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Controlling Electron Spin to Realise a Greener Future

Kevin Sewell[1,*]

[1] *Tyndall National Institute, University College Cork, Ireland.*

[*] *Corresponding author: 121103407@umail.ucc.ie*

At a Glance

The Information and Communication Technology (ICT) sector is consuming an ever-increasing amount of electricity. Most electronic devices are composed of billions of transistors, which are made of materials called semiconductors. Semiconducting devices can be engineered to hold properties that suit the device's function. One relatively unexplored property is electron spin, which, if it can be controlled, may be manipulated to increase the efficiency of semiconducting devices, particularly regarding data transfer and storage. I want to examine whether spin polarisation (the degree to which the spin of electrons aligns with a given direction) can be controlled. This is achieved by understanding the electron-scattering processes by which electrons change their spin polarisation in time. The ultimate potential impact of this research is leaner, greener telecommunications and computing.

Keywords: Physics, Spintronics, Computation, Technology, Scattering, Light, Germanium.

"The whole of science is nothing more than a refinement of everyday thinking."
— Albert Einstein

The need to understand electron spin

Currently, the Information and Communication Technology (ICT) sector uses 4-10% of global electricity use and generates 1.5-5% of greenhouse gas emissions. This includes user devices, data centres, and communication networks. The ever-increasing demand for ICT will cause an increase in global ICT energy use in the future, leading to further air, water and thermal pollution. It is therefore critical to produce more eco-friendly but effective telecommunication systems. Telecommunication devices are composed of semiconductors, which have conductivity between that of a conductor (metal) and an insulator. They are the foundation for smartphones, computers, and other electronic devices due to their ability to control and manage the flow of electric current in electronic equipment and devices. Examples of semiconducting materials are silicon and Germanium, both of which are Group-IV materials in the periodic table.

There are many well explored variables that alter the properties of various semiconductors. It is known that the efficiency of semiconductors can be influenced by manipulating electron spin, a field of study known as ”spintronics.”, which is still an active area of research, and the extent of its potential impact on semiconductor efficiency is yet to be fully realised. The aim is that electron spin can be used as an effective new alternative logic variable that can lead to higher-performance logic devices with lower power consumption.

How to understand electron spin

Electrons can either have spin-up or spin-down. They undergo a “spin-flip” if they transition from having spin-up to spin-down or vice versa. Electron spin plays a vital role in determining the electronic and magnetic properties of a material. I believe that by manipulating the spin of electrons, the flow of charge through the material can be controlled, leading to more efficient electronic devices with reduced power consumption and higher processing speeds. So, what exactly is it I am trying to do regarding electron spin? Let us first establish the relationship between electrons and light. When electrons jump to a higher orbit in an atom, light gets absorbed, and when electrons drop to a lower orbit, light gets emitted. I must also convey that in quantum mechanics, electrons exhibit wave-like properties and can be treated as waves. In that sense, electrons exhibit polarisation, which specifies the geometrical orientation of the wave oscillations. Polarised light waves only vibrate in one plane. Our research centres on the circular polarisation of light, whereby the light wave has a constant magnitude and is rotating at a constant rate in a plane perpendicular to the wave direction, as seen in Figure 1. I seek to map the ways the generation of circularly polarised light can be controlled in an alloy called Germanium-tin (GeSn). I achieve this by understanding the electron-scattering processes by which electrons change their spin polarisation in time. Let us examine ways in which electrons can scatter.

