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SEARCH FOR HALF METALLICITY IN HEUSLER ALLOY Fe_2NiAl FOR SPINTRONIC APPLICATION USING DENSITY FUNCTION THEORY

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ABSTRACT
Fast, durable, non-volatile and inexpensive data storage in electronic devices is greatly desired both for work and entertainment. Components that can provide these qualities continue to be developed by material scientists as companies continue to compete to produce devices possessing these qualities. Giant Magnetoresistance (GMR) and Tunnel Magnetoresistance (TMR) are properties that would greatly contribute to a device having these qualities. Half metals have attracted interest for their potential use in Metallic Tunneling Junctions (MTJ's) fabrication, as well as spintronics due to their ability to provide full polarization of conduction electrons hence high GMR and TMR values. Heusler alloys, some of which exhibit half metallic character are intermetallic compounds which would be suitable in fabrication of MTJ's with high GMR and TMR values. The electronic structure of Heusler alloy Fe_2NiAl was investigated using first principle calculations of the density functional theory (DFT); the energy of exchange and correlation was treated by the generalized gradient approximation (GGA). Preliminary results point to the electronic structure of the alloy having a gap in the majority band, hence exhibiting desirable half metallic ferromagnetic character. This will contribute in design and fabrication of MTJ's used in magnetic random access memory (MRAM) currently occupying a great deal of effort of material designers in spintronics technology.

Keywords: Half metal, Spintronic, Giant magnetoresistance, Haussler alloys, Density functional theory, Magnetic random access memory

INTRODUCTION
Spintronics is an emerging technology exploiting both the intrinsic spin of the electron and its associated magnetic moment in addition to its fundamental electronic charge in solid state devices (Klaer, 2012). Spin dependent electron transport phenomena in solid state devices has led to discoveries which include spin polarized electron injection from a ferromagnetic metal to a normal metal, Magneto Resistance (MR) in particular, Giant Magneto Resistance (GMR) and Tunnel Magneto Resistance (TMR). MR is sensitive to spin polarization and is applied in making Metallic Tunneling Junctions (MTJ) with very high MR values. Some of the metal based spintronic devices include TMR and GMR devices such as read heads of modern

hard drives with higher head sensitivity, able to read weak magnetic signals and spin transfer torque devices. Another device is the Magneto Resistive Random Access Memory (MRAM), which is nonvolatile, has low power usage and good shock robustness (Lacaze and Lacroix, 2014). Others are spin wave logic devices which utilize the phase to carry information. Interference and spin wave scattering are utilized to perform logic operations. In 2012, IBM scientists mapped the creation of persistent spin helices of synchronized electrons persisting for more than a nanosecond. This opened new paths to investigate for using electron spin for information processing (Markoff, 2012). Others include magnetic field sensors, biosensors, microelectromechanical systems (MEMS) and compasses in consumer devices such as mobile phones and tablet computers amongst others (Parker, 2003).

Half metals have a metallic band structure for one spin channel and an insulating band gap at the Fermi level for the opposite spin. This provides a complete polarization of conducting electrons. The first material to be predicted to be half metallic ferromagnets were Cl_b type half Heusler alloys NiMnSb and PtMnSb, whose half metallic character was discovered by de Groot using first principles calculation based on Density function theory (DFT) in 1983 (Luo, Zhu, Ma, et al., 2008). Half metallic ferromagnets have a 100% spin polarized current. They can be used as spin filters and as spin injectors for magnetic random access memories and other spin dependent devices as an alternative to ferromagnetic 3d metals, which have a spin polarization of 40% - 50% and cause problems due to a large difference between the resistances of metal and semiconductor substrates (Luo, Zhu, Liu, et al., 2008). If MTJ's are made using half metallic materials with spin polarization of one, MR values would become infinite, hence the importance of half metallic thin films (Parker, 2003).

Heusler alloys have been found to exhibit half metallic behavior (Luo, Zhu, Liu, et al., 2008). From experiment, majority of Heusler compounds order ferromagnetically in stoichiometric composition and saturate in weak applied fields. They have a major advantage due to their structural similarity to binary semiconductors used industrially and their high curie temperatures as compared to other half metallic materials (Galanakis, Özdoğan, Şaşıoğlu, and Aktaş, 2008).

In view of this, the electronic structure of Fe_2NiAl is investigated using first principle calculations of the density functional theory (DFT) in which the energy of exchange and correlation is treated by the generalized gradient approximation (GGA). The findings from this study will sensitize industry players about the potential applications of Fe_2NiAl in technology.

METHOD OF CALCULATION

The first principles calculations of the electronic structure were performed using DFT. The GGA exchange correlation functional was used to calculate the total energy using pseudopotentials and plane waves. The Kohn and Sham single electron equation, equation 1 that yields the electron density was solved. The irreducible part of the Brillouin zone was divided using a grid of 12 x 12 x 12 points.

