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RESEARCH ARTICLE

FERROMAGNETISM OF FCC Co_n/Ni (111) OVER LAYERS WITH GGA AND GGA+U

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ABSTRACT

In this work We have investigated the magnetic ordering of Co_n/Ni systems with a first-principle calculation of the Density Functional Theory (DFT) ferromagnetic (FM) face-centered cubic (fcc) of Cobalt Co_n on Ni substrate for n=1-3 over layers. The relaxed ion, relaxed ion + volume, and non-relaxed electronic structures of the Co_n/Ni (111) crystallographic orientations are determined with generalized gradient approximation (GGA) and generalized gradient approximation + Hubbard (GGA+*U*). The onset of magnetism depends on the faces considered. The magnetism is most favored with GGA+U_{Ni} than with GGA calculations due to the strong correlations of Hubbard. The observed trends can be explained as in earlier studies in terms of the hybridization between d states of Ni substrate, also some interesting specific behavior of the magnetization in the fcc Co_n/Ni (111) overlayers with different layers has been observed.

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INTRODUCTION

Intensive experimental (Liebermann *et al*., 1970, Bergmann, 1978, Weller *et al*., 1995 and Tischer *et al*., 1995) and theoretical (Tersoff *et al.,* 1982 and Hjortstam *et al*., 1996) studies of Surface and interface for transition metals have focused on how the magnetic moments are modified in size and/or orientation in such ultrathin films from both fundamental and technological points of view. In our previous study, Cobalt (Co) and Nickel (Ni) are a 3d transition-metal that exhibits a ferromagnetic (Fm) groundstate in their bulk form, with magnetic moments of 1.595 and 0.591 μB for GGA, while for GGA+U are 1.785 and 0.659 μB respectively (Mohammed *et al*., 2010). Experimentally evidence of the magnetically dead layers of Ni in sputter-grown Ni/Pt multilayers, studied with room-temperature magnetic circular dichroism and temperature-dependent superconducting quantum interference device magnetometry (Sang-Koog *et al*., 2001). They found that the magnetic state of Ni/Pt interfaces is quite different from the bulk one due to the changed electronic structure. Also NiMnGa half-Heusler alloy films have been deposited on Si(100) substrates by the pulsed laser deposition technique at temperatures ranging from 450 to 650 ◦C (Zhu *et al*., 2005). X-ray diffraction and atomic force microscopy observation show the phase structure and surface morphology of these films are different. From theoretical points of view, (Husain *et al*., 2003) have investigated the exchange bias effect in micron-sized ferromagnetic wires made from Co and $Ni_{80}Fe_{20}$ films. The wires were fabricated using optical lithography, metallization by sputtering and lift-off technique. The onset of exchange biasing effect is found to be 70 and 15 K for the Co and $Ni_{80}Fe_{20}$ wires, respectively. Also, The surface electronic structure of Co(0001), Co(111), and 2Co/Cu(111) is studied using a parametrized tight-binding Hamiltonian with s, p, and d orbitals in the basis (Barral *et al*., 2005). They compare the calculated local density of states in the vacuum region near the surface with the differential conductance dI/dV obtained with scanning tunneling microscopy (STM). In addition to that, Single crystal Co/Ni (111) superlattices with perpendicular magnetic anisotropy interested the magnetic memories switched with a rather small spin-torque current (Gimbert *et al*., 2011). And they show that the number of the states depends on the Co layer thickness.

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Also they found that the spin magnetic moment increases at the interfaces or at the surface. In the other hand (Gimbert *et al*., 2011) used a surface-dedicated first-principles method calculated the electronic structure in Co/Ni (111) overlayers with a Co thickness varying between 1 and 5 monolayers, They found that the energy of the surface states is the same for all the overlayers thicker than 2 CoMLs, while the number of quantum-well (QW) states increases with the Co thickness. Also, The calculated one- and two-atom layers of cobalt on a copper (111) surface was performed in a tight-binding scheme, with single-site, full orbital interactions treated self-consistently (Victora *et al*., 1983). They were examined Antiferromagnetic and ferrimagnetic states with a two-atom periodicity. And they found a new type of "spatially modulated" state, and the ferromagnetic state was found to have the lowest total energy. Beside that (Ernst *et al*., 2000) were reported on Korringa-Kohn-Rostoker Green's function calculations for the ground-state moments of ultrathin Ni films on Cu(001) and on four monolayers (ML) Co/Cu(001). They found that for Ni on a ferromagnetic substrate, such as 4 ML Co/Cu(001), no reduction of the magnetic moment occurs, so that Ni at the interface retains its bulk value.

