coupling. Generally, it is classed into two distinct contributions: the intrinsic, bandstructure driven, and the extrinsic, scattering induced, mechanism. I will put it into relation to similar effects such as the anomalous Hall, Spin Nernst[1], and Edelstein effect all similar in their microscopic origin.

In the following I will introduce our numerical tool which is based on a multiple-scattering Greens function method solving the electronic structure of the impurity and surface problem fully relativistically. The electronic transport is solved exploiting the Boltzmann equation providing microscopic insight into the various mechanisms, separating intrinsic and extrinsic contributions.[2] However, I will carefully compare our results to methods exploiting the Kubo formalism as well as putting them in relation to experimental observations.[3]

In the final part of my talk I will present material specific calculations which lead to predictions of material systems to maximise the effect.[4] In combination with our calculations for thin films[5] it enables us to identify conditions to enhance the effect in various circumstances. These results are supported, at least partially, by experimental evidence.[6] Finally, I will contrast the material specific transport parameters with our calculations for the spin relaxation time.[7] This quantity is crucial for the integration of materials in devices since it defines the life time of the transported spins as well as the spin injection and absorption efficiency at interfaces which is essential for future applications.

REFERENCES

[1] K. Tauber, M. Gradhand, D.V. Fedorov, I. Mertig; *Extrinsic spin Nernst effect from first principles*; Phys. Rev. Lett. **109**; 026601 (2012)
[2] M. Gradhand, DV. Fedorov, P.Zahn, and I. Mertig; *Extrinsic spin Hall effect from first principles*; Phys. Rev. Lett. **104**, 186403 (2010)
[3] K. Chadova, D. V. Fedorov, C. Herschbach, M. Gradhand, I. Mertig, D. Kdderitzsch, and H. Ebert, *Separation of the individual contributions to the spin Hall effect in dilute alloys within the first-principles Kubo-Steda approach*, Phys. Rev. B **92**, 045120 (2015)
[4] M. Gradhand, D.V. Fedorov, P. Zahn, I. Mertig, Y. Otani, Y. Niimi, L. Vila, A. Fert; *Perfect alloys for spin Hall current induced magnetization switching*, Spin **2**; 1250010 (2012)
[5] C. Herschbach, D. V. Fedorov, M. Gradhand, and I. *Mertig, Colossal spin Hall effect in ultrathin metallic films*, Phys. Rev. B **90**, 180406(R) (2014)
[6] Y. Niimi, Y. Kawanishi, D. H. Wei, C. Deranlot, H. X. Yang, M. Chshiev, T. Valet, A. Fert, and Y. Otani, *Giant Spin Hall Effect Induced by Skew Scattering from Bismuth Impurities inside Thin Film CuBi Alloys*, Phys. Rev. Lett. **109**, 156602 (2012)
[7] M. Gradhand, DV. Fedorov, P.Zahn, and I. Mertig; *Spin Hall angle versus spin diffusion length: Tailored by impurities*; Phys. Rev. B, **81**, 245109 (2010)

Mechanisms of perpendicular magnetic anisotropy and Dzyaloshinskii-Moriya interaction in magnetic layered structures

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Spin-orbit coupling based phenomena such as perpendicular magnetic anisotropy (PMA) and Dzyaloshinskii-Moriya interaction (DMI) at interfaces between ferromagnetic (FM) metal and nonmagnetic (NM) insulator or metal have been an object of increased interest for spintronics including spin orbitronics in a view of ultra-dense information storage and spintronic devices such as MRAM. In this talk mechanisms responsible for PMA and DMI are elucidated from first-principles for Co(Fe)|MgO and Co|Pt interfaces, respectively.

First, the nature of PMA control at Fe|MgO interfaces is unveiled by evaluating the orbital and layer resolved contributions to magnetic anisotropy in Fe/MgO interfaces and MTJs with different interfacial conditions [1,2]. Mechanisms of the optimisation of the effective anisotropy as well as of its electric field control are discussed [3,4].

Next, the main features and microscopic mechanisms of DMI behavior in Co/Pt bilayers are clarified by analyzing DMI and corresponding spin-orbit energy distributions across the structure [5]. The thickness dependencies as well as the impact of interfacial mixing on DMI values in Co/Pt and other FM/NM interfaces is analyzed and discussed. Furthermore, several approaches for DMI enhancement and manipulation will be presented including, in particular, physical mechanisms of DMI behavior in Pt/Co/MgO structures [6,7]. Finally, a possibility of electric field control of DMI in such structures will also be presented [6]. These results clarify underlying mechanisms of DMI at FM/NM bilayers and should help optimizing material combinations for skyrmion- and DW-based storage and memory devices [7].

REFERENCES

[1] H. X. Yang, M. Chshiev, B. Dieny, A. Manchon, J. H. Lee, K. H. Shin, *First-principles investigation of the very large perpendicular magnetic anisotropy at Fe|MgO and Co|MgO interfaces*, Phys. Rev. B **84**, 054401 (2011).

[2] A. Hallal, H. X. Yang, B. Dieny, and M. Chshiev, *Anatomy of perpendicular magnetic anisotropy in Fe/MgO magnetic tunnel junctions: First-principles insight*, Phys. Rev. B 88, 184423 (2013).

[3] A. Hallal, B. Dieny, and M. Chshiev, *Impurity-induced enhancement of perpendicular magnetic anisotropy in Fe/MgO tunnel junctions*, Phys. Rev. B 90, 064422 (2014).

[4] H. X. Yang, A. D. Vu, A. Hallal, N. Rougemaille, J. Coraux, G. Chen, A. K. Schmid, and M. Chshiev, *Anatomy and Giant Enhancement of the Perpendicular Magnetic Anisotropy of Cobalt-Graphene Heterostructures*, Nano Lett. 16, 145 (2015).

[5] F. Ibrahim, H. X. Yang, A. Hallal, B. Dieny, and M. Chshiev, *Anatomy of electric field control of perpendicular magnetic anisotropy at Fe/MgO interfaces*, Phys. Rev. B 93, 014429 (2016).

[5] H. X. Yang, A. Thiaville, S. Rohart, A. Fert, and M. Chshiev, *Anatomy of Dzyaloshinskii-Moriya Interaction at Co/Pt Interfaces*, Phys. Rev. Lett. 115, 267210 (2015).

[6] H. X. Yang, O. Boulle, V. Cros, A. Fert and M. Chshiev, *Controlling Dzyaloshinskii-Moriya Interaction via Chirality Dependent Layer Stacking, Insulator Capping and Electric Field*, arXiv:1603.01847.

[7] O. Boulle et al, *Room-temperature chiral magnetic skyrmions in ultrathin magnetic nanostructures*, Nature Nanotechnology 11, 449 (2016).

Antiferromagnetic Spintronics

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Revealing the Hidden Structural Phases of FeRh and Electric Field Control of Magnetization Direction across the Metamagnetic Transition

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Recent experiments on FeRh thin films epitaxially grown on ferroelectric $BaTiO_3$ or piezoelectric substrates have provided evidence of an isothermal electric-field control of the magnetic phase transition between the low-temperature antiferromagnetic (AFM) and high-temperature ferromagnetic (FM) phase driven via piezoelectirc bi-axial strain[1-2]. These results raise the intriguing question of the effect of strain on tuning the interplay between FM and AFM spin correlations and hence the stability of the FeRh phases. In the first part of my talk I will discuss the results of *ab initio* electronic structure calculations which reveal that tetragonal distortion has a dramatic effect on the relative stability of the various magnetic structures (C-, A-, G-, A'-AFM, and FM) of FeRh giving rise to a wide range of novel stable/metastable structures and magnetic phase transitions between these states. We predict that the cubic G-AFM structure, which was believed thus far to be the ground state, is metastable and that the tetragonally expanded G-AFM is the stable structure. The low energy barrier separating these states suggests phase coexistence at room temperature. We propose a novel A'-AFM phase to be the global ground state among all magnetic phases which arises from the strain-induced tuning of the exchange interactions. The results elucidate the underlying mechanism for the recent experimental findings of electric-field control of magnetic phase transition driven via tetragonal strain. The novel magnetic phase transitions open interesting prospects for exploiting strain engineering for the next-generation memory devices.

Electric field induced switching of magnetism, as opposed to current-driven spin transfer torque magnetization switching, can lead to a new paradigm enabling ultra-low power, highly scalable, and nonvolatile magnetoelectric random access memory (MeRAM) [3–4]. Manipulation of the AFM magnetization direction of ultrathin (~ 1nm) FeRh/insulator bilayers in the AFM or FM phase by purely electric field means (rather than E-field induced strain), is of fundamental importance for the operation of the next- generation ultra-low power MeRAM and has not been investigated thus far. In the second part of my talk I will discuss results of *ab initio* electronic structure calculations which reveal that the voltage-controlled magnetic anisotropy (VCMA) of ultrathin FeRh/MgO bilayers exhibits distinct linear or nonlinear behavior across the metamagnetic transition depending on the Fe- or Rh-interface termination. We predict that the AFM Fe-terminated phase undergoes an electric field (E-field) *magnetization switching* with large VCMA efficiency and a spin re- orientation across the metamagnetic transition. In sharp contrast, while the Rh-terminated interface exhibits large out-of-plane (in-plane) MA in the ferromagnetic (AFM) phase, its magnetization is more rigid to external E-field due to the large Rh spin-orbit coupling. These findings demonstrate that manipulation of the AFM magnetization direction via purely E-field means (rather than E-field induced strain) can pave the way toward ultra-low energy *AFM-based* magnetoelectric random access memory devices.

REFERENCES

[1] R. O. Cherifi, V. Ivanovskaya, L. C. Phillips, A. Zobelli, I. C. Infante, E. Jacquet, V. Garcia, S. Fusil, P. R. Briddon, N. Guiblin, A. Mougin, A. A. *Ünal*, F. Kronast, S. Valencia, B. Dkhil, A. Barth*élé*my, and M. Bibes, *Electric-field control of magnetic order above room temperature,* Nat. Mater. **13**, 345 (2014).

[2] Z. Q. Liu, L. Li, Z. Gai, J. D. Clarkson, S. L. Hsu, A. T. Wong, L. S. Fan, M.-W. Lin, C. M. Rouleau, T. Z. Ward, H. N. Lee, A. S. Sefat, H. M. Christen, and R. Ramesh, Full Electroresistance Modulation in a Mixed-Phase Metallic Alloy, Phys. Rev. Lett. **116**, 097203 (2016).

[3] Y. Shiota, T. Nozaki, F. Bonell, S. Murakami, T. Shinjo, and Y.Suzuki, *Induction of coherent magnetization switching in a few atomic layers of FeCo using voltage pulses*, Nature Mater. **11,** 39 (2012).
[4] V. Ong, Nicholas Kioussis, D. Odkhuu, P. Khalili Amiri, K. L. Wang, and Gregory P. Carman , *Giant voltage modulation of magnetic anisotropy in strained heavy metal/magnet/insulator heterostructures*, Phys. Rev**. B 92,** 020407 (2015).

