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Magnetising computer-simulated copper

Lattice stretching and depletion of electrons - when is it possible for perfectly ordered simple metals to become ferromagnetic?

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Introduction

Copper
29
Cu
63.546

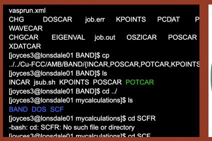
This research project is an investigation into what happens when the structure of copper is altered at the nanoscale, with the specific aim of making the copper ferromagnetic. Copper (chemical symbol *Cu*, left) is a non-magnetic metal found in group 11 on the periodic table. It is an excellent conductor of both electricity and heat and has many uses.

Ferromagnetism is the property of being magnetic - a ferromagnet has an extremely strong magnetic field. If successfully magnetised, the copper could be used to (e.g.) create longer-lasting computer hard drives.

VASP

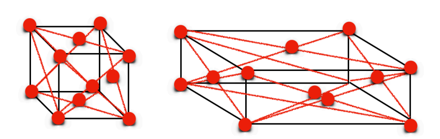
The copper was simulated on VASP (Vienna Ab initio Simulation Package), a software that allows nanophysical parameters to be altered and calculations to be carried out.

VASP was run on the Lonsdale cluster of the Trinity Centre for High Performance Computing (TCHPC), which was accessed using Linux commands in Terminal (below left).



```
vasprun.xml
CHG       DOSCAR    job.err   KPOINTS   PCDAT     P
WAVECAR
CHGCAR    EIGENVAL  job.out   OSZICAR   POSCAR
XDATCAR
[joyces3@lonsdale01 BAND]$ cp
../../Cu-FCC/AMB/BAND/{INCAR,POSCAR,POTCAR,KPOINTS
[joyces3@lonsdale01 BAND]$ ls
INCAR  jsub.sh  KPOINTS  POSCAR  POTCAR
[joyces3@lonsdale01 BAND]$ cd ../
[joyces3@lonsdale01 mycalculations]$ ls
BAND  DOS  SCF
[joyces3@lonsdale01 mycalculations]$ cd SCFR
-bash: cd: SCFR: No such file or directory
[joyces3@lonsdale01 mycalculations]$ cd SCF
```

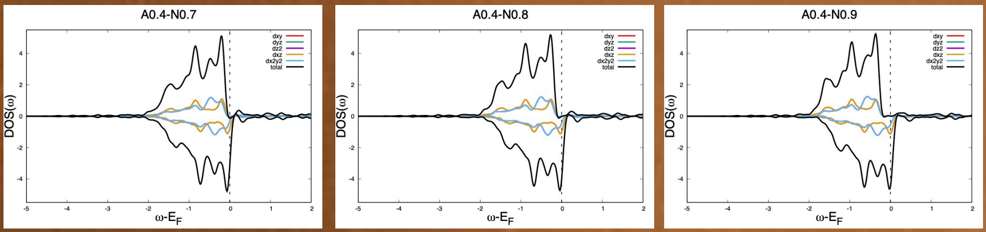
Atomic Structure



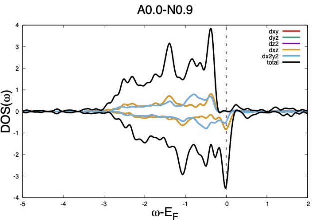
Two properties of the copper atoms were altered during the course of this research. The first - *N* - was the number of electrons depleted from the atom. The values of N used ranged from 0.7 to 0.9, increasing in steps of 0.02. The second variable, *A*, refers to the lattice constant: above is a rough approximation of how the crystal lattice structure of copper would be "stretched out" by changing this value. Copper has a face-centred cubic structure, which is why the atoms are in the centre of each face of the cubes. The values of A were -0.4, -0.2, 0.0, 0.2 and 0.4.

Graphs

The graph titles below refer to the values of the variables used - e.g. "A0.4-N0.7" means a lattice constant of 0.4, and 0.7 electrons depleted.