COMPUTATIONL METHODS

All calculations have been performed with VASP (Vienna ab initio Simulation Package) (Kresse *et al*., 1993, 1994, 1996 and 1999), a first principles plane-wave code based on spin-polarized density functional theory. The interaction between ions and valence electrons was described by the projector augmented-wave (PAW) method (Blochl, 1994). The Kohn-Sham equations were solved via iterative matrix diagonalization based on the minimization of the norm of the residual vector to each eigenstate and optimized charge- and spin-mixing routines (Wood *et al*., 1985, Johnson, 1988 and Pulay, 1980). The generalized gradient corrections added in form of Perdew-Wang functional PW91 (Perdew *et al*., 1992) were chosen for the exchange correlation function for the GGA. The spin interpolation of (Vosko *et al*., 1980) was also used to correct the strong electronic correlation, a simple rotationally invariant DFT+*U* version proposed by (Anisimov *et al*., 1991 and Dudarev *et al*., 1998) and implemented in VASP (Bengone *et al*., 2000) was used as GGA+*U*. In this method, the parameters *U* and *J* did not enter separately, only the difference *U*-*J* was meaningful.

Table 1. The GGA and GGA+U Magnetic moments (in Bohr magnetons, μB) of F Co_n/Ni (111) orientation for n = 1-3 over layers

State	n	non-relaxed				relaxed ion+volume			
		Ni	Co			Ni	Co		
		(I)	(S)	(S-1)	(S-2)	(I)	(S)	(S-1)	(S-2)
GGU	1	0.663	1.788	1.724	1.539	0.664	1.739	1.635	1.644
	2	0.642	1.707	-1.583		0.659	1.687	1.551	
	3	0.632	0.323			0.636	-1.464		
GGA+U_{Co}	1	0.558	1.927	1.847	1.930	0.573	1.892	1.799	1.880
	2	0.524	1.779	1.872		0.549	1.744	1.825	
	3	0.622	1.905			0.605	1.863		
GGA+U_{Ni}	1	0.665	1.779	1.724	1.602	0.663	1.739	1.695	1.608
	2	0.642	1.707	-1.103		0.659	1.687	0.329	
	3	0.660	0.276			0.650	-1.558		
GGA+U_{Co}+U_{Ni}	1	0.558	1.927	1.847	1.930	0.573	1.892	1.795	1.880
	2	0.524	1.779	1.872		0.552	1.745	1.825	
	3	0.622	1.905			0.605	1.863		