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_i^2}+\frac{\partial^2}{\partial y_i^2}+\frac{\partial^2}{\partial z_i^2}\right)+V_{H(r)}+V_{xc(r)}+V_r\right]\psi_i(r_i)=\epsilon_i\psi_i(r_i) \qquad (1)$$

Where, $V_{H(r)}$ is the Hatree potential, $V_{xc(r)}$ is the correction to self interaction in $V_{H(r)}$ as well as exchange and correlation contributions to the single electron equations. V_r is the interaction between an electron and the collection of atomic nuclei.

The solution to equation 1, ψ_i is used to determine the density of electrons $n(r)=2\sum_i \psi^*{}_i(r)\psi_i(r)$ a function of 3 coordinates and contains physically observable information. The total energy calculated includes the sum of one electron energies and double counting corrections (Sholl and Steckel, 2011).

The single electron Kohn-Sham equations were solved using the self consistent approach according to the algorithm shown in Figure 1.

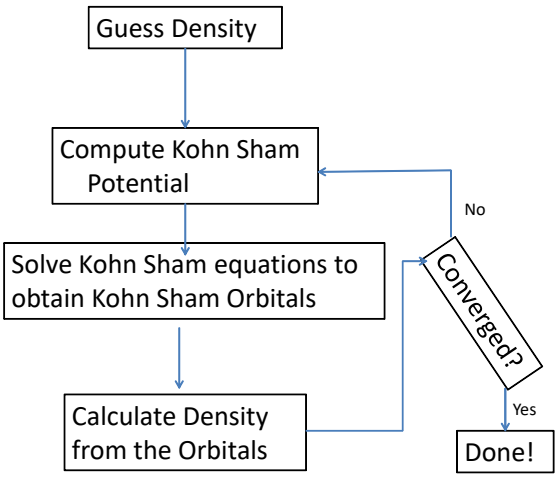

Figure 1: Kohn-Sham DFT Algorithm

To solve the Kohn Sham equation, $V_{H(r)}$needs to be defined. To define $V_{H(r)}$, $n(r)$ needs to be known. To know $n(r)$, $\psi_i(r)$needs to be known. To know $\psi_i(r)$, the Kohn Sham equation needs to be solved. To break this cycle, the problem is treated in an iterative way as outlined in the following algorithm;

(i) Define an initial trial $n(r)$

(ii) Solve the Kohn Sham equation to find $\Psi_i(r)$

(iii) Calculate $n(r)$ defined by Kohn Sham single particle wave functions from step (ii)

$$n_{ks}(r) = 2\sum_i |\psi_i(r)|^2$$

(iv) Compare $n_{ks}(r)$ with $n(r)$. If the same, then this is the ground state electron density and it can be used to compute the total energy. If not equal, update $n(r)$ and continue from step (ii). This process should lead to a solution of the Kohn Sham equation that is self consistent. However, the exchange correlation energy needs to be known (Sholl and Steckel, 2011).

RESULTS AND DISCUSSION

Self consistent calculations for Fe, Ni and Al were done (Giannozzi et al., 2009) . The crystal structures of Fe obtained had the expected body centered cubic structure as shown in figure 2.

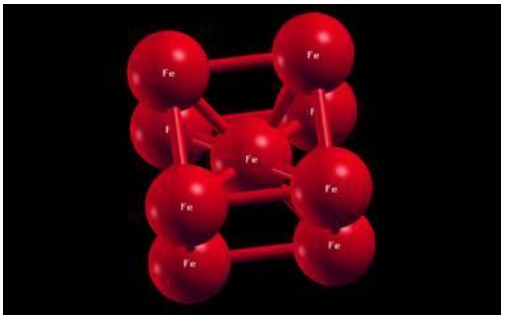

Figure 2: Crystal structure for Fe
The crystal structure for Ni was found to be the face centered cubic structure as shown in figure 3.

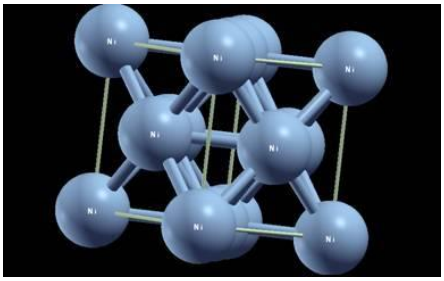

Figure 3: Crystal structure for Ni

Both the lattice parameters for Fe and Ni obtained are slightly less than expected. The crystal structure for Al was the face centered cubic as shown in Figure 4.

