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Investigation of the Magnetic, Electronic and Structural Properties of Nickel, Cobalt, and Iron Thin Layers on Silicon (001) Substrate

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ABSTRACT

In spintronic new science, the attempts have been focused on the use of spin of electron in addition to the electron charge to create a wider and new application for microelectronic components. Moreover, one of the main issues in the spintronic is finding the appropriate sources to produce and inject the bipolar spin current from a ferromagnetic substance into semiconductors, which is called spin-injection operation. Therefore, it is necessary to grow a thin ferromagnetic layer on the semiconductor.

Nowadays, the use of silicon substrates has been considered in the production of thin ferromagnetic layers such as cobalt, nickel, and iron (Ni-Co-Fe) layers. In this system, due to the electronegativity similarity of Ni-Co-Fe and silicon, there is a strong interaction between Ni-Co-Fe and silicon atoms. In the present study, Nickel, Cobalt and Iron layers were selected as ferromagnetic metals and silicon as a semiconductor substrate.

The aim of this study is to find the optimal location of cobalt, nickel, and iron atoms on silicon and investigate magnetic properties. The calculations are based on the primary quantum principles and in the framework of the density functional theory (DFT). Kohn-Sham equations have been solved using full-potential linearized augmented plane wave (FP-LAPW) and wien2k software.

Keywords: *Density functional theory, Ferromagnetic, Thin layer, Spintronic, Semiconductor*

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INTRODUCTION

The thin layers have special properties that vary considerably from those of their respective materials in volumetric state. This difference emerges from their geometric shape, physical dimensions, and microstructure. In addition, these characteristic properties of thin layers can be adjusted and modified to a large extent to achieve the desired physical characteristics. These features form the basis for development of applications of thin layers in various devices. Some of these applications are in submicron dimensions such as microelectronic circuits with very high density and so on. In fact, thin layers are essential parts in many modern electronic and optical instruments. Taking into account the numerous advantages of thin layers, it can be predicted that in the near future, the era of volumetric materials will end and most of the devices will be designed and made using the thin layer technology (Prinz et al., 1995; Gtistis et al., 2002)

Characteristics of thin layers:

When a solid material is in the thin layer form, it is formed on an appropriate solid support (substrate) with a small thickness layer. This layer may be achieved directly by a physical process like evaporation-condensation or through an electrochemical or chemical reaction. It should be noted that the small thickness of these layers is not the only contributor to their special and prominent properties, rather the microstructure of these layers, which is created through their unique formation process of continually increasing the initial structural parts one after the other, is more important. The features of thin layers and the importance of investigating the behavior of two-dimensional solids have gained particular interest in such a way that the thin layer is widely used in numerous modern electro-optic components in the manufacture of micro-valves, micro-pumps, smart micro-pipes, Nano-robots, Nano Chengs, etc. In addition, it can be used in aircraft industry, medical engineering, tissue engineering, cardiac angiography operation, and orthodontics. Magnetic-optic characteristics of thin ferromagnetic layers are of great importance in optical switching and (Hortamani et al.,2004;Grffith et al.,1990)

Another interesting application of the thin layers are in transistors. Transistor is an electronic solid-state device made of semiconductor materials such as silicon and germanium (Zwier phzycki et al.,2003)

Spintronic:

In addition to rotation around the nucleus, electron also has a rotating motion around itself that is called the “electron spin”, meaning the rotation of electron. Spintronic has several components, including the injection of a bipolar spin current with a specific spin direction into the semiconductor (Asada et al., 1997).

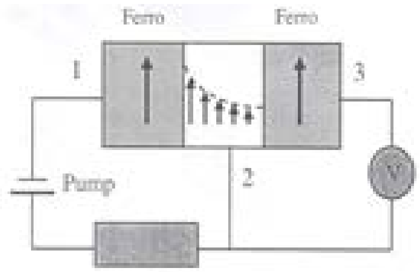

Figure 1. Injection of bipolar spin current

When a semiconductor is covered with a ferromagnetic material such as cobalt, nickel, or iron, and the resulting structure is placed in a circuit like figure 1, then the current generated in the magnetic field will penetrate into the semiconductor, which is called the spin current. The main purpose of injecting ferromagnetic materials into the semiconductor is to use these thin ferromagnetic layers as a source for bipolar spin current; this process is called spin injection (Brown et al., 2000; Blaha et al., 2001).

Supercell Silicon containing cobalt, nickel, and iron thin layer:

Nickel, cobalt, and iron are ferromagnetic materials with a strong interaction with silicon, hence they can induce a spin current into semiconducting silicon. The placement of Ni-Co-Fe atoms in different situations will lead to different properties. Therefore, one of the objectives in this study is to find the best position for these atoms in order to minimize energy consumption and increase stability of the structure. Based on the wien2k program, and considering that the appropriate supercell silicon contains 8 layers and a vacancy of 10 Bohr (Smart et al.,1996) the Ni-Co-Fe atoms were placed on both sides (parallel to the xy plane). If the Ni-Co-Fe atoms are placed in the highest layer instead of the silicon atoms, the bridge site is created, however if the the Ni-Co-Fe atoms are shifted as 0.5 along the X direction, the top site will be created.