General switching voltages for magnetic tunnel junctions with in-plane and/or perpendicular-to-plane anisotropy free layers

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We analytically calculate the switching voltages for MgO-based magnetic tunnel junctions for the generalized case where the free layer has two generic "intrinsic" fields oriented along orthogonal directions. The magnetization of the reference layer and the applied field are assumed to be parallel to one of the two intrinsic field axis. Both the in-plane and the field-like spin-torque terms are taken into account, with the field-like torque assumed to have a quadratic dependence on the applied voltage and to favour the antiparallel state [1]. The switching voltages thus determined can be particularized for different geometries by replacing the two generic intrinsic field terms with the appropriate expressions for the anisotropy and demagnetizing fields, according to the specific free and reference layer configuration considered. The results are consistent with numerical integration of the Landau-Lifshitz-Gilbert equation with the relevant spin-torque terms.

For in-plane MgO-based magnetic tunnel junctions, one of the two intrinsic fields of the free layer corresponds to the (negative) demagnetizing field, which pulls the magnetization of the free layer towards the film plane. The orthogonal intrinsic field component is the easy-axis anisotropy, parallel to the current polarization and the external field direction. We demonstrate that in this configuration the quadratic dependence of the field-like torque on the applied voltage can cause back-hopping (a somewhat obscure behaviour characteristic to tunnel junctions, whereby reliable switching to the desired state is achieved for applied voltages of the order of the critical voltage, but a larger applied bias induces a telegraph-noise behaviour [2, 3]). For perpendicular anisotropy tunnel junctions without in-plane shape anisotropy, the only intrinsic field present in the free layer is parallel the effective anisotropy, parallel to the reference layer direction. In this case, we find that neither back-hopping, nor spin-transfer driven steady stare precession are expected, as evidenced by experimental results [4]. Finally, if an in-plane shape anisotropy is considered in addition to the effective perpendicular anisotropy, a variety of canted states are predicted [5].

REFERENCES

[1] C. Heiliger and M. Stiles, *Ab Initio Studies of the Spin-Transfer Torque in Magnetic Tunnel Junctions*, Phys. Rev. Lett. **100**, 186805 (2008).

[2] J. Z. Sun, , M. C. Gaidis, G. Hu, E. J. O'Sullivan, S. L. Brown, J. J. Nowak, P. L. Trouilloud and D. C. Worledge, *High-bias backhopping in nanosecond time-domain spin-torque switches of MgO-based magnetic tunnel junctions*, J. Appl. Phys. **105**, 07D109 (2009).

[3] T. Min, J. Z. Sun, R. Beach, D. Tang and P. Wang, *Back-hopping after spin torque transfer induced magnetization switching in magnetic tunneling junction cells*, J. Appl. Phys. **105**, 07D126 (2009).

[4] J.J. Nowak, R. P. Robertazzi, J. Z. Sun, G. Hu, David W. Abraham, P. L. Trouilloud, S. Brown, M. C. Gaidis, E. J. O'Sullivan, W. J. Gallagher, and D. C. Worledge, *Demonstration of Ultralow Bit Error Rates for Spin-Torque Magnetic Random-Access Memory With Perpendicular Magnetic Anisotropy*, IEEE Magn. Lett. **2**, 3000204 (2011).

[5] Kerstin Bernert, Volker Sluka, Ciarán Fowley, Jürgen Lindner, Jürgen Fassbender and Alina M. Deac, *Phase diagrams of MgO magnetic tunnel junctions including the perpendicular spin-transfer torque in different geometries*, Phys. Rev. B **89**, 134415 (2014).

The search for new materials for spintronics

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The development of novel materials is a strong enabler for any technology, and in fact technology and materials innovation cannot be separated. Unfortunately the process of finding new materials, optimal for a given application, is a lengthy, often unpredictable and has a low throughput. Here we describe a systematic pathway to the discovery of novel materials, which demonstrates an unprecedented throughput and discovery speed. The method can be applied to any materials class and any potential application, so that can enable progress in quantum and classical technologies alike. Here I will use the example of magnetism to introduce the main features of the method, and I will demonstrate the discovery of several new high-performance magnets.

Based on an extensive electronic structures library of Heusler alloys containing 236,115 prototypical com- pounds, we have filtered those alloys displaying magnetic order and established whether they can be fab- ricated at thermodynamical equilibrium1. Specifically, we have carried out a full stability analysis for in- termetallic Heuslers made only of transition metals. Among the possible 36,540 prototypes, 248 are found thermodynamically stable but only 20 are magnetic. The magnetic ordering temperature, TC, has then been estimated by a regression calibrated on the experimental TC of about 60 known compounds. As a final validation we have attempted the synthesis of a few of the predicted compounds and produced two new magnets. One, Co_2MnTi, displays a remarkably high T_C in perfect agreement with the predictions, while the other, Mn_2PtPd, is a complex antiferromagnet. Our work paves the way for large-scale design of novel magnetic materials at unprecedented speed.

REFERENCES

1 Stefano Sanvito, Corey Oses, Junkai Xue, Anurag, Tiwari, Mario Zic, Thomas Archer, Pelin Tozman, Munuswamy Venkatesan, J. Michael D. Coey and Stefano Curtarolo, Accelerated discovery of new magnets in the Heusler alloy family, under review.

Contributed Talks

Structural and metal-insulator transitions in Ge-Sb-Te phase-change materials

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Phase-change materials (PCMs) are capable of switching very rapidly and reversibly between the amorphous and crystalline phase at high temperature. Yet, the two phases are stable at room temperature and exhibit pronounced optical and electrical contrast. These unique properties have resulted in applications in electronic non-volatile random access memories, where heating is induced by the Joule effect.
In this talk, I will present our recent work, based on density functional theory simulations, about the structural and electronic properties of the technologically most important family of PCMs, namely the Ge-Sb-Te compounds. I will first give an introduction on the structural transitions and metal-insulator transitions which occur in crystalline Ge-Sb-Te materials as a function of annealing temperature or stoichiometry. Then I will discuss our simulations, which have shed light on the microscopic mechanisms responsible for these transitions and on the nature of the electronic states in the insulating phase.
These findings open up the possibility of exploiting the multiple phases of crystalline Ge-Sb-Te to develop multilevel memory cells, which would dramatically increase the storage density of PCM-based devices.

REFERENCES

[1] T. Siegrist, P. Jost, H. Volker, M. Woda, P. Merkelbach, C. Schlockermann, and M. Wuttig, *Disorder-induced localization in crystalline phase-change materials*, Nat. Mater. **10**, 202 (2011).

[2] W. Zhang, A. Thiess, P. Zalden, R. Zeller, P. H. Dederichs, J.-Y. Raty, M. Wuttig, S. Blügel, and R. Mazzarello, *Role of vacancies in metal-insulator transitions of crystalline phase-change materials*, Nat. Mater. **11**, 952 (2012).

[3] W. Zhang, M. Wuttig, and R. Mazzarello, *Effects of stoichiometry on the transport properties of crystalline phase-change materials*, Sci. Rep. **5**, 13496 (2015).

[4] I. Ronneberger, W. Zhang, H. Eshet, and R. Mazzarello, *Crystallization properties of the $Ge_2Sb_2Te_5$ phase-change compound from advanced simulations*, Adv. Funct. Mater. **25**, 6407 (2015).

[5] V. Bragaglia, F. Arciprete, W. Zhang, A. M. Mio, E. Zallo, K. Perumal, A. Giussani, S. Cecchi, J. E. Boschker, H. Riechert, S. Privitera, E. Rimini, R. Mazzarello, and R. Calarco, *Metal-insulator transition driven by vacancy ordering in GeSbTe phase change materials*, Sci. Rep. **6**, 23843 (2016).

[6] B. Zhang, W. Zhang, Z. Shen, Y. Chen, J. Li, S. Zhang, Z. Zhang, M. Wuttig, R. Mazzarello, E. Ma, and X. Han, *Element-resolved atomic structure imaging of rocksalt $Ge_2Sb_2Te_5$ phase-change materials*, Appl. Phys. Lett. **108**, 191902 (2016).

Phonon scattering induced by line defects in silicon viewed from Atomic-Greens-Function approach

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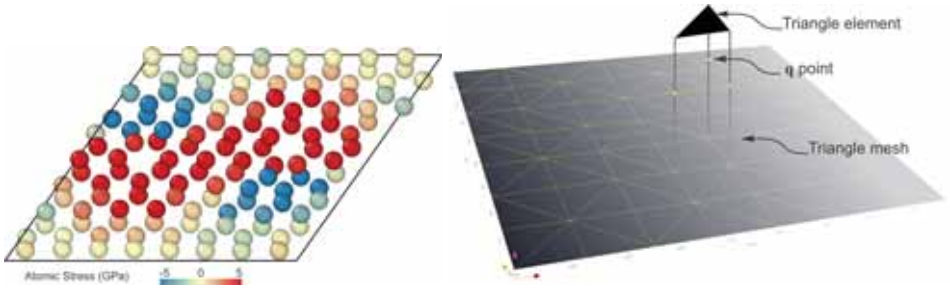
When reduced to small scale, the thermal transport behavior of devices is not only dependent on the materials' intrinsic properties. Predicting the thermal conductivity is an inherent multi-scale problem. It requires the quantification of phonon scattering strength caused by various types of defects e.g. vacancies, interfaces and dislocations, inside the materials. For the defects that strongly perturb their atomic environment, the Born approximation of the associated perturbation to the system will fail. The Atomic-Green's-Function approach has been demonstrated to be an efficient way to evaluate such phonon scattering events[1].

For one-dimensional line defects, e.g. dislocations, as shown in Fig. 1(a), we demonstrate a formalism, where the three-dimensional Brillouin Zone (BZ) is divided into parallel two-dimensional planes perpendicular to the defect line direction. A triangulation mesh is adopted to discretize each of the two-dimensional BZ planes. This treatment allows us to split the three-dimensional domain into independent two-dimensional domains and obtain Greens function in defected super-cell. By summing all the results of the planar subdomains, the T-matrix and scattering cross section are obtained.

We will illustrate this strategy by setting up an atomic model of a quadrupolar arrangement of edge dislocations in silicon using linear elastisity theory. The frequency frequency dependence of the scattering rate is calculated and it is discussed how this form the basis of a all-scale calculation of the thermal conductivity.



(a) (b)

FIG. 1: (a) Atomic structure of a dislocation dipole in Stiling-Weber[2] silicon. Atoms are colored by atomic stress. (b) Triangulation scheme to calculate 2D Green's function on a q plane.

References

[1] NA Katcho, J Carrete, Wu Li, and N Mingo. Effect of nitrogen and vacancy defects on the thermal conductivity of diamond: An ab initio green's function approach. *Physical Review B*, 90(9):094117, 2014.
[2] F.H. Stillinger and T.A. Weber. Computer simulation of local order in condensed phases of silicon. *Phys. Rev. B*, 31(8):5262, 1985.

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Devices with learning capability based on ferroelectricity as state variable

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Devices with memory and learning capabilities are key elements to implement bio-inspired neuro-computing platforms in low-power embedded systems. Unfortunately, neural networks are still mapped into highly inefficient hardware platforms, so that new technologies and materials are needed to enable information processes with state variable other than charge. Ferroelectric (FE) polarization (P) is highly appealing for use as state variable, because: *i)* it is purely electric, *ii)* can be altered via low power voltage pulses and *iii)* ensures long-term endurance. In this paper I will discuss two classes of device classes with learning capabilities, based on: (i) on conventional FE oxides and (ii) novel ferroelectric semiconductors with giant Rashba.