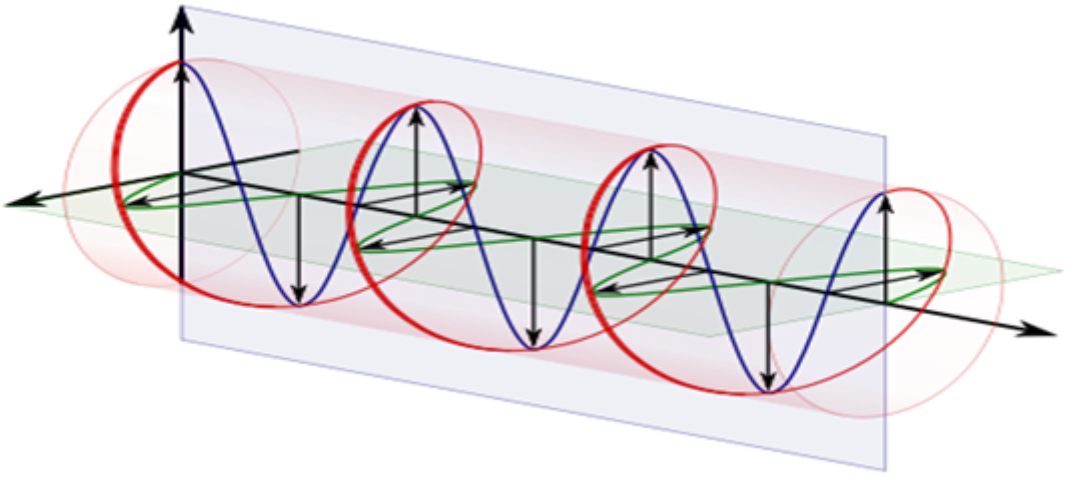

Figure 1: Circularly polarised light waves.

Scattering

Scattering is the change in the direction of motion and velocity of a particle (or wave) due to interactions with one another. Scattering can occur with various types of particles or waves, such as photons, electrons, neutrons, protons, and even waves like sound or light. Charge carriers, such as electrons, which travel through a semiconductor, can be scattered by all manners of disorders or "imperfections" such as alloying, vacancies (the absence of an atom in a periodic crystal), and phonons (which are vibrations in a periodic arrangement of atoms). I want to establish, for instance, if you vary the Sn content in GeSn, will alloy scattering affect the spin-orientation of electrons? I will also examine to what extent phonons assist electron spin-flips in these alloys.

If a relationship is established between the various scattering processes and spin-flips, it will open up a new way to control spin, allowing us better control of how electrons move through semiconductors. Subjecting the material to compressive or tensile strain could also affect the scattering and, therefore, the spin-orientation. As well as strain, doping (which is the introduction of impurities) and nano-structuring can alter the spin-orientation by influencing the scattering, so there are many variables to examine.

Density Functional Theory

The parameters that determine the different scattering processes that affect electron spin are calculated using Density Functional Theory (DFT) codes. DFT is a quantum-mechanical method used to calculate the electronic structure of atoms, molecules, and solids. Its affordability and high-performance ratio mean large molecular systems can be analysed accurately, making it the most used electronic structure method. Examples of the parameters calculated using DFT codes are primarily the molecular and crystal structure but also the bandgaps (the energy ranges where no electronic states exist), the effective masses (the mass a particle such as an electron seems to have when responding to forces or interacting with other electrons), and alloy scattering parameters, which are potentials that determine the strength with which an electron scatters from one location to another. Several software options are available for DFT calculations, including ABINIT (which I use), Quantum ESPRESSO, and VASP.

More specific applications

The overall aim, as discussed, is to explore the possibilities in using electron-spin as a new logic variable that can be controlled to produce more efficient semiconductor devices. I work with the semiconductor GeSn, which can be used in transistors, light sources, and low-resistivity contacts, but there are potentially several more specific applications. If electron spin does prove to be an effective new logic variable, further developments could be realised in polarisation modulation, which in essence serves as an added degree of freedom for modifying carrier waves. This makes it ideal in realising simple transceivers (which are devices that are a combination of a radio transmitter and receiver) and play a crucial role in modern communication.[1]

The direction of spin of photons and electrons is tied to the handedness (see Figure 2) of circularly polarised light. Circular dichroism (CD) is the differential absorption of left- and right-handed circularly polarised light and is the basis of a type of spectroscopy that can be used to determine the handedness (chirality) of molecules. Some semiconductors have a chiral structure. They can interact with circularly polarized light in interesting ways due to their chiral nature. When circularly polarized light interacts with chiral materials, it can lead to differences in absorption or emission of the light depending on its handedness. Analysing the CD spectra of these materials can provide insights into the electronic and optical properties of chiral semiconductors. This could lead to advancements in light-emitting diodes (LEDs), which are used in most light-emitting devices, and laser diodes, which are used in optical communications, barcodes, laser pointing, laser printing, surgical instruments, and spectroscopy.