If the position of Ni-Co-Fe atoms does not change along the z-axis, the result is the 1ML single layer mode. However, if the nickel, cobalt, and iron atoms lowered down to the same level as the first layer of silicon, this is called the 0.5ML of the first layer. The other case, in which nickel, cobalt, and iron are positioned between the first and second layer of silicon, is called interlayer 0.5ML (second layer). The most stable state will be obtained through comparing these states (Table 1).

Formation energy:

The formation energy is the energy required to make a supercell like silicon with a coating of ferromagnetic materials such as cobalt, nickel, and iron, which is obtained from pure and bulk supercell. The total energy is obtained through relation 1:

$$E_{form} = E_{tot} - N\,\mu - \gamma_{Si}\,A \qquad (1)$$

Since γ_{si}, N, μ are the same for all 6 states, so, to compare the formation energy and find a stable state based on the minimum formation energy, comparing only the total energy associated with each state will be enough. Tables 1, 2, and 3 are the total energy of the bridge site and top site of iron, cobalt, and nickel atoms, respectively.

Comparing the total energy of these states, it can be observed that the total energy associated with the second layer "0.5ML interlayer of the bridge site" is less than the other states, hence its formation energy will be less.

Table 1. Iron atom

E (tot)	1ML	First layer 0.5 ML	Interlayer 0.5 ML
Bridge site	-0.134727	-0.361339	-0.362246
Top site	-0.221151	-0.273610	-0.273017

Table 2. Cobalt atom

E (tot)	1ML	First layer 0.5 ML	Interlayer 0.5 ML
Bridge site	-0.548082	-0.541855	-0.794143
Top site	-0.448712	-0.680030	-0.738595

Table 3. Nickel atom

E (tot)	1ML	First layer 0.5 ML	Interlayer 0.5 ML
Bridge site	-0.785212	-0.756415	-0.854602
Top site	-0.658741	-0.815014	-0.821301

Spin bipolar percentage:

The electron spin density of states (DOS) in the fermi level is a criterion for bipolarity of the system. This means that the spin current can be estimated and compared in different systems determining the polarizability rate at the fermi level. The higher this rate, the greater bipolar spin current. The polarizability rate is obtained through the following relation:

$$P = \left[\frac{DOS(down) - DOS(up)}{DOS(down) + DOS(up)}\right] \times 100 \qquad (2)$$

DOS curve:

The following points can be derived from the electron density of states (DOS) curve. DOS curve in figures (2) and (3) refers to the steady state of the "bridge site of 0.5ML" interlayer in two cases of the spin up and down of iron atoms. It is observed that atoms with a downward spin have a higher contribution to the spin-bipolar current and fermi level compared to the atoms with upward spin.

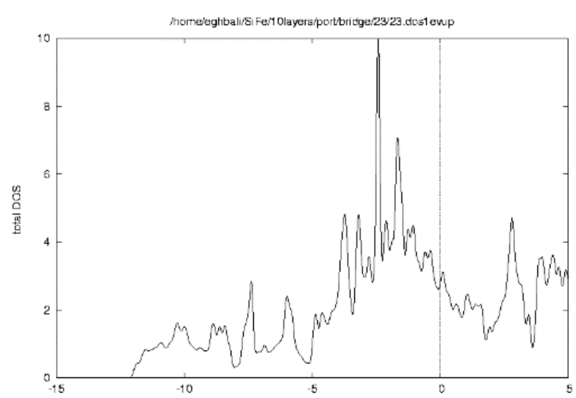

Figure 2. electron density of states DOS (up) of iron atoms

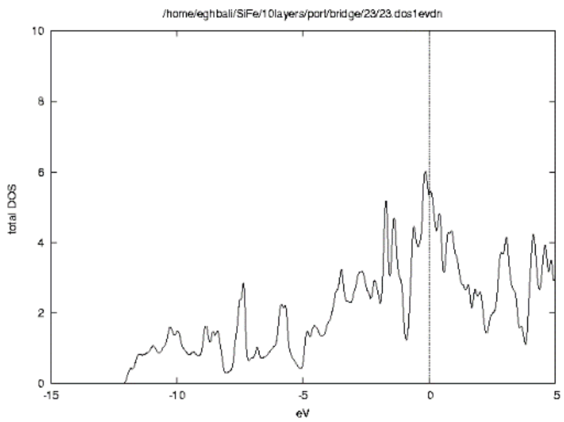

Figure 3. electron density of states DOS (down) of iron atoms

Moreover, the following points can be extracted from the electron state density curve. Figures 4 to 7 of the DOS curve are related to the steady state of the "bridge site of 0.5ML" interlayer in two cases of the spin up and down of Cobalt and Nickel atoms. It can be seen that atoms with a downward spin have a higher contribution to the spin-bipolar current and fermi level compared to the atoms with upward spin.