As regards conventional FE oxides, the most promising architecture is that of ferroelectric tunneling junctions (FTJs), where a huge change of the tunneling resistance (TER) is obtained upon reversal of the polarization state (from P_{up} to P_{dn}) in the ferroelectric barrier. The actual resistance depends on the story of voltage pulses, thus implementing the learning capability. Since the discovery of the memristive behaviour of FTJs in proof of concept devices [1] there has not been a sizable advancement in the related technology. In this paper I will present some recent results obtained on micron-sized tunnelling junctions involving epitaxial $BaTiO_3$ (BTO) barriers. In particular I report on TER of $Pt/BaTiO_3/La_{0.7}Sr_{0.3}MnO_3$ (Pt/BTO/LSMO) purely ferroelectric tunnel junctions. [2] Record values of TER, up to 3 x 10^4 %, have been found at room-temperature on large-area junctions (A = 4 to 900 μm^2), made using standard lithography techniques. Beyond this, a radically new experimental observation is made. It is found that the capacitance of the junctions is bias-voltage and frequency dependent, due to the modification of the barrier thickness arising from the modulation of a depletion layer existing close to the BTO/LSMO interface.

Ferroelectric Rashba semiconductors (FERSC), [3] instead, hold potential for the integration of memory and computing functionalities within the channel of the very same transistor. Being ferroelectric, FERSC show an internal effective electric field and lack inversion symmetry. As such, in the presence of spin-orbit coupling which breaks spin-degeneracy, they show a k-dependent spin-splitting in some regions of the Brillouin zone owing to the (bulk) Rashba effect. What is relevant is that the spin direction in each sub-band can be fully reversed upon reversal of the ferroelectric polarization, thereby allowing its electrical control. In perspective, these unique features can be exploited in FERSC transistors, where the non-volatile FE configuration is the state variable electrically controlled by gate voltage pulses, which determines the transconductance (computing functionality) via bulk Rashba and charge-to-spin-to charge conversion. In this paper I will review o the state of the art of research on GeTe, [4,5] the father compound of FERSC, and illustrate some device architectures currently under investigation.

REFERENCES

[1] A. Chantbouala *et al.*, Nature Mater. **11**, 860 (2012)

[2] Greta Radaelli, Diego Gutiérrez, Florencio Sánchez, Riccardo Bertacco, Massimiliano Stengel and Josep Fontcuberta, "*Large Room-Temperature Electroresistance in Dual-Modulated Ferroelectric Tunnel Barriers*", Advanced Materials, 27, 2602–2607 (2015)

[3] Di Sante, D., Barone, P., Bertacco, R. and Picozzi, S., "*Electric Control of the Giant Rashba Effect in Bulk GeTe*", Advanced Materials 25 (4), 509-513 (2013)

[4] L. Liebmann, C. Rinaldi, … , R. Calarco, S. Picozzi, R. Bertacco, M. Morgenstern, "*Giant Rashba Type Spin Splitting in Ferroelectric GeTe(111)*", *Adv. Mater.* **28**, 560 (2016).

[5] C. Rinaldi, J. C. Rojas-Sánchez, R. N. Wang, Y. Fu, S. Oyarzun, L. Vila, S. Bertoli, M. Asa, L. Baldrati, M. Cantoni, J.-M. George, R. Calarco, A. Fert and R. Bertacco, "*Evidence for spin to charge conversion in GeTe(111)*", *Appl. Phys. Lett. Mater.* **4**, 032501 (2016).

Electron transport simulations for resistive switching memory devices

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Reversible resistive switching between high-resistance and low-resistance states in metal-spacer-metal heterostructures makes them very interesting for applications in random access memories. The change of resistance is typically obtained either by a phase change in the spacer or by creating a conductive filament in insulating oxide spacers. While recent experimental work has shown that inserting a metallic "oxygen scavenger" layer between the positive electrode and the oxide improves device performance, the fundamental understanding of how the scavenger layer modifies heterostructure properties is lacking. We use density functional theory combined with the non-equilibrium Green's function formalism implemented in the *Smeagol* code [1,2] to calculate thermodynamic properties and conductance of TiN/HfO_2/TiN heterostructures with and without Ta scavenger layer [3]. We show that Ta insertion lowers the formation energy of oxygen-deficient low-resistance filaments, while maintaining a high ratio between resistances of high- and low-resistance states. We evaluate how motion of oxygen atoms from the metal to the filament can block filament-conductance in HfO_{2-x}, and discuss those results in the context of experimental observations. We will conclude by outlining an emerging memory technology based on the combination of piezoelectric and piezoresistive materials (http://www.petmem.eu/).

REFERENCES

[1] A. R. Rocha, V. M. Garcia-Suarez, S. W. Bailey, C. J. Lambert, J. Ferrer, and S. Sanvito , Phys. Rev. B **73**, 085414 (2006), *Spin and molecular electronics in atomically generated orbital landscapes*, Phys. Rev. B **88**, 165112 (2013).

[2] I. Rungger and S. Sanvito , *Algorithm for the construction of self-energies for electronic transport calculations based on singularity elimination and singular value decomposition*, Phys. Rev. B, **78**, 035407 (2008).

[3] X. Zhong, I. Rungger, P. Zapol, H. Nakamura, Y. Asai, and O. Heinonen, *The effect of Ta "oxygen scavenger layer" on HfO2-based resistive switching behavior: thermodynamic stability, electronic structure, and low-bias transport*, Phys. Chem. Chem. Phys. **18**, 7502 (2016).

Spectroscopic fingerprint of resistive switching oxide interfaces probed by bulk sensitive photoemission spectroscopy

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A large variety of transition metal oxides exhibit different resistance states at opposite polarities upon electrical stimulation, an effect potentially relevant for Resistance Random Access Memory (RRAM) [1]. Although some agreement has been reached on the importance of the oxygen vacancies role and of their redox process under applied electric field, knowledge of the microscopic details of such process, in particular near the active interface(s), is relatively limited.

Hard x-ray photoemission spectroscopy (HAXPES), thanks to a probing depth as large as 5 to 10 nm, is able to probe in a chemical sensitive, non-destructive way a buried interface in a device-ready system. We present HAXPES results from resistive switching layered oxide interfaces Ti/PCMO ($Pt/Ti/Pr_{0.5}Ca_{0.5}MnO_3/SrRuO_3$), including in-operando measurements, i.e. measurements while applying field, where we observe modifications of the spectroscopic features under electroforming treatment. Formation of Titanium oxide is promoted through migration of oxygen ions from the PCMO to the Ti layer/electrode and a reversible redox reaction at the interface is observed, both governing the formation and the shortening of an insulating tunnel barrier [2,3]. Moreover, it is shown that the oxygen content and the interface quality are intrinsically important to device behavior [4].
Present results provide a spectroscopic proof of the correlation between redox-state occurring at the Ti/PCMO interface, as due due to voltage-induced oxygen drifting, and charge carrier transport since the initial electroforming treatment, thus clarifying the relevant number of physical parameters needed to model and built a device.

REFERENCES

[1] R. Waser, M. Aono, *Nanoionics-based resistive switching memories* Nat. Mater. ***6***, 833 (2007).

[2] A. Herpers, C. Lenser, C. Park, F. Offi, F. Borgatti, G. Panaccione, S. Menzel, R.Waser, R. Dittmann, *Spectroscopic Proof of the Correlation between Redox-State and Charge-Carrier Transport at the Interface of Resistively Switching Ti/PCMO Devices* Adv. Mater. **26** , 2730 (2014) .

[3] F. Borgatti, C. Park, A. Herpers, F. Offi, R. Egoavil, Y. Yamashita, A. Yang, M.Kobata, K. Kobayashi, J. Verbeeck, G. Panaccione, R. Dittmann, *Chemical insight into electroforming of resistive switching manganite heterostructures*, Nanoscale **5**, 3954 (2013).

[4] A. Regoutz, I. Gupta, A. Serb, A. Khiat, F. Borgatti, T.-L. Lee, C. Schlueter, P. Torelli, B. Gobaut, M. Light, D. Carta, S. Pearce, G. Panaccione, and T. Prodromakis, *Role and Optimization of the Active Oxide Layer in TiO2-Based RRAM,* Adv. Funct. Mater. **26**, 507 (2016).

Surface Chemical Modification of Semimetal Nanowires for Schottky Barrier Diodes

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Semimetallic α-tin is known to become semiconducting when patterned below a critical length due to quantum confinement. Exploitation of this size-dependent variation in electronic properties has been proposed in the design of dopant free Schottky barrier nanowire field effect transistors [1]. In this work, we employ density functional based methods to further explore the impact of crystal orientation, wire diameter, surface passivation, and uniaxial stress on the electronic structure of α-Sn nanowires. It is found that control over the nanowire energy band gap and electron affinity is possible by appropriate choice of structural parameters and surface termination.

Results show applications for ultra-scaled CMOS device concepts to enable complex logic devices operating near atomic limits. Nanowire-based field effect transistors are a promising candidate for replacing or extending current CMOS technology as the ability to implement gate-all-around architectures provides optimal electrostatic control and thus low power consumption in the OFF state. A device based on semimetallic α-Sn in which quantum confinement effects are exploited to create a semiconducting region has already been proposed [1]. In the present work, we apply density functional theory and non-equilibrium Green's function methods in order to explore the electronic structure and transport properties of single crystalline α-Sn nanowires of 1 and 3 nm diameter grown along [100], [110], and [111] crystallographic orientations. It is found that the threshold size at which the semimetal to semiconductor occurs depends on nanowire orientation and can be significantly controlled via surface chemistry. This modification of electronic properties, including band gaps and electron affinities, can be exploited in the design of ultra-scaled electronic devices by allowing greater flexibility in the engineering of interfaces with desired band offsets.

In particular, our study demonstrates the formation of Schottky junctions by locally switching between semimetallic and semiconducting behavior along a single crystal α-Sn nanowire with a uniform diameter by varying the surface chemistry along the nanowire's length [2]. This novel Schottky diode design can be extended to molecular-scale Schottky barrier nanowire field effect transistors; enabling fabrication of ultra-scaled devices without the introduction of substitutional doping, nor the need to form heterogeneous junctions, and without the need for forming wide-narrow regions within a single nanowire.

Atomistic simulations based on non-equilibrium Green's functions predict devices with these characteristics to show rectification ratios in excess of 10^3 at molecular length scales.

REFERENCES

[1]L. Ansari, G. Fagas, J.P. Colinge, and J.C.Greer, "A proposed confinement modulated gap nanowire transistor based on a metal (tin)", *Nano Letters*, vol. 12, pp. 2222-2227, 2012.

[2] A. Sanchez-Soares and J. C. Greer. "Nanowire surface modification". UK Patent 1605814.1 (filed)

Magnetisation reversal in CoFeB-MgO tunnel junctions via atomistic modelling

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Magnetic Random Access Memory (MRAM) is a non-volatile memory technology utilizing a magnetic tunnel junction (MTJ) to sense the magnetic state. A promising material for MRAM is a MTJ consisting of CoFeB/MgO due to its strong thermal stability, low damping and high tunneling magnetoresistance [1]. Given the strong variation of the properties at the atomic level, here we investigate the intrinsic material properties of CoFeB/MgO structures using an atomistic spin model [2]. The system we simulate consists of a single high anisotropy monolayer in contact with MgO, which causes the perpendicular magnetic anisotropy (PMA), and a thicker soft bulk layer. We have then systematically investigated the effects of temperature, system size and thickness on the coercivity of the system and on the reversal modes of the magnetisation. We find that the switching of the magnetisation is incoherent for diameters larger than 30 nm at each temperature, although the mechanism is different. At relatively high temperatures the switching is thermally activated: the thermal fluctuations allow nucleation sites at the edge of the disk, where the domain is formed and subsequently propagates through the material, while at low temperature the magnetisation reverses at the centre of the disk (Figure 1 (left)). Notwithstanding these differences the mean coercivity shows a constant trend, as expected for a nucleation-like reversal. When the critical single domain size is approached, thermal fluctuations cause the magnetisation to reverse at smaller fields and the system tends toward superparamagnetic behaviour, leading to a reduction in the mean coercive field. At the same sizes but low temperature, the stability of the system increases and the reversal becomes coherent (Figure 1 (right)). Moreover, an intrinsic thermal switching field distribution (TSFD) caused by the temperature emerges from the simulations. This TSFD plays an important role since it imposes a limit to the accuracy which the magnetisation reversal can be accessed at finite temperature with, particularly from the experimental side.