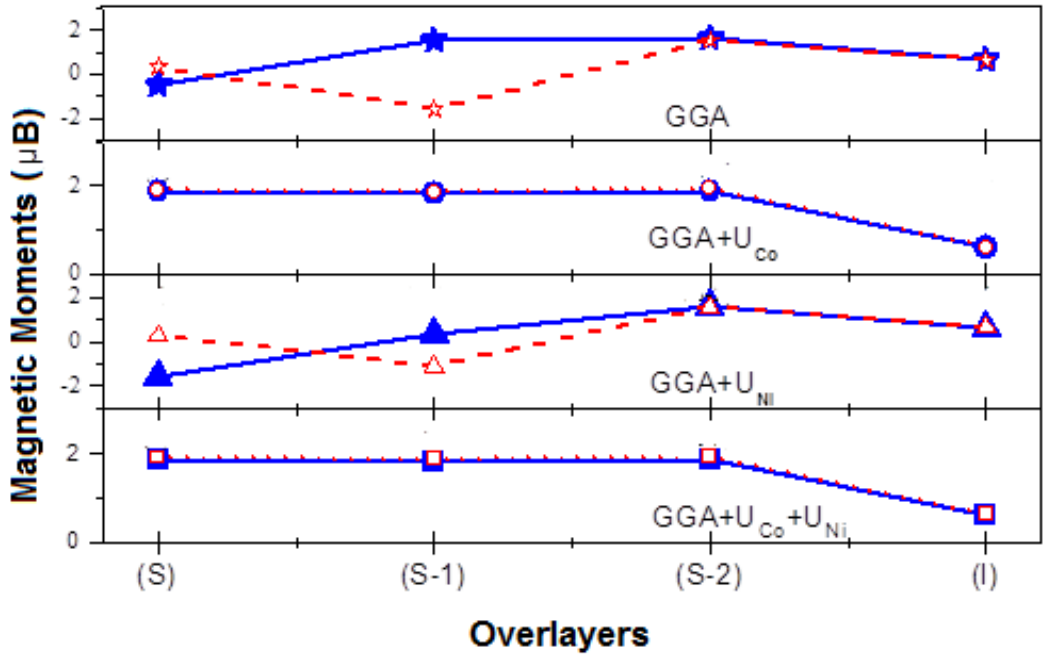

Fig. 1. Oscillatory magnetic moments of three over layers for Co_n/Ni (111) orientation (n=3). Solid symbols straight lines for relaxed and open symbols dotted lines for non-relaxed. Star for GGA, Circle for GGA+U_{Co}, triangle for GGA+U_{Ni} and Square for GGA+U_{Co}+U_{Ni} respectively

Table 2. The GGA and GGA+*U* Total Charge (in coulomb, C) of F Co_n/Ni (111) for n = 1-3 over layers

State	n	non-relaxed				relaxed ion+volume			
		Ni (I)	(S)	Co (S-1)	(S-2)	Ni (I)	(S)	Co (S-1)	(S-2)
GGU	1	9.011	7.959	8.098	8.172	9.123	8.086	8.214	8.220
	2	9.017	7.993	7.968		9.105	8.088	8.231	
	3	9.064	8.040			9.093	8.097		
GGA+U_{Co}	1	9.028	7.982	8.102	8.129	9.127	8.083	8.223	8.193
	2	9.023	8.006	8.165		9.103	8.104	8.227	
	3	9.041	8.014			9.080	8.064		
GGA+U_{Ni}	1	9.030	7.981	8.098	8.143	9.124	8.082	8.214	8.211
	2	9.017	7.993	8.119		9.105	8.088	8.259	
	3	9.048	8.037			9.100	8.079		
GGA+U_{Co}+U_{Ni}	1	9.028	7.982	8.102	8.129	9.127	8.083	8.230	8.193
	2	9.023	8.006	8.165		9.104	8.104	8.227	
	3	9.041	8.014			9.080	8.064		

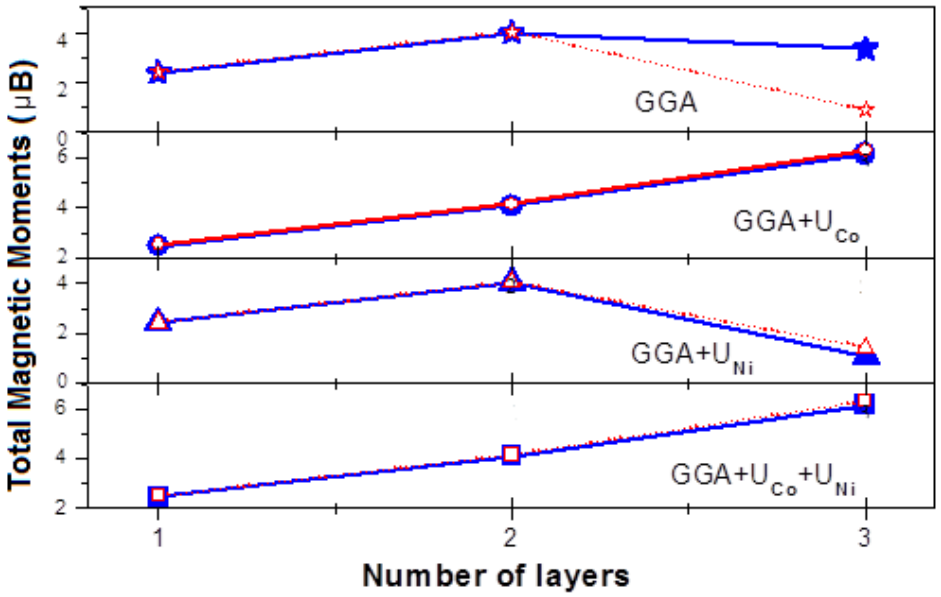

Fig. 2. Total magnetic moments (in Bohr magnetons, μB) of Co_n/Ni (111) orientation for n = 1-3 over layers. Solid symbols straight lines for relaxed and open symbols dotted lines for non-relaxed. Star for GGA, Circle for GGA+U_{Co}, triangle for GGA+U_{Ni} and Square for GGA+U_{Co}+U_{Ni} respectively

