Research Project Proposal (1000 words max.)

Title

The title for the proposed project is "**Lattice stretching and depletion of electrons - when is it possible for perfectly ordered simple metals to become ferromagnetic?**"

Abstract

This research project is an investigation into what happens when the structure of certain metals is altered at the nanoscale, with the specific aim of changing the physical properties of these metals in order to make them magnetic - or, in some cases, more magnetic. This will be done by using a highspeed computing system to simulate the quantum properties of these metals through setting up calculations evaluating several experiments, supervising them while they run and then analysing and interpreting the results.

Introduction and Background

The three metals to be analysed during the course of this experiment are copper, nickel, and palladium. On the Periodic Table, these have the symbols Cu, Ni, and Pd, respectively. These three metals have been chosen as they all have face-centered cubic structures, which means they have the same type of atomic arrangement - a tightly packed cubic lattice. This is important as it allows the three elements to be similarly analysed and their reactions to the experiments to be compared.

Magnetism is a property that some materials have - that of being magnetic. Ferromagnets have the strongest magnetic fields of any magnetic materials, and ferromagnetism is the strongest type of magnetism. Of the three metals in this experiment, regular copper is completely unmagnetic, nickel is ferromagnetic, and the magnetic susceptibility of palladium is linked to its hydrogen content.

Stoner's Criterion is a yes-or-no criteria to tell whether a metal should be a ferromagnet or not. Through using the density of states to calculate an integral, it indicates if the Fermi level is above or below a certain threshold - which gives a good indication of the presence or absence of magnetic properties in any given particular metal. The Fermi level is the amount of work that is needed for one electron to be added to a system, and the density of states is a mathematical function that describes the probability density of the state of a system at different energies.

Previous Research

Investigations into this field have been undertaken by researchers previously - for example by Dr Oscar Cespedes at the University of Leeds - but not from the same angle and not by using the same methods that are proposed in this research project.

Methodology

The three metals - copper, nickel and palladium - that are to be looked at during this research (with the objective of making them more magnetic) would be entirely simulated on Trinity College Dublin's High Performance Computing System, which would allow calculations such as analysing where the Fermi level is in relation to the density of states to be performed. The Vienna Ab initio Simulation Package (VASP) - a computer programme designed to model materials at an atomic scale - will be used to determine a density function for the simulated metals and their altered versions with removed electrons, which will allow us to determine which metals are perfectly ferromagnetic, and which ones are perfectly not. The expected result is that the theoretical electron depletion will make the metals more ferromagnetic.

A number of plots will be obtained from this experimental research - including one that plots the strain as a percentage change in length against the material-adjusted number of electrons removed from the structure.

The fact that this experiment will be entirely simulated on a computing system means that it would be easily done remotely online, if COVID-19 restrictions meant that physical access to Trinity College Dublin was not possible.

Detailed Project Plan

The six-week plan for this project is as follows:

Week 1: Arrange set-up for computer simulations of the three types of metals on the high performance computing system. Ensure that all is ready to begin the experiment, that all calculations are initialised, that the system is working properly etc. Confirm that the properties of the metals are correctly inputted on the system, and determine that the simulations mathematically resemble the elements in their physical form.

Week 2: Launch calculations on the computing system. Run tests to double-check that the simulations are working as expected, and supervise system over the week to ensure that the calculations are running correctly. Closely monitor the completion of the calculations to ensure a high degree of accuracy in their computing.

Week 3: Begin collecting results of calculations completed during Week 2. The simulation will keep running during this time, but more and more results will be obtained every day.

Week 4: A continuation of Week 3, further gathering results of calculations until they have all been computed - concluding the simulation aspect of the experiment.

Week 5: Plot obtained calculation results - including the density of states, the phase diagram result, the Fermi level and Stoner's Criterion analysis.

Week 6: Conclude experiment by evaluating and analysing results and plots, completing a final write-up and drawing meaningful conclusions about the achievements of the experiment, using the original aims and goals as headings with which to measure the experiment's success. Note how the actual results are similar to and differ from what the expected results were at different stages in the experiment, and come to a conclusion on the effectiveness of electron depletion on the materials' ferromagnetism.

Implications of Research

This research has major implications in the field of quantum computing, with particular related applications in the area of quantum semiconductors. If metals can theoretically be made to be more magnetic in a lasting way - or even given magnetic properties where none existed before - this would have many applications in nanoelectronics and solid state physics, allowing the lattice structure of materials with face-centered cubic structures to be modified in such a way that they gain more applications - e.g. to create longer-lasting computer hard drives.