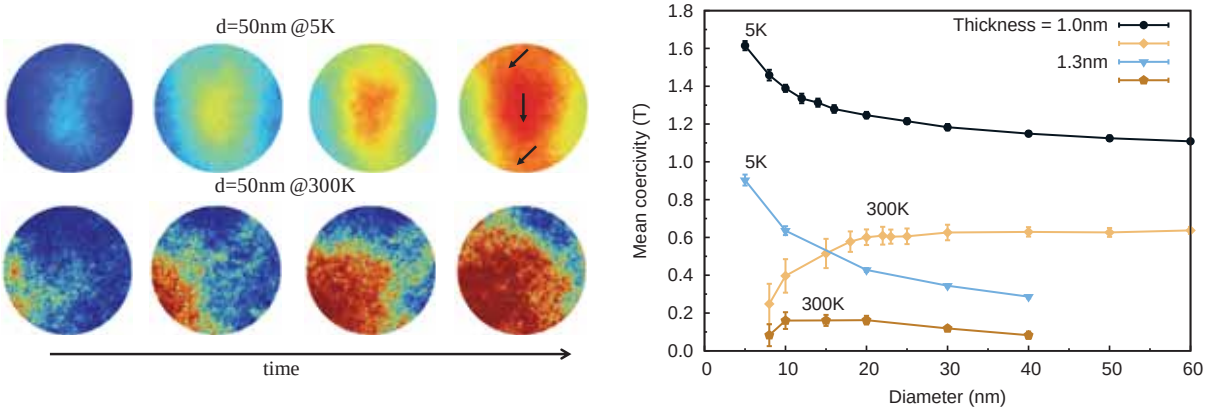

Figure 1: (Left) Evolution of the spin configurations during the switching at 5 and 300 K for a particle size of 50 nm and 1 nm thick. The thermal energy causes the reversal to start from the edge of the dot, while at low temperature the nucleation origin is the centre. (Right) Mean coercivity as function of the particle size for different temperatures.

ACKNOWLEDGEMENT

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REFERENCES

[1] Ikeda,S. et al. A perpendicular-anisotropy CoFeB–MgO magnetic tunnel junction. Nature Materials 9, 721–724 (2010).

[2] R. F. L. Evans, W. J. Fan, P. Chureemart, T. A. Ostler, M. O. A. Ellis and R. W. Chantrell J. Phys.: Condens. Matter 26, 103202 (2014).

Manipulation of a spin current in a lateral spin valve

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Recent advancement in nanofabrication and growth allows the utilisation of spin-polarised electrons in transport and dynamics, resulting in the development of spintronic devices [1]. In the spintronic devices, the key technologies are injection, manipulation and detection of spin-polarised electron in a non-magnetic media with high efficiency.

Conventionally such a spin-polarised electron current has been injected into a non-magnetic material by flowing an electrical current through a ferromagnetic layer. However, its spin polarisation is dependent upon the interfacial properties, such as conductance matching, junction resistance and interfacial resonant states. We have been investigated a series of lateral spin-valves to demonstrate their geometrical ratchet effect on spin-current signal amplification and modulation [2].

We calculated diffusive electron transport in a LSV, consisting of 100-nm-wide Ni81Fe19 (Py) wires bridged by a 100-nm-wide Cu wire, using our simple model. Here, the central part of the Cu wire was modified into the following geometrical ratchet shapes with allowing 50 nm separation between the Py wires and the ratchets; (i) one or two-pairs of right-angled triangles (base: $100 \leq b \leq 450$ nm and height: $0 \leq h \leq 100$ nm) and (ii) one or two-pairs of obtuse-angled triangles (base: $100 \leq b \leq 450$ nm, height: $0 \leq h \leq 100$ nm and the distance between the top ends and base ends of the triangular: 50 nm). We found that the spin amplification takes its maximum for the single-paired right- and obtuse-angled triangles with b=250 nm and h=75 and 80 nm, respectively.

The above LSV devices were fabricated by conventional electron-beam lithography and lift-off processes. Two Py nanowires were designed to be 30 nm thick and 200 nm wide with different shapes at their ends (square and sharp) to induce a difference in their magnetisation-reversal fields. These wires were bridged by a Cu nanowire (70 nm thick and 100 nm wide). We demonstrated spin-current amplification in a lateral spin-valve (LSV) using a geometrical ratchet effect. Two Py nanowires were designed to be 30 nm thick and 200 nm wide bridged by a Cu nanowire (70 nm thick and 100 nm wide). Here, the central part of the Cu wire was modified into the following geometrical ratchet shapes with allowing 50 nm separation between the Py wires and the ratchets. We measured over 700% spin-current amplification for the right-angled triangles with 100 nm base and 60 nm height.

Acknowledgments

This work has been partially funded by JST-PRESTO and EPSRC (EP/I000933/1 and EP/M02458X/1).

References

[1] A. Hirohata and K. Takanashi, *J. Phys. D: Appl. Phys.* **47**, 193001 (2014).

[2] R. M. Abdullah *et al.*, *J. Phys. D: Appl. Phys.* **47**, 482001(FTC) (2014).

Multi-scale spin dynamic simulations of current-induced switching in magnetic tunnel junctions

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Using spin transfer torque (STT) to switch the free ferromagnetic layer of a magnetic tunnel junction (MTJ) without the need for external magnetic fields would improve the scalability of MRAM. The magnetisation dynamics driven by STT is usually modelled using the Landau-Lifshitz-Gilbert-Slonczewski equation[1,2] but here we present a combined approach using ab initio methods to calculate the STT and the dynamics performed with atomistic spin dynamics. At the microscopic scale we employ the density functional theory combined with the non-equilibrium Green's function technique, as implemented in the Smeagol code,[3] to calculate the spin-transfer torque (STT) in the MTJ as function of the angle of misalignment, θ, and the applied finite bias V. This then provides direct input to finite-temperature atomistic spin dynamics augmented with additional STT[2]. Different methods of mapping the ab-initio STT are also considered, i.e that the torque is individual to each spin or the layer average determines the torque.

Using this methodology we investigate a Co/MgO/Co MTJ for which the results are shown in figure 1. From the *ab initio* calculations the STT shows a significant decay into the Co free layer with the largest torque on the first atomic layer and oscillating in sign for further layers. Figure 1.(a-c) shows the bias dependence and the angular dependence of the torque which is then mapped to the atomistic spin model. Due to the strong exchange coupling the different mapping methods show little variation but indicate atomic resolution is important for nanoscale systems. At the dynamics stage uniaxial anisotropy is incorporated and the critical bias voltage required to cause switching against it is calculated. Above the critical bias voltage the switching time drops inversely with bias as shown in figure 1.(d). The switching is also investigated at finite temperatures; this shows a significant reduction in the critical voltage due to thermal excitations over the anisotropy energy barrier.

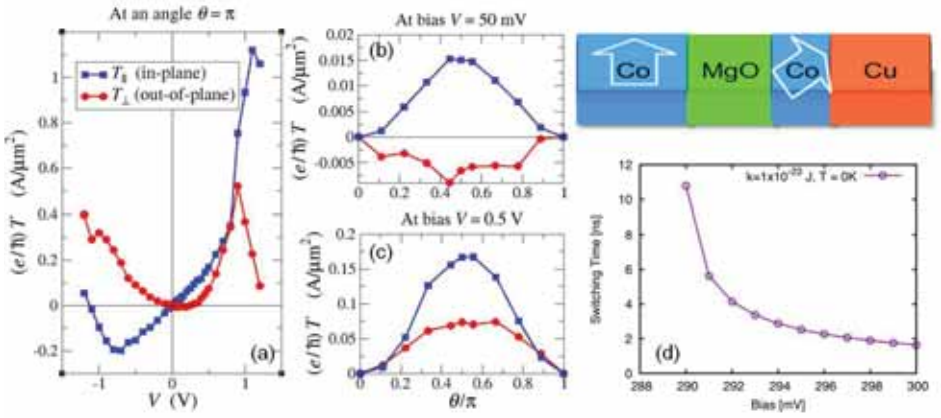

FIG. 1: *Ab initio* STT as function of (a) the bias voltage, for $\theta = \pi$, (b,c) the misalignment angle θ, for $V = 50$ mV and $V = 0.5$ V, respectively. (d) Switching time of the free layer magnetisation showing a critical voltage of 290 mV.

[1] J. Slonczewski, J. Magn. Magn. Mater. **159**, L1 (1996).
[2] A. Brataas, A. D. Kent, and H. Ohno, Nat. Mater. **11**, 372 (2012).
[3] A. R. Rocha, V. M. Garcia-Suarez, S. Bailey, C. Lambert, J. Ferrer, and S. Sanvito, Phys. Rev. B **73**, 085414 (2002).

The zero-moment half metal: How could it change spin electronics ?

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The Heusler compound Mn_2Ru_xGa (MRG) is thought to be the first example of a fully compensated half metal [1], where the Mn is occupies two inequivalent crystallographic positions which have the same sublattice magnetization, but opposite magnetic alignment yielding zero net moment [2]. We have demonstrated how interplay between the Ru concentration *x*, the precise Mn:Ga ratio and substrate-induced biaxial strain may be varied to obtain perfect magnetic compensation and diverging coercivity around room temperature [3,4]. Magnetic compensation is coupled with a high Fermi-level spin polarisation ($P > 50$ %) determined by point-contact Andreev spectroscopy, which leads to high tunnel magnetoresistance (TMR) ratios of ~40 % [5].

A zero-moment half metal is free from demagnetising forces and creates no stray field. It is therefore particularly suited to memory applications where cross talk between neighbouring cells must be suppressed. Furthermore the effective damping is expected to be weak on account of the lack of coupling of the magnetisation with the surrounding space during switching.

An upper limit of switching speed is limited by the Larmor precession frequency of the material, $f = H_{eff}$ where H_{eff} is an effective field created by anisotropy or exchange. In ferrimagnetic materials this field scales as the reciprocal of the net magnetisation (for the ferromagnetic mode) or the product of the anisotropy and exchange fields (for the exchange mode). When , as in MRG, both frequencies are expected to lie in the terahertz region, between 0.3 and 5 THz.

Oscillators based on spin torque transferred from a magnetic polarizer layer to another with MRG has the potential to pave the way not only to ultra-fast, low-power memory applications, but also to extremely broad-band data transfer by opening up the terahertz range of the electromagnetic spectrum, hitherto inaccessible for chip-based data communications.