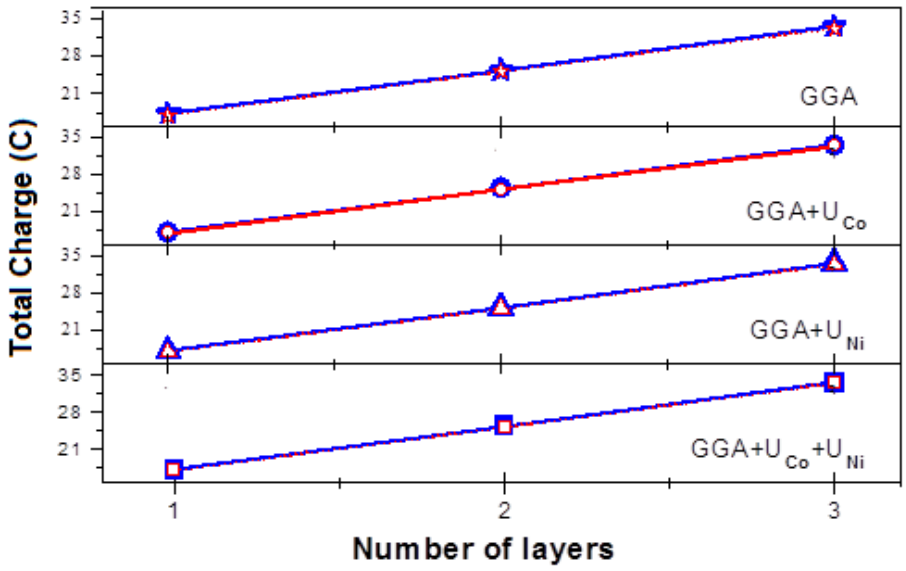

Fig. 3. Total charge (in coulomb, C) of Co_n/Ni (111) orientation for n = 1-3 overlayers. Solid symbols straight lines for relaxed and open symbols dotted lines for non-relaxed. Star for GGA, Circle for GGA+U_{Co}, triangle for GGA+U_{Ni} and Square for GGA+U_{Co}+U_{Ni} respectively

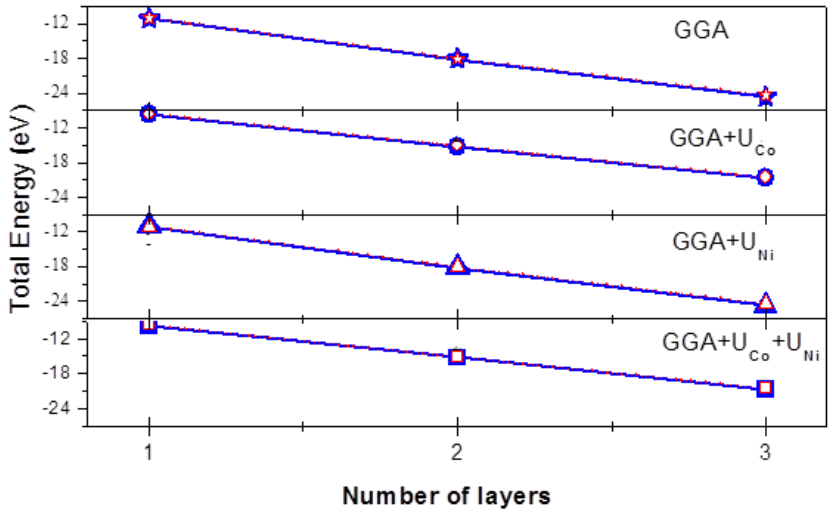

Fig. 4. Total energy (in electron Volt, eV) of Co_n/Ni (111) orientation for n = 1-3 over layers. Solid symbols straight lines for relaxed and open symbols dotted lines for non-relaxed. Star for GGA, Circle for GGA+U_{Co}, triangle for GGA+U_{Ni} and Square for GGA+U_{Co}+U_{Ni} respectively