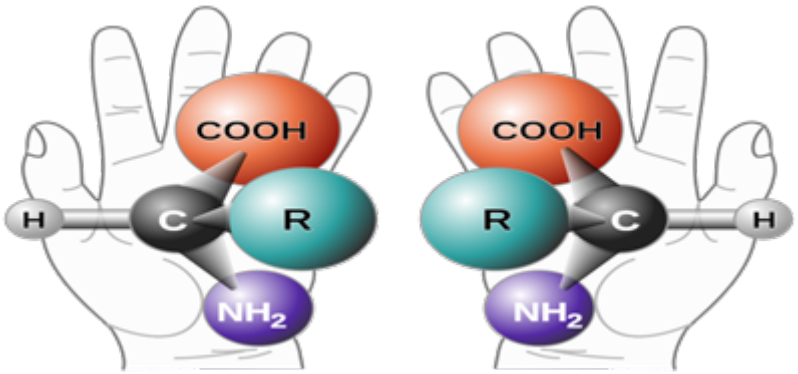

Figure 2: Chiral objects, displaying left- and right-handedness.

Most recent developments

Previous work

There are recent papers that explore the theory of spin flips by electron-phonon scattering and impurity scattering in silicon. This is one of the most important sources of spin relaxation in group-IV semiconductors like GeSn or silicon. These models establish important relations between the electron energy levels (or electronic band structure) and experimental findings. In most models, the spin lifetimes are left as a free parameter to be determined by experiment. I want to calculate them from first principles (that is, to use fundamental definitions and axioms for the problem at hand) to gain a true understanding of their control.

Many of the properties of GeSn remain unknown. Bandgaps have been calculated using different theories, and the results correlate well. Effective masses have only been calculated in part. Crucial to understanding spin polarisation are the alloy scattering parameters, which have not been previously determined, and phonon parameters, which have been calculated for Germanium but not GeSn. Early research (first from Murphy-Armando and Fahy[2] and now furthered by my own calculations) suggests GeSn possesses a higher mobility than Germanium; that is to say, electrons move quicker through GeSn, making it more efficient.

Our findings thus far, and what is to follow

I have calculated the alloy scattering parameters for GeSn and will soon examine how they affect the electron spin. The effect of phonon scattering on spin-flips remains undetermined, but I plan to calculate the phonon parameters for GeSn using first principles methods.[3] Once it has been established how various forms of scattering affect the spin-orientation of electrons, I will examine how strain, alloying, doping, and nano-structuring affect the spin-flips, and whether the spin-flips can be controlled by these variables. I have also begun calculating some optical properties of GeSn, which are also important in understanding spin polarisation. Such properties include the dielectric function, which is a measure of the degree to which a material can be polarised, and the absorption coefficient, which equates to the reciprocal of the depth of penetration of radiation into a bulk solid.

Conclusion

To help solve the issue regarding energy consumption caused by the ICT sector, I aim to explore if electron-spin can be used as a new logic variable, which can be manipulated to make electronic devices more efficient and greener through improved control of current. I do this by understanding the ways in which electrons scatter through a semiconducting material, with a particular focus on GeSn. The impact of the different scattering forms on the spin polarisation can help us understand how the spin states are best controlled through alloying, strain, and other variables to realise more efficient devices. Findings will be used by experimental collaborators to grow new Germanium alloy materials which can be engineered into devices to enable lower energy data transfer.

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Declaration of Interests

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Author Bio

Kevin is a third-year PhD student in Computational Physics. He graduated with a BA in theoretical physics from TCD and a MSc in mathematical science from UCD. Kevin tutored in maths in UCD before embarking on his PhD, in which he is seeking to understand the electron-scattering processes by which electrons change their spin polarisation in time. He is based in Tyndall National Institute and UCC. He has presented his work in conferences in France and Italy. He hopes his work can lead to greener and leaner telecommunication and computing.

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