References

[1] H. Kurt, K. Rode, P. Stamenov, M. Venkatesan, Y.-C. Lau, E. Fonda, and J. M. D. Coey, Phys. Rev. Lett. **112**, 027201 (2014), http://link.aps.org/doi/10.1103/PhysRevLett.112.027201.

[2] D. Betto, N. Thiyagarajah, Y.-C. Lau, C. Piamonteze, M.-A. Arrio, P. Stamenov, J. Coey, and K. Rode, Phys. Rev. B **91**, 094410 (2015).

[3] N. Thiyagarajah, Y.-C. Lau, D. Betto, K. Borisov, J. Coey, P. Stamenov, and K. Rode, Appl. Phys. Lett. **106**, 122402 (2015).

[4] M. Žic, K. Rode, N. Thiyagarajah, Y.-C. Lau, D. Betto, J. M. D. Coey, S. Sanvito, K. J. O'Shea, C. A. Ferguson, D. A. MacLaren, et al., Phys. Rev. B **93**, 140202 (2016), http://link.aps.org/doi/10.1103/PhysRevB.93.140202.

[5] K. Borisov, D. Betto, Y.-C. Lau, C. Fowley, A. Titova, N. Thiyagarajah, G. Atcheson, J. Lindner, A. M. Deac, J. M. D. Coey, et al., Applied Physics Letters **108**, 192407 (2016), http://scitation.aip.org/content/aip/journal/apl/108/19/10.1063/1.4948934.

NVM Workshop, Trinity College, Dublin (Ireland), 29th June-1st July 2016

Title of the talk: “The first ever real bistable memristor”

Presenter: Dr. A. Ascoli

Coauthors: R. Tetzlaff and L.O. Chua

Abstract:
L. Chua has recently introduced a purely mathematical memristor model [1], which, under DC and AC periodic stimuli, experiences memory erase effects [2] in each of the basins of attraction [3] of its 2 locally stable state space attractors. This work presents the first ever real memristor [4] with similar bistable steady state DC and AC dynamics. A deep theoretical analysis, based on the application of concepts from nonlinear dynamics theory (Poincaré section analysis [5]) and circuit [6] and system [7] theoretic techniques (study of the Driving Point characteristics [8]) unveils the basic mechanisms lying behind the emergence of non-unique asymptotic behaviour in the proposed electronic circuit, which falls into the class of extended memristors [9].

References:
[1] L. O. Chua, “If It’s Pinched, It’s a Memristor,” Special Issue on Memristive Devices, Semiconductor Science and Technology, vol. 29, no. 10, 104001 (42 pp.), 2014
[2] A. Ascoli, R. Tetzlaff, L. O. Chua, J. P. Strachan, and R. S. Williams, “History erase effect in a non-volatile memristor”, IEEE Trans. Circuits and Systems-I, Reg. Papers, vol. 63, no. 3, pp. 389-400, March 2016, DOI: 10.1109/TCSI.2016.2525043
[3] A. Ascoli, R. Tetzlaff, L. O. Chua, “The first ever real bistable memristors - Part I: theoretical insights on local fading memory”, TCAS-II, in press
[4] A. Ascoli, R. Tetzlaff, L. O. Chua, “The first ever real bistable memristors - Part II: design & analysis of a local fading memory system”, TCAS-II, in press
[5] S. H. Strogatz, “Nonlinear dynamics and chaos,” Perseus Books, 1994
[6] L. O. Chua, C. A. Desoer, and E. A. Kuh, “Linear and nonlinear circuits,” McGraw Hill, New York, 1985
[7] L. O. Chua, “Introduction to nonlinear network theory,” Mc Graw-Hill, 1969
[8] L. O. Chua, “CNN: a paradigm for complexity,” Word Scientific Publishing Co Pte Ltd, 1998, ISBN: 981-02-3483-X
[9] L. O. Chua, “Everything you wish to know about memristors but are afraid to ask,” Radioengineering, vol. 24, no. 2, pp. 319–368, 2015

Posters

Ab initio simulations of material applicability for 2D A-RAM memory devices

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After the isolation of graphene [1] two dimensional (2D) materials have taken the spotlight as future active components in the design and fabrication of nanoscale devices, due to the extraordinary variety of their electronic properties and to the possibility of stacking different layers in a seamless way to create the so called van der Waals (vdW) heterostructures [2].

One of their most exciting applications is the design and optimization of 2D MOSFETs for their further use as A-RAM memory cells [3, 4]. In such cells, the binary value is given by the current flowing through the bridge connecting source and drain, which is controlled by the holes accumulated between the gate and the bridge under a negative gate bias.

The vdW heterostructures studied on this work aim to simulate one of such devices, using graphene as a conduction bridge, MoS_2 as the charge-storage layer and h-BN as an insulator. Using the SIESTA method [5], two devices were studied, designed by stacking the materials in two different ways: graphene – MoS_2 – h-BN h-BN and graphene – h-BN – MoS_2 . For the first system, the interaction between the graphene and the MoS_2 layer is negligible and the bridge channel remains metallic, while on the second one the interaction of graphene with h-BN induces a gap of a few meV on the graphene layer, thus turning the system semiconducting. In both cases the charge distribution on each layer has been calculated, showing that the charge transference between the layers remains small even under the effect of a -0.5 V/Å electric field.

To asses the performance of such heterostructures as a potential A-RAM memory cell conductance calculations were performed by using the TranSIESTA [6] code, based on Non-Equilibrium Green's Functions, on a system formed by a bottom layer of 2D graphene and a top layer of either a MoS_2 or a h-BN ribbon. Our results show that the graphene – MoS_2 system remains metallic regardless of the applied voltage between the electrodes, whereas the device containing a h-BN ribbon keeps a metallic *plateau* near the Fermi level even in the presence of the applied bias.

REFERENCES

[1] K. S. Novoselov et al, Science **306**, 666-669 (2004).
[2] A. K. Geim and I. V. Grigorieva, Nature **499** , 419 (2013).
[3] N. Rodriguez et al, IEEE Electron Dev. Lett. **31**, 972 (2010).
[4] N. Rodriguez et al, IEEE Trans. Electron Dev. **58**, 2371 (2011).
[5] J. M. Soler et al, J. Phys.: Condens. Matter **14**, 2745 (2002).

[6] M. Brandbyge et al, Phys. Rev. B **65**, 165401 (2002).

Simulation of the electronic mobility dependence of the RESET operation for bipolar resistive switching

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Redox-based resistive memories (ReRAM) based on the valence change mechanism (VCM) can be switched between a high resistance state (HRS) and a low resistance state (LRS). Switching operations from the HRS into the LRS are called SET while the reversed process is known as RESET. Both switching operations are depend strongly on the material system, cell structure and the experimental operation mode.

Our electrical measurements reveal that the defect states formed from oxygen vacancies are close to the conduction band. Consequently, oxygen vacancies are treated as mobile donors. Therefore, a model is implemented based on the drift-diffusion equation for oxygen vacancies and electrons. Additionally, the internal temperature is calculated using the heat transfer equation. It could be shown that this model is able to explain the nature behind the gradual RESET [1,2].

In this presentation, we will show simulation studies of VCM-type memories. The simulated device structure consists of one insulating ionic conduction layer, commonly built from different transition metal oxides, sandwiched between two metal electrodes. In our model, we assume a filamentary region with a high concentration of mobile oxygen vacancies, which are shifted due to opposite driving forces during the RESET or SET operation. We can show that this RESET is strongly depending on the electrical current and as a consequence on the electron mobility. It reveals that this is a result of Joule heating and the temperature-dependent hopping transport process of the oxygen vacancies. Hence, we will show that the electron mobility has an influence on the oxygen vacancy motion during the RESET. Additionally, the oxygen vacancy concentration influences the electron concentration. The oxygen vacancy concentration itself could possibly influence the electronic mobility due to the increasing impurity scattering, which was neglected so far. In order to investigate this effect, we employ an atomistic model using DFT and the non-equilibrium Green's function formalism using the software tool QuantumWise. We calculate the transmission spectrum of an atomistic wire built from $SrTiO_3$ consisting of a 4x4x6 supercell. We will discuss the electronic transmission spectrum for a variation in the position of single oxygen vacancy. Using the Landauer formalism and transferring recently developed models for nanowires, we are able to calculate the energy dependent electronic mean free path of the given structure [3,4].

REFERENCES

[1] A. Marchewka, R. Waser, and S. Menzel, "Physical Simulation of Dynamic Resistive Switching in Metal Oxides Using a Schottky Contact Barrier Model," *2015 International Conference On Simulation of Semiconductor Processes and Devices (SISPAD), 9-11 September, Washington*

Three-terminal Memristive MoS_2 Switch Fabricated with Helium Ion Beam

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The precise modification of the properties of low-dimensional advanced materials will play a key role in the development of future planar electronic devices and on-chip technologies. For example, a reproducible approach for the fabrication of new-generation resistive switches has great consequences for prototyping novel non-volatile memory storage in resistive RAM (ReRAM), and uncovering fundamental physics which governs material behaviour on the nanoscale. These new generation devices promise low power consumption, high endurance, non-destructive read-out operation and offer a simple cell structure as well as potential for high scalability. Sangwan et al. [1] have demonstrated memristive behaviour in single-layer MoS_2 when an appropriate electroforming process is used to pre-treat the device. Resistive switching properties are enhanced by the introduction of a back-gate, expanding on L. Chua's original memristor proposal [2] and introducing a 3-terminal arrangement for memristive on-chip devices which could revolutionise nanoelectronics.

We report a controllable and reproducible methodology for fabricating a memristive switch based on few-layer mechanically exfoliated molybdenum disulfide layered crystals. A sub-2 nm helium ion beam is employed to introduce sulfur vacancies in the specimen whose I-V characteristics can be tested through electron beam lithography (EBL)-deposited contacts, and modulated through a back-gate terminal operating through the doped substrate underneath the device.
When a He^+ ion beam of probe size $\sim$ 1.5 nm is used to mill a bisecting boundary in the MoS_2 flake, the electrical response is that of a bipolar resistive switch. The degree of high and low resistance states is shown to be tunable by the application of a back-gate voltage through the device, similar to that of a field-effect transistor. The exact form of filamentary switching and the nature of the switching interface created by the helium ion beam is yet to be determined. Sulfur vacancy filamentary switching is the likely candidate, due to previous work showing preferential sputtering of S from He^+ ion beam-irradiated MoS_2 [3].

1 References

[1] V. K. Sangwan, D. Jariwala, I. S. Kim, K.-S. Chen, T. J. Marks, L. J. Lauhon, and M. C. Hersam, "*Gate-tunable memristive phenomena mediated by grain boundaries in single-layer MoS_2*", Nature Nanotech., 2015.

[2] *"Memristor - The missing circuit element."* [Online]. Available: http://www.cpmt.org/scv/meetings/chua.pdf. [Accessed: 26-Jan-2016].

[3] D. S. Fox, Y. Zhou, et al., *"Nanopatterning and Electrical Tuning of MoS 2 Layers with a Subnanometer Helium Ion Beam,* Nano Lett., 2015.

D.C, USA, 2015, pp. 297-300.

[2] A. Marchewka, B. Roesgen, K. Skaja, H. Du, C. L. Jia, J. Mayer, V. Rana, R. Waser, and S. Menzel, "Nanoionic Resistive Switching Memories: On the Physical Nature of the Dynamic Reset Process," *Adv. Electron. Mater.*, vol. 2, pp. 1500233/1-13, 2016.