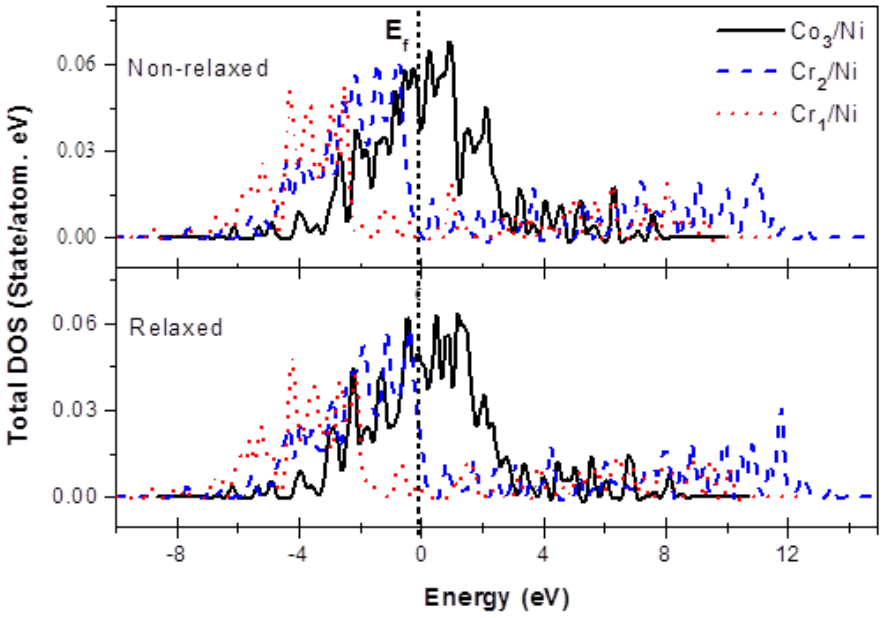

Fig. 5. Total DOS of Co_n/Ni (111) orientation for n = 1-3 over layers, for non-relaxed and relaxed GGA calculations respectively. Solid lines for Co_3/Ni, dashed line for Co_2/Ni and dotted line for Co_1/Ni respectively

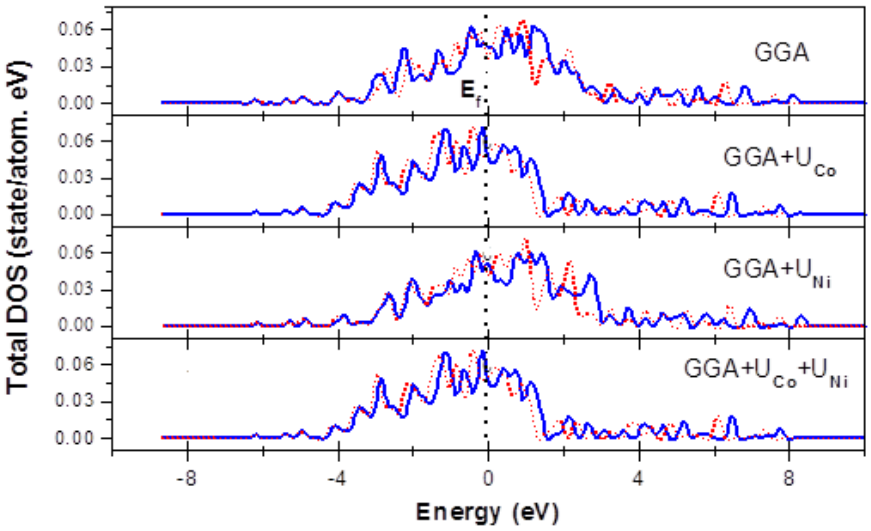

Fig. 6. Total DOS of Co_n/Ni (111) orientation for n=3 over layers, for GGA, GGA+U_{Co}, GGA+U_{Ni} and GGA+U_{Co}+U_{Ni} respectively. Solid lines for relaxed and dotted lines for non-relaxed cases

Parameters *U* and *J* represented on-site Coulomb interaction energy and exchange energy respectively. *J* was kept to 1 eV for both Co and Ni, with a value of *U-J*=1.8 and 2.4 eV respectively (Mohammed *et al*., 2010 and Rohrbach *et al*., 2003) was used in our calculations. A detailed desc*rip*tion of the DFT+*U* method can be found in (Trimarchi *et al*., 2005). All results reported in this work were carried out on a surfaces face-central-cubic ferromagnetic supercell including Co_n/Ni (111) orientation for n = 1-3 overlayers. Convergence tests have been checked carefully both for plane wave cutoff energy and k points sample, a plane-wave set expanded in energy cutoff 270 eV and k-points sample with a mesh of points 9x9x1 generated by the scheme of Monkhorst and Pack (Monkhorst *et al*., 1976) can ensure the total energies difference is less than 3 meV/atom. For total energy and DOS calculation, the integration over the Brillouin zone was performed using the linear tetrahedron method with blochl corrections (Jepsen *et al*., 1971, and Methfessel *et al*., 1989).