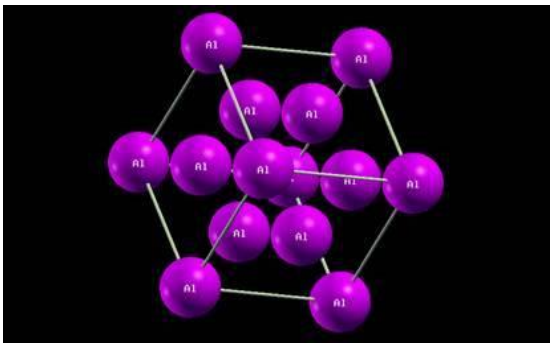

Figure 4: Crystal structure for Al

The partial density of states for Ni was also calculated. Figure 5 displays the dominance of d states at the fermi level

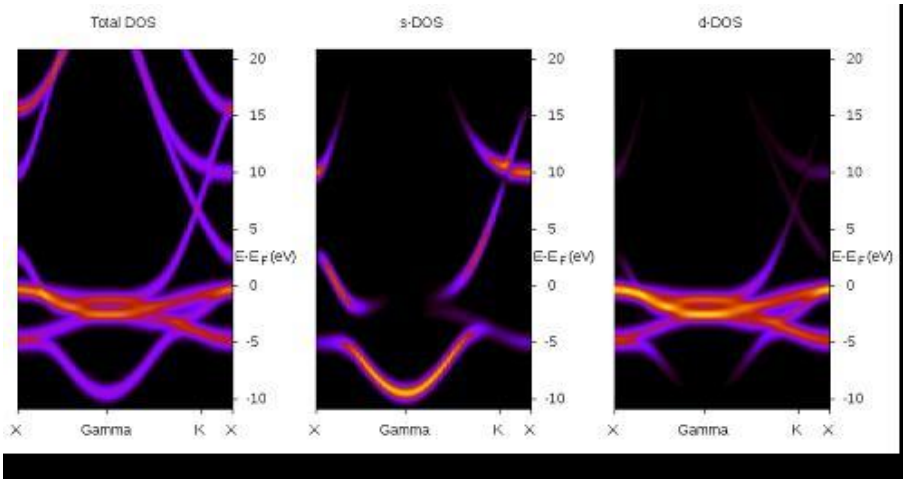

Figure 5: PDOS for Ni majority states

Due to the slightly contracted lattice, d-d hybridization of Fe and Ni states is expected to result in a band gap for the minority states at the fermi level. The electronic structure calculated for Fe_2NiAl using the full potential linear Augmented plane wave method, revealed a pseudo gap as shown in figure 6.

The calculated magnetic moments were 4.25 μB per formula unit (Doumi et al., 2015). This is quite close to an integer giving indications that the alloy possesses a half metallic character. According to the Slater Pauling rule for predicting if a Heusler alloy is half metallic or not, a value of 5 μB per formula unit for Fe_2NiAl would be expected. This suggests a half metallic ferromagnetic character. This is as expected, as the structure is found to be the Hg_2CuTi structure, similar to half heusler structure in which covalent band gaps are commonly exhibited.

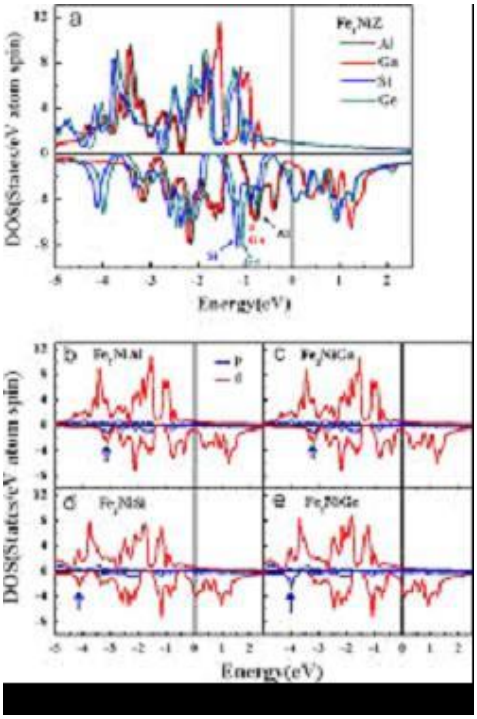

Figure 6: Density of States of FeNiAl: Source – Doumi et al., 2015

The bands formed are mostly of the d states of Fe and Ni, while the p states of Al participate in the hybridization.

CONCLUSION

Heusler alloy Fe_2NiAl promises to be one of the materials that will enable material scientists to fabricate components displaying high GMR and TMR values due to its spin polarization. This will greatly contribute to advances in spintronics technology. In addition, the significant role of lattice parameter in hybridization is brought out by this study, a physical property which is controlled at the atomic level and can therefore not be investigated experimentally but can be investigated computationally, displaying the power of computational studies.

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