[3] Troels Markussen, Riccardo Rurali, Antti-Pekka Jauho, and Mads Brandbyge. "Scaling Theory Put into Practice: First-Principles Modeling of Transport in Doped Silicon Nanowires" *Phys. Rev. Lett. 99, 07680*, 2007.

[4] Troels Markussen, Antti-Pekka Jauho, and Mads Brandbyge. "Electron and phonon transport in silicon nanowires: Atomistic approach to thermoelectric properties" *Phys. Rev. B 79, 035415*, 2009.

Effect of strain, thickness, and local surface environment on electron transport properties of oxygen terminated copper thin films

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Electron transport is studied in surface oxidized single-crystal copper thin films with a thickness of up to 5.6 nm by applying density functional theory and density functional tight binding to determine electron transmission probabilities. The variation of the electron transmission as a function of the copper film thickness as well as the different contributions to the overall electron transmission as a function of depth into the films is examined. Transmission at the oxidized copper film surfaces is found to be universally low. Films with thickness greater than 2.7 nm exhibit a similar behavior in local transmission per unit area with depth from the film surface; transmission per unit area initially increases rapidly and then plateaus at a depth of approximately 0.3-0.5 nm away from the surface, depending on surface facet.

Given previous reports from surface reconstruction mechanisms observed in copper films [1] and copper nanowires [2] suggesting tensile surface strain induced by presence of oxygen could be significant at sub 10 nm dimensions, the impact of tensile strain on the electronic transport properties of sub 5nm copper thin films is studied. It is found that unstrained films tend to exhibit a higher transmission per unit area than corresponding films under tensile strain.

The effects of different surface facets on electronic transport properties is assessed. Structures based on (100) and (110) surface reconstructions are investigated [1,3]: Thin films with the Cu(100)c(2x2)-O surface reconstruction are found to exhibit improved conductance than films with exposed Cu(110) facets and p(2x1)-O surface reconstructions.

The results are related to the ability to scale metal interconnects for sub 5 nm technologies.

REFERENCES

[1] N. Bonini *et al.*, Surface Science **600**, 5074 (2006)

[2] S.L.T. Jones *et al.*, Phys. Rev. B **92**, 115413 (2015)

[3] F. Besenbacher and J.K. Norskov, Progress in Surface Science **44**, 5 (1993)

Non-equilibrium transport using order-N methodes

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Combining non-equilibrium green's functions (NEGF) techniques with density functional theory (DFT) derived electronic structure has proven to be capable of providing an accurate atomistic picture of the charge and heat transport in nano-structured devices [1,2]. The NEGF approach provides thereby the possibility to describe not only ballistic but also non-linear transport [3]. So far it has been mostly applied to single molecule junctions, while larger devices are mostly treated using a tight-binding approach [4]. Here, we aim to incorporate the NEGF formalism into the framework of order-N electronic structure theory as provided by the O(N) code conquest [5]. Using Conquest as DFT framework in combination with our NEGF approach allows to compute devices with channel materials containing up to tens of thousands or even hundreds of thousands of atoms.

REFERENCES

[1] S. K. Lee, M. Bürkle, R. Yamada, Y. Asai and H. Tada, *Thermoelectricity at the molecular scale: a large Seebeck effect in endohedral metallofullerenes*, Nanoscale, 7, 20497 (2015).

[2] M. Bürkle, T.J. Hellmuth, F. Pauly, and Y. Asai, *First-principles calculation of the thermoelectric figure of merit for [2,2]paracyclophane-based single-molecule junctions*, Phys. Rev. B 91, 165419 (2015)

[3] Y. Asai, Theory of local heating in single molecular bridge junctions, Phys. Rev. B 84, 085436 (2011).

[4] M. Luisier and G. Klimeck, *Atomistic full-band simulations of silicon nanowire transistors: Effects of electron-phonon scattering*, Phys. Rev. B 80, 155430 (2009).

[5] D. R. Bowler and T. Miyazaki, *O(N) methods in electronic structure calculations*, Rep. Prog. Phys.75, 036503 (2012).

Transmission through correlated heterostructures with half-metallic

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Half-metallic materials are of particular importance for achieving spin dependent transport properties for various spintronic applications. We study a (001) oriented heterostructure of epitaxial grown NiMnSb on Au and evaluate the transmission within the combined Density Functional and Dynamical Mean Field Theory. We use the recent two step LDA+DMFT implementation in combination with SMEAGOL [1]. Electronic correlations [2,3,4] induce minority spin states in the half-metallic gap and significantly reduce the spin polarization of bulk NiMnSb. Although the same depolarization effect appears in the heterostructure geometry, no significant change is seen in the transmission coefficient. These results demonstrate the localized nature of the many-body induced states in the half-metallic gap.

[1] L. Chioncel et. al., Phys. Rev. B 92, 054431 (2015)

[2] M. Katsnelson et. al., Rev. Mod. Phys. 83, 315 (2008)

[3] L. Chioncel et. al., Phys. Rev. B 68, 144425 (2003)

[4] H. Allmaiere al., Phys. Rev. B 81, 054422 (2010)

First-principles finite-bias spin-transfer torque in magnetic tunnel junctions

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The spin-transfer torque (STT) underpins the operation of what is probably one of the most promising candidates for scalable, non-volatile memory technologies, the STT-MRAM. In these data storage units, the switching in each magnetic tunnel junction (MTJ) cell is driven by spin-polarised currents as opposed to strain magnetic fields in conventional MRAM cells. Accurate quantitative material-specific predictions of the switching currents in MTJs are hence key to the development of STT-MRAM.

We consider the most widely-studied and technologically relevant MTJ, the Fe|MgO|Fe, and explore the STT within an *ab initio* finite-bias transport method. The latter is based on the density-functional theory and the non-equilibrium Green's function approach (DFT+NEGF) as implemented in the Smeagol[1] code. We have implemented a steady-state local formulation of STT based on the exchange field of the current-carrying electrons[2]. The main computational bottleneck in this type of calculations is typically the self-consistency under current-carrying conditions. Our aim is to compare the numerical efficiency and accuracy of such method in both self-consistent and non-self-consistent calculations, as well as their sensitivity to system size and details in the electronic structure in order to establish a feasible approximate computational scheme to be used in massive automated (high-throughput) material optimisation algorithms for STT-MRAM.

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[1] A. R. Rocha, V. M. Garcia-Suarez, S. Bailey, C. Lambert, J. Ferrer, and S. Sanvito, Phys. Rev. B **73**, 085414 (2002).

[2] P. M. Haney, D. Waldron, R. A. Duine, A. S. Núñez, H. Guo, and A. H. MacDonald, Phys. Rev. B **76**, 024404 (2007); C. Heiliger and M.D. Stiles, Phys. Rev. Lett. **100**, 186805 (2008) .

First-principles finite-bias schemes for spin-transfer torque

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School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2, Dublin (Ireland)

Ivan Rungger
Materials Division, National Physical Laboratory, Teddington, TW11 0LW, United Kingdom

Spin-transfer torque (STT) arises every time a spin-polarized current flows through a heterogeneous magnetic system and it underpins the operation of what is probably one of the most promising candidates for scalable, non-volatile memory technologies, the STT-MRAM. In these data storage units, the switching in each magnetic tunnel junction (MTJ) cell is driven by spin-polarised currents as opposed to stray magnetic fields in conventional MRAM cells. Accurate quantitative predictions for the switching currents in realistic MTJs are hence key to the development of STT-MRAM. Such modelling, however, poses a multi-scale problem as atomistic detail of the structure is essential together with the effect of the device environment, e. g. external magnetic field, finite temperature, defects, etc.

We present here the microscopic end of our in-house multi-scale MTJ-modelling scheme (see abstract by M. Ellis *et al.*). We consider the most widely-studied and technologically relevant MTJ, the Fe|MgO|Fe stack (figure 1), and explore a number of technically different formulations for the STT within an *ab initio* finite-bias transport method. This is based on the density-functional theory and the non-equilibrium Green's function approach (DFT+NEGF) as implemented in the Smeagol[1] code. Investigated are two of the most widely used steady-state formulations of STT: 1) the one based on the exchange field generated by the current-carrying electrons[2] and 2) the non-local variant based on the spin-current divergence[3]. We establish a quantitative equivalence of the two methods of evaluating the STT. The main computational bottleneck in this type of calculations is typically the self-consistency under current-carrying conditions but the two methods show different sensitivity to small variations of the charge distribution in the junction. The accuracy and the computational cost of the *ab initio* STT methods are key factor for the development of massive automated (high-throughput) material optimisation algorithms for STT-MRAM.

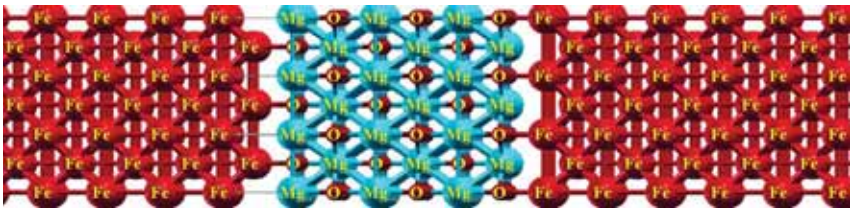

Figure 1. Atomistic cartoon of the Fe—MgO—Fe junction.

[1] A. R. Rocha, V. M. Garcia-Suarez, S. Bailey, C. Lambert, J. Ferrer, and S. Sanvito, Phys. Rev. B **73**, 085414 (2002).
[2] P. M. Haney, D. Waldron, R. A. Duine, A. S. Nunez, H. Guo, and A. H. MacDonald, Phys. Rev. B **76**, 024404 (2007); C. Heiliger and M.D. Stiles, Phys. Rev. Lett. **100**, 186805 (2008) .
[3] A. Kalitsov, M. Chshiev, I. Theodonis, N. Kioussis, and W. H. Butler, Phys. Rev. B **79**, 174416 (2009).

Topological torques in magnetic skyrmions and vortices

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The search for efficient electrical manipulation of magnetic textures has recently received a major boost with the recent realization of room temperature magnetic skyrmions[?] . A striking feature of current-driven skyrmion motion is the extremely low critical current at which it is observed in MnSi[1] and GeMn[3]. Indeed, critical current as low as 10^2A/cm^2 has been recorded implying that skyrmions can be moved by current four orders of magnitude smaller than in conventional current-driven domain wall motion. An interesting property of two- (or three-) dimensional textures such as skyrmions and vortices is that a spin-polarized carriers feel an emerging electromagnetic field on the form

$$E_i^s = s\frac{\hbar}{2e}\mathbf{m}\cdot(\partial_t\mathbf{m}\times\partial_i\mathbf{m}), \tag{1a}$$

$$\mathbf{B}^s = -s\frac{\hbar}{2e}\mathbf{m}\cdot(\partial_x\mathbf{m}\times\partial_y\mathbf{m})\mathbf{z}. \tag{1b}$$

The electric field is proportional to the first derivative in time and space therefore a moving magnetic texture induces a charge current and a self-damping. Interestingly, the effect of the magnetic field has been overlooked since it requires a second order derivative in space, and is generally considered as small. This magnetic field creates a local ordinary Hall current, so that the spin-dependent charge current driven by the external electric field reads

$$\mathbf{j}_e^s = \sigma_0^s\mathbf{E} + \sigma_0^s\mathbf{E}^s + \frac{\sigma_H^s}{B_\mathrm{N}}\mathbf{E}\times\mathbf{B}^s, \tag{2}$$

where the first term is the regular spin-dependent drift, the second term is driven by the emergent electric field and the third term is the (spin-dependent) Hall effect induced by the magnetic texture, or so-called topological Hall effect[?] . This topological Hall current is accompanied by a topological spin Hall current which is expected to induce a sizable torque on the magnetic texture.