Above are three examples of graphs that I plotted. E_F - the Fermi energy - is plotted on the x-axis, while the density of states (DOS) is on the y-axis. I have chosen to include three graphs with a fixed A-value (0.4) to allow for comparison between them as the N-value increases - note how the high and low peaks both move farther away from the centre dotted line as more electrons are depleted. I obtained graphs for every possible combination of A and N - 55 graphs in total. On the right for visual comparison there is a graph that has a different lattice constant, but a fixed electron depletion, to the graph on the above right. To calculate E_x, the distance between the Fermi energies, I measured between the first upward peak and the first downwards peak from the left, and then repeated for the second and third peaks.



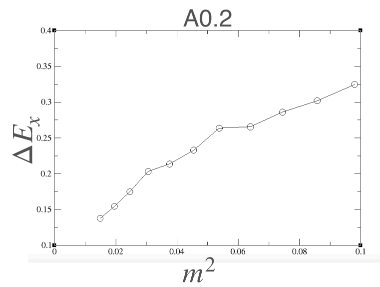
Table

Below is a small section of a table with the measured values from VASP (the magnetic moment m) and the graph values for the first, second and third peaks with their mean - "*avg x*", meaning ΔE_x.

	x (up)	x (down)	x diff	avg x	m	m^2
A-0.4-N0.7	-0.25	-0.15	-0.1	0.10566	0.091	0.00828
(peak 2)	-0.737	-0.63	-0.107			
(peak 3)	-1.14	-1.03	-0.11			
A-0.4-N0.72	-0.285	-0.146	-0.139	0.13033	0.128	0.01638
	-0.72	-0.58	-0.14			
	-1.122	-1.01	-0.112			
A-0.4-N0.74	-0.31	-0.11	-0.2	0.20066	0.16	0.026
	-0.77	-0.564	-0.206			
	-1.16	-0.964	-0.196			

Final Graphing

Here is the final graph for the lattice constant 0.2. This graph has 11 points plotted, one for each input value of N. As expected, the fit is roughly linear, so it is likely that the copper has been magnetised.



Calculations

After obtaining a numerical value for the slope of the final graphs, I calculated the Stoner criterion as below. The Stoner criterion is a single yes-or-no value that indicates whether a particular metal will act as a ferromagnet - if the criterion is greater than or equal to 1 then magnetic properties are present. It does this through evaluating the Fermi level from the density of states and the Fermi energy.

$$I \times \mathrm{DOS}(E_F) \geq 1,$$

where I is the slope of the graph and $\mathrm{DOS}(E_F)$ is the density of states at the Fermi energy. The values of I for A-values 0.0, 0.2 and 0.4 were all ~2.25, for A = -0.4 the value was ~2.7, and for A = -0.2, I was equal to approximately 4.819.

Conclusion

In conclusion, yes, it is possible to magnetise simulated copper by depleting electrons and manually changing the value of the lattice constant. From the use of the Stoner criterion, density of states and Fermi level, it is possible to mathematically determine when the metal has successfully been magnetised.

One element of note from the end results is that the graphs obtained for A = -0.2 and A = 0.0 contained points that didn't precisely match the linear fit - this is something with much potential to be further investigated and understood.

Sources

All graphs, tables and images are original asides from the VASP logo (in "VASP") - [www.vasp.at], and the copper spool image (in "Introduction") - [www.medicalnewstoday.com/articles/288165] .

G. Kresse and J. Furthmüller, *VASP the GUIDE*, Vienna (2005) - L. MacEnulty and D. O'Regan, *Calculation of the Magnetostatic Energy in Spin Density Functional Theory*, Dublin (2020) - M. Sigrist, *Solid State Theory*, Heidelberg (2010) - K. Capelle, *A Bird's-Eye View of Density-Functional Theory*, São Paulo (2006) - J. Perdew, A. Ruzsinszky, L. Constantin, J. Sun and G. Csonka, *Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed*, Budapest (2008) - K. Burke et al., *The ABC of DFT*, California (2007).

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