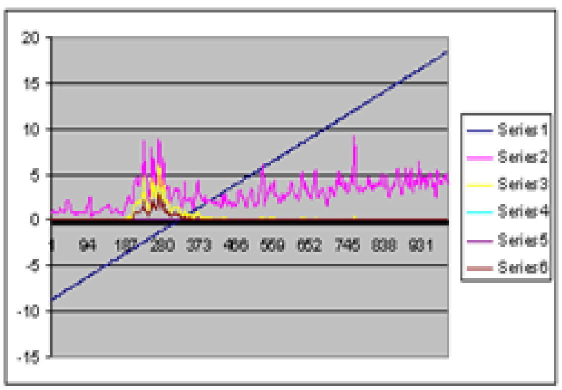

Figure 4. electron density of states DOS (up) of cobalt atoms

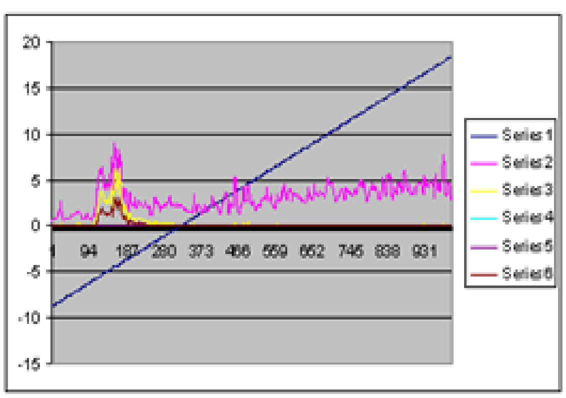

Figure5. electron density of states DOS (down) of cobalt atoms

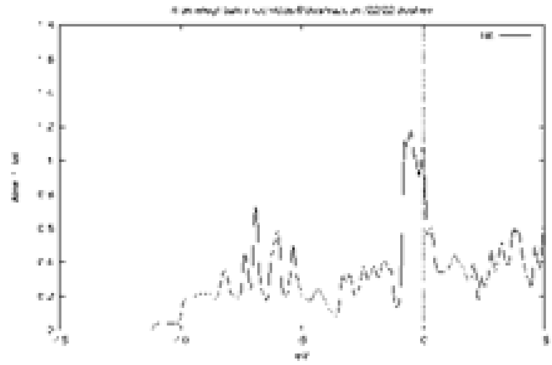

Figure 6.electron density of states DOS (up) of nickel atoms

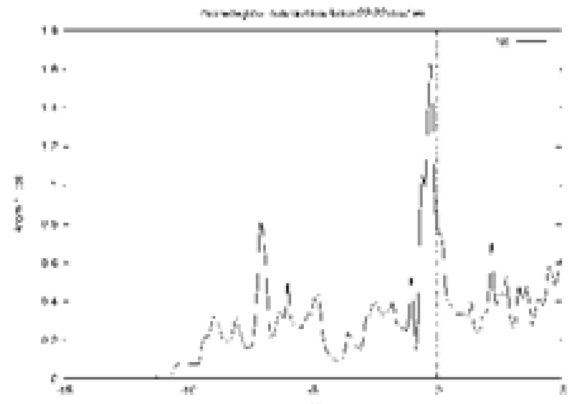

Figure 7.electron density of states DOS (down) of nickel atoms

Furthermore, calculation and comparison of the shapes of the orbital d reveals that this orbital plays a more significant role in spin current in comparison to s (Table 4).

Table 4. Bridge site of 0.5ML interlayer of iron atom

	Tot	Atom1tot	Atom4tot	Atom4d
DOS (up)	2.743636	0.129148	0.646859	0.308393
DOS (down)	5.347407	0.096475	2.926004	1.453433
P	32.18	-14.48	63.79	64.99

Magnetic bipolar torque:

The bipolar magnetic torque in the isolated and bulk states is larger than 1 and is equal to 4 for the iron atom in the isolated state, in addition, its bulk bipolar magnetic torque is 2.2 μ_β and the bridge site "0.5ML interlayer" in the steady state has been obtained as 3.74140 and 5.5 has been obtained for cobalt and nickel. Therefore, we approach an isolated atom in these states, meaning that by increasing the distance between the atoms, the magnetic bipolar torque will increase, and on the other hand, coating of these atoms increases the magnetic properties of the supercell silicon.

Summary of results:

1. Since the total energy of supercell silicon containing the coating of these atoms in the interlayer bridge site 0.5ML is

less than other states, therefore, this state is in the minimum energy and stable state.
2. Since before the relaxation, atoms occupy the silicon position at the highest layer, but after relaxation, silicon atoms pull the nickel, cobalt and iron atoms toward themselves to extent that nickel, cobalt and iron atoms are placed in a minimum state, and they are located in the second layer.
3. By investigation and comparing spin bipolar percentages for bridge site and top site conditions, it can be concluded that the position of nickel, cobalt and iron atoms in the top site has a higher contribution to bipolar spin current. Electrons with down spin have higher contribution to spin-bipolar current than up-spin electrons.
4. The orbital d of cobalt, nickel, and iron atoms are more effective in bipolar spin current.

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