In this work, I investigate the nature of topological Hall effect, topological spin Hall effect and its associated torque in both ferromagnetic and antiferromagnetic skyrmions. To do so, I used both analytical derivations and numerical calculations within nonequilibrium Green's function formalism implemented on a tight-binding model[4].

First, I will compute topological Hall spin and charge currents in ferromagnetic skyrmions and show how these mechanisms produce a large non-adiabatic torque[?] . Second, I will investigate the nature of these topological currents in antiferromagnetic skyrmions. I will show that the cancellation of the effective magnus force in antiferromagnetic skyrmions results in zero topological charge Hall effect but a non-vanishing topological spin Hall effect. Interestingly, in insulating antiferromagnets this topological spin Hall effect can become very large, up to two orders of magnitude higher than their ferromagnetic counterpart. The topological spin Hall effect in antiferromagnetic skyrmions results in a large non-adiabatic torque, similar to their ferromagnetic counterpart.

REFERENCES

[1] O. Boulle, *et al*, Nature Nanotechnology **11**, 449-454 (2016); C. Moreau-Luchaire, *et al*, Nature Nanotechnology **11**, 444-448 (2016); S. Woo, *et al*, Nature Materials **15**, 501-506 (2016).
[2] F. Jonietz, *et al*, Science **330**, 1648-1651 (2010).
[3] X. Z. Yu, *et al*, Nature **465**, 900-904 (2010); T. Schulz, *et al*, Nature Physics **8**, 301-304 (2012).
[4] A. Neubauer *et al*, Phys. Rev. Lett. **102**, 186602 (2009).

[5] A. Bisig, *et al*, arXiv:1511.06585 (2015).
[6] C. W. Groth *et al*, New J. Phys. **16**, 063065 (2014).

Investigation of Anomalous Hall effect on Ni-B thin films

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The research on magnetic sensor is an area that has rapidly grown over the last decade. Anomalous Hall effect (AHE) emerges as effective tool for measuring the magnetic characteristics of thin films and magnetic nanostructures [1]. Here, we investigate the Anomalous Hall effect in thin films of Ni-B prepared by electroless deposition. Deposition was carried out on polymer substrates 'cross-patterned' for Van der Pauw measurements. Figure 1, shows a measurement of Hall resistivity as a function of applied field for ferromagnetic films made of Ni-B. At high magnetic field the saturation of the effect can be observed indicating the ferromagnetic nature of the deposit.

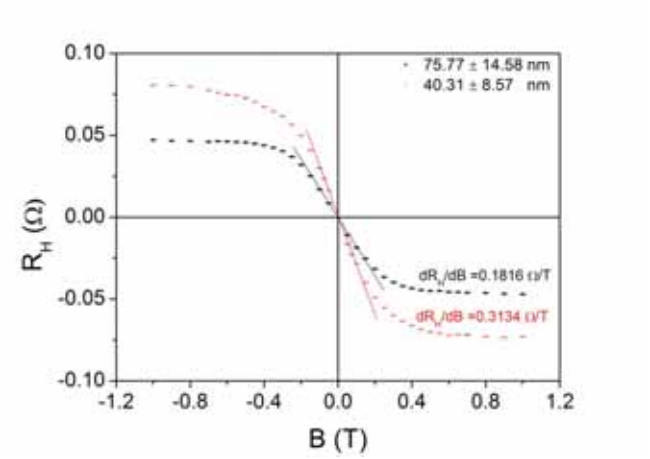

Figure 1. Hall resistance dependence on the film thickness of Ni-B films prepared by electroless deposition.

A systematic investigation of the dependence of the anomalous Hall effect on film thickness is carried out. The data also shows that decreasing the thickness of the Ni-B film leads to an increase in field sensitivity to a maximum measured sensitivity of about 0.3 Ω/T. Nanoscale films are of high interest due to their increased field sensitivity and application in high density magnetic recording devices.

Acknowledgment:

This work is supported by Science Foundation Ireland (12/IP/1692).

REFERENCES

[1] A. Gerber, A. Milner, M. Karpovsky, B. Lemke, H.-U. Habermeier, J.Tuaillon-Combes, M. Negrier, O.Boisron, P. Melinon, A. Perez, J. Magn. Magn. Mater. **242-245** (2002) 90-97

Combined Computational and Experimental Study of Liquid Phase Change Materials

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Employing large scale ab initio molecular dynamics (AIMD) and reverse Monte-Carlo (RMC) modeling together with experiments, we investigate selected phase change materials (PCM) in liquid and supercooled liquid state, addressing their structural, electronic and kinetic properties. Detailed knowledge about the liquid state of the PCMs is crucial for the elucidation of the switching process in both directions, namely the amorphous-to-crystalline and crystalline-to-amorphous transition: The amorphization occurs by local melting and the devitrification is connected to the high fragility [1] of the supercooled liquid state.

Our computational models of liquid PCMs contain about 500 atoms. The simulations are performed using a second generation Car-Parrinello-like method [2] and a nonlocal exchange-correlation functional (vdW-DF2) [3] that provides an improved description of van der Waals interactions. X-ray diffraction (XRD), neutron diffraction with isotopic substitution (NDIS) and oscillating-cup viscometer measurements [4] are carried out to determine the structure factors and the viscosity of the liquid state, respectively. We also perform reverse Monte-Carlo simulations [5].

Our analysis of the AIMD model trajectories [6] provides total/partial radial distributions, bond angle distributions (BADs), angular-limited three body correlations (ALTBC) and XRD/NDIS structure factors, as well as values for the diffusivity and the viscosity, for a set of temperatures ranging from 800 K to 1250 K. In the following, we discuss the properties of the PCM $Ge_2Sb_2Te_5$ in the liquid state. The AIMD structure factors obtained from vdW-DF2 simulations are in better agreement with experiments than GGA ones. The structure factor displays a prominent first peak followed by a smaller second peak. Together with the peaks of the BADs being centered around 90°, this indicates octahedral order [7]. The ALTBC distributions show significant Peierls distortion, which decreases with increasing temperature. Furthermore, we extract the diffusivity as a function of temperature from linear fits to the mean square displacements and determine the viscosities using the Stokes-Einstein relation. The estimated viscosities are in fair agreement with the viscometer measurements. In particular, fits of the Arrhenius function to the viscosity yield comparable values for the activation energy E_a. Overall, our study shows that AIMD simulations are capable to reproduce the experimental results well.

REFERENCES

[1] J. Orava, A.L. Greer, B. Gholipour, D.W. Hewak, and C.E. Smith, *Nat Mater* **11,** 279–283 (2012).

[2] T. Kühne, M. Krack, F. Mohamed, and M. Parrinello, Phys. Rev. Lett. **98** (2007) 066401

[3] K. Lee, E.D. Murray, L. Kong, B.I. Lundqvist, and D.C. Langreth, *Phys Rev B* **82,** 081101 (2010)

[4] R. Roscoe and W. Bainbridge, *Proc Phys Soc* **72,** 576–584 (1958).

[5] R.L. McGreevy and L. Pusztai, *Mol Simulat* **1,** 359–367 (1988).

[6] M. Schumacher, H. Weber, P. Jóvári, Y. Tsuchiya, T.G.A. Youngs, I. Kaban, and R. Mazzarello, Structural, electronic and kinetic properties of the phase-change material $Ge_2Sb_2Te_5$ in the liquid state, to be published in *Sci. Rep.*

[7] C. Steimer, V. Coulet, W. Welnic, H. Dieker, R. Detemple, C. Bichara, B. Beuneu, J.-P. Gaspard, and M. Wuttig, *Adv Mater* **20,** 4535–4540 (2008)

Atomistic simulation of thermal transport in GeTe nanowires

E. Bosoni [1], D. Campi [1], D. Donadio [2], S. Caravati [1], G. C. Sosso [3], and M. Bernasconi [1]

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[2] Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany
[3] Thomas Young Centre, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom

Chalcogenide alloys such as the $Ge_2Sb_2Te_5$ (GST) and GeTe compounds are of interest for applications in non-volatile phase change memories (PCM) thanks to their ability to undergo a fast and reversible phase transformation between the crystalline and amorphous phase upon Joule heating [1]. The set of the memory correspond to the melting and subsequent amorphization of the crystal, while the reset process correspond to the recrystallization of the amorphous phase. In recent years, the use of nanowires in PCM devices has been proposed to physically confine heat and current [2]-[3]. This could lead to a better scalability of the memory and also to a lower energy requirement for the writing/erasing process. An additional technological advance would be the realization of a multistate memory using core-shell nanowires [4].

Thermal transport is a key property for the device operation, as the writing/erasing process strongly depends upon heating dissipation and transport. Moreover, transport is strongly affected by the reduction of dimensionality.

In this contribution, we report on lattice thermal conductivity of a 6.5 nm diameter GeTe nanowire, calculated using non-equilibrium molecular dynamics (NEMD) simulations [5]. To this end, we used an interatomic potential generated with a Neural Network method [6]. An analysis of the phonon dispersion relations and lifetimes has been carried out in order to understand the origin of the significant reduction in the thermal conductivity obtained for the nanowire with respect to the bulk.

REFERENCES

[1] M. Wuttig and N. Yamada, Nature Materials 6, 824 (2007)
[2] S.H. Lee, D.K. Ko, Y. Jung and R. Agarwal, Appl. Phys. Lett. 89, 223116 (2006)
[3] S. Meister, H. Peng, K. McIlwrath, K. Jarausch, X.F. Zhang and Y. Cui, Nano Lett. 6, 1514 (2006)
[4] Y. Jung, S.H. Lee, T. Jenning and R. Agarwal, Nano. Lett. 8, 2056 (2008)
[5] F. Muller-Plathe, J. Chem. Phys. 106, 6082 (1997)
[6] G. C. Sosso, D. Donadio, S. Caravati, J. Behler, and M. Bernasconi, Phys. Rev. B 86, 104301 (2012)

Day 1 (June 29th, 2016)

8:30-11.00 *Registration*

9:15-9:30 Welcome

Keynote Lecture (Chair: Blanka Magyari-Kope)

9:30 – 10:00 "Revolution in Semiconductor Memories --- and the radical transformation of semiconductor business models as Moore's Law ends", **Rahul Sud** (Silicon Capital)

Session 1: Current Memory Technology (Chair: Blanka Magyari-Kope)

10:00-10:30 "Atomistic simulations of phase change materials for data storage", **Marco Bernasconi** (*Department of Materials Science, University of Milano-Bicocca, Milano, Italy*)

10:30-11:00 "Relativistic Ferroelectrics: a novel class of multifunctional materials", **Silvia Picozzi** (*Consiglio Nazionale delle Ricerche, CNR-SPIN L'Aquila c/o Univ. "G. D'Annunzio", 66100 Chieti, Italy*)

11:00-11:30 Coffee Break

Session 2: Phase Change Memory (Chair: Marco Bernasconi)

11:30-11:45 "Structural and metal-insulator transitions in Ge-Sb-Te phase-change materials", (contributed) **Riccardo Mazzarello**, (*Institute for Theoretical Solid State Physics, JARA-FIT and JARA-HPC, RWTH Aachen, Germany*)

11:45-12:00 "*Phonon scattering induced by line defects in silicon viewed from Atomic-Greens-Function approach*", **Tao Wang**[1], Jesus C. Montana[2], Natalio Mingo[2], and Georg K. H. Madsen[1], (contributed) (***1*** *Computational Materials Discovery (CMD), Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany,* ***2*** *LITEN, CEA-Grenoble, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France)*

12:00-12:15 "Devices with learning capability based on ferroelectricity as a state variable", **Riccardo Bertacco** (contributed) (*Department of Physics, Politecnico di Milano, Via G. Colombo 81, 20133 Milano, Italy)*

12:15-14:00 Lunch

Session 3 Resistive RAM I **(Chair: Ivan Rungger & Sergiu Clima)**

14:00-14:30 "Simulation and Modelling of the Switching Dynamics in Electrochemical Metallization and Valence Change Memory Cells", **Stephan Menzel** (*RWTH Aachen University and FZ Juelich, Aachen, Germany*)

14:30-15:00 "Atomic disorder – intrinsic source of variability in RRAM materials", **Sergiu Clima** (*IMEC, B-3001, Leuven, Belgium*)

15:00-15:30 "First principles simulations of doping effects on RRAM forming and switching characteristics" **Blanka Magyari-Kope** (Stanford University, USA)

15:30-16:00 Coffee Break

16:00-16:30 "Simulating Oxygen Vacancies in Transition Metal Oxides for Resistive Switching Applications", **Sebastian Wicklein** (SanDisk)

16:30-16:45 "Electron transport simulations for resistive switching memory devices" (contributed)**, Ivan Rungger**[1], Xiaoliang Zhong[2], Peter Zapol[3], Hisao Nakamura[3], Yoshihiro Asai[3], and Olle Heinonen[2]

[1]National Physical Laboratory, Teddington, TW11 0LW, United Kingdom; [2]Argonne National Laboratory, Lemont, IL, USA; [3]AIST, Tsukuba, Japan

16:45-17:00 "Spectroscopic fingerprint of resistive switching oxide interfaces probed by bulk sensitive photoemission spectroscopy", (contributed) **Giancarlo Panaccione**[a], Piero Torelli[a], Francesco Borgatti[b] ([a] *Consiglio Nazionale delle Ricerche (CNR), IOM- Lab. TASC, Trieste, Italy,* [b]*Consiglio Nazionale delle Ricerche (CNR), ISMN, Bologna, Italy)*

17:30-19:00 Poster Session

POSTER SESSION (12 total)

RRAM

R1 “Ab initio simulations of material applicability for 2D A-RAM memory devices”
Ernesto R. Ortiz, Blanca Biel and Francisco Gámiz
Departamento de Electrónica y Tecnología de Computadores, Facultad de Ciencias, Campus de Fuente Nueva, Universidad de Granada, 18071, Granada, Spain

R2 “Simulation of the electronic mobility dependence of the RESET operation for bipolar resistive switching”
Carsten Funck[1], Peter Schmidt[4], Manfred Martin[3], Rainer Waser[1,2] and Stephan Menzel[2]
1 Institut für Werkstoffe der Elektrotechnik II, RWTH Aachen University
2 Peter Grünberg Institut, Forschungszentrum Jülich
3 Institut für Physikalische Chemie, RWTH Aachen University
4 Physikalische Chemie, TU Darmstadt

R3 “Three-terminal Memristive MoS_2 Switch Fabricated with Helium Ion Beam”
Jakub Jadwiszczak[1], Darragh Keane[2], John J. Boland[2], and Hongzhou Zhang[1]
1 School of Physics, CRANN, Trinity College Dublin, Ireland
2 School of Chemistry, CRANN, Trinity College Dublin, Ireland

R4 “Effect of strain, thickness, and local surface environment on electron transport properties of oxygen terminated copper thin films”
Alfonso Sanchez-Soares, Sarah L. T. Jones and James C. Greer
Tyndall National Institute, University College Cork, Dyke Parade, Cork, Ireland

R5 “Non-equilibrium transport using order-N methods”
Marius Ernst Bürkle and Yoshihiro Asai
Research Center for Computational Design of Advanced Functional Materials, AIST, Central 2, Umezono 1-1-1, Tsukuba, Ibaraki 305-8568, Japan

MRAM

M1 “Transmission through correlated heterostructures with half-metallic ferromagnets”
C. Morari, A. Prinz-Zwick, M. Radonjic, R.-J. Zhang, I. Rungger, W. Appelt, L. Chioncel, U. Eckern
University of Augsburg, Germany

M2 “First-principles finite-bias spin-transfer torque in magnetic tunnel junctions”
Mario Galante, Maria Stamenova, and Stefano Sanvito
School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2, Dublin (Ireland)

M3 “First-principles finite-bias schemes for spin-transfer torque”
Maria Stamenova[1], Ivan Rungger[2] and Stefano Sanvito[1]
1 School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2, Dublin (Ireland)
2 Materials Division, National Physical Laboratory, Teddington, TW11 0LW, United Kingdom

M4 “Topological torques in magnetic skyrmions and vortices”
Collins Ashu Akosa, Papa Birame Ndiaye, and Aurelien Manchon
Physical Science and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia

M5 Investigation of Anomalous Hall effect on Ni-B thin films

Cian McKeown, Fernando M. F. Rhen
Department of Physics and Energy, Materials and surface Institute, University of Limerick, Ireland

M6 "HfO_2 and SiO_2 as barriers in magnetic tunnelling junctions"
Gokaran Shukla, Thomas Archer and Stefano Sanvito
School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2, Dublin (Ireland)

M7 "Ab-initio electron transport: the Smeagol code"
Ivan Rungger, Alex Reily Rocha, Thomas Archer, Maria Stamenova, Andrea Droghetti, C. Das Pemmaraju and Stefano Sanvito
School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2, Dublin (Ireland)

Phase Change

P1 "Combined Computational and Experimental Study of Liquid Phase Change Materials"
Mathias Schumacher
Institute for Theoretical Solid State Physics, RWTH Aachen, 52056 Aachen, Germany

P2 "Atomistic simulation of thermal transport in GeTe nanowires", E. Bosoni [1], D. Campi [1], D. Donadio [2], S. Caravati [1], G. C. Sosso [3], and M. Bernasconi [1] *[1] Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Via R. Cozzi 53, I-20125 Milano, Italy [2] Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128,Mainz,Germany, [3] Thomas Young Centre, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom*

Day 2 (June 30th, 2016)

Session 4: Resistive RAM II (Chair: Stefano Sanvito)

9:00-9:30 "Non-equilibrium transport theory from single molecules to nanoelectronics devices: examples of non-volatile memory cells" **Yoshihiro Asai** (*Research Center for Computational Design of Advanced Functional Materials, AIST, Central 2, Umezono 1-1-1, Tsukuba, Ibaraki 305-8568, Japan*)

9:30-10:00 "Forming processes of OxRRAMs" **Phillipe Blaise** (CEA-Grenoble)

10:00-10:30 "Electron injection Facilitated Defect Creation in Amorphous Oxide", **David Z. Gao**, Manveer Munde, and Alexander L. Shluger (*Physics and Astronomy, University College London, WC1E 6BT, United Kingdom*)

10:30-11:00 "Multiscale modeling of electron-ion interactions for engineering novel electronic devices and materials", **Luca Larcher** (University of Modena and Reggio Emilia & MDLabs, Inc).

11:00-11:30 Coffee Break

11:30-12:00 "Ab-initio Insight into Vacancy Formation and Diffusion in Resistive RAM Oxides" **Derek Stewart** (HGST, A Western Digital Company)

12:00-12:30 "Extended horizons: true atomistic simulations of junctions, interfaces and surfaces", **Anders Blom** (QuantumWise, Denmark)

12:30-12:45 "Surface Chemical Modification of Semimetal Nanowires for Schottky Barrier Diodes", (contributed) **Alfonso Sanchez-Soares** and James C. Greer, (*Tyndall National Institute, University College Cork, Dyke Parade, Cork, Ireland*)

12:45-14:30 *Lunch & Group Picture*

Session 5 Novel MRAM (Chair: Nick Kioussis)

14:30-15:00 "Ferroelectric tunnel junctions: Mechanisms for the tunneling electroresistance effect", **Evgeny Tsymbal** (Department of Physics and Astronomy, University of Nebraska, Lincoln, Nebraska 68588, USA)

15:00-15:30 "Contributions to impurities and surfaces to the device design", **Martin Gradhand** (University of Bristol)

15:30-16:00 Coffee Break

16:00-16:30 "Mechanisms of perpendicular magnetic anisotropy and Dzaloshinskii-Moriya interaction in magnetic layered structures", **Mairbek Chshiev** (SPINTEC CEA Grenoble)

16:30-16:45 "Magnetization reversal in CoFeB-MgO tunnel junctions via atomistic modelling", **Andrea Meo**, Phanwadee Chureemart, S. Wang, Roman Chepulskyy, Dmytro Apalkov, Roy W. Chantrell (University of York) (contributed)

19:00 Conference Dinner

Day 3 (July 1st, 2016)

Session 6 Spinning UP MRAM (Spin Transfer Torque RAM and Perpendicular Magnetic Anisotropy) **(Chair: Derek Stewart)**

9:00-9:30 "Antiferromagnetic spintronics", **Tomas Jungwirth** (Institute of Physics, Czech Republic)

9:30-10:00 "Revealing the Hidden Structural Phases of FeRh and Electric Field of Magnetization Direction across the Metamagnetic Transition", **Nick Kioussis** (*W. M. Keck Computational Materials Theory Center, California State University Northridge, Northridge, CA 91330 USA*)

10:00-10:30 "General switching voltages for magnetic tunnel junctions with in-plane and/or perpendicular-to-plane anisotropy free layers", **Alina Deac** (*Institute of Ion Beam Research and Materials Research, Helmholtz Zentrum Dresden-Rossendorf e V, Dresden, Germany*)

10:30-11:00 "The search for new materials for spintronics" **Stefano Sanvito,** *School of Physics and CRANN, Trinity College, Dublin 2, Ireland*

11:00-11:30 Coffee Break

11:30-11:45 "Manipulation of a spin current in a lateral spin valve"
R. M. Abdullah,[1] B. A. Murphy,[2] A. J. Vick,[2] M. Samiepour [1] and **A. Hirohata** [1] (contributed)
[1] *Department of Electronics, University of York*
[2] *Department of Physics, University of York*

11:45-12:00 "Multi-scale spin dynamic simulations of current-induced switching in magnetic tunnel junctions", **Matthew Ellis**, Maria Stamenova and Stefano Sanvito (contributed) *School of Physics and CRANN, Trinity College, Dublin 2, Ireland*

12:00-12:30 "The zero-moment half metal: How could it change spin electronics?"
Karsten Rode, Gwenaël Atcheson and Plamen Stamenov and **J.M.D Coey**
School of Physics, AMBER and CRANN, Trinity College, Dublin 2, Ireland

12:30-12:45 "The first ever real bistable memristor"
A. Ascoli, R. Tetzlaff and L.O. Chua, (contributed)
TU Dresden, Germany

12:45-13:00 *Closing Remarks*