RESULTS AND DISCUSSION

A number of experimental (Liebermann *et al*., 1970, Bergmann, 1978, Weller *et al*., 1995 and Tischer *et al*., 1995) and theoretical (Tersoff *et al*., 1982 and Hjortstam *et al*., 1996) studies of Surface and interface for transition metals have focused on how the magnetic moments are modified in size and/or orientation in such ultrathin films from both fundamental and technological points of view. In our calculations, we investigate the magnetic ordering of Co_n/Ni (111) orientation, for n=1-3 overlayers. And we found that the ion relaxation does not change atomic sphere charge and magnetic moments of all our study cases, while the ion + volume relaxation change atomic sphere charge and magnetic moments of our study cases for both GGA and GGA+*U* with the oscillatory ordering. Here we will show the calculated results for relaxed ion + volume and non-relaxed Co_n/Ni (111) surfaces for n = 1-3 overlayers. In this work we used the lattice constants of our previous DFT calculations for fcc bulk Co and Ni (Mohammed et al., 2010), which produce a ferromagnetic solution. For Ni the lattice constant, magnetic moment are 3.53 Å, 0.591 μB for GGA, while for GGA+*U* (*U-J* = 2.4 eV) the obtained values are 3.51 Å, 0.659 μB, respectively. While for Co the lattice constant, magnetic moment are 3.52 Å, 1.595 μB for GGA, while for GGA+*U* (*U-J* = 1.8 eV) the obtained values are 3.55 Å, 1.785 μB, respectively. Table 1, show us the Magnetic moments of one independent atom per plane of Co_n/Ni (111) orientation for n = 1-3 relaxed and non-relaxed overlayers with GGA and GGA+*U* respectively. From this table we see that the magnetic moment of the Co overlayers are Enhanced due to the presence of a Ni interface. However, as the number of Co overlayers increases, the surface local magnetic moments decrease for GGA and GGA+U_{Ni} calculations, while for GGA+U_{Co} and GGA+U_{Co}+U_{Ni} calculations the magnetic moments ocillatroy decrease. Our calculations indicate that AF coupling is observed in the Co-rich region and F coupling in the Ni-rich region which in good agreement with our previous study of Cr/Mn systems (Mohammed *et al*., 2002). Also table 1 shows that the magnetic moments for GGA+U_{Co} and GGA+U_{Co}+U_{Ni} quit similar for relaxed and non-relaxed cases for different Co overlayers. Table 2, show us the total charge (in coulomb, C) of F Co_n/Ni (111) orientation for n = 1-3 overlayers for relaxed and non-relaxed cases with GGA and GGA+*U* respectively.

From this table we see that the total charge of the Co overlayers are oscillatory Enhanced due to the presence of a Ni interface. However, as the number of Co overlayers increases, the surface total charge increase. In addition to that table 2 shows that the total charge for GGA+U_{Co} and GGA+U_{Co}+U_{Ni} quit similar for relaxed and non-relaxed cases for different Co overlayers. In fig. 2 The total magnetic moments of F Co_n/Ni (111) orientation for n = 1-3 overlayers with GGA, GGA+U_{Co}, GGA+U_{Ni} and GGA+U_{Co}+U_{Ni} was reflected. The figure shows that the total magnetic moments increase with increasing the number of layers for GGA+U_{Co} and GGA+U_{Co}+U_{Ni} which they are almost have the same values. While for GGA and GGA+U_{Ni} from n=1 to 2 increase then it decrease from n=2 to 3 du to the new AF coupling that observed in the Co-rich region for Co (S-1) layer as shown in table 1. In addition to that fig. 3 shows the total charge of F Co_n/Ni (111) orientation for n = 1-3 overlayers with GGA, GGA+U_{Co}, GGA+U_{Ni} and GGA+U_{Co}+U_{Ni} respectively.

From fig. 3 we found that the total charge increase with increasing the number of Co layers for all cases of our study. The Total energy with the number of Co overlayers of Co_n/Ni (111) orientation for n = 1-3 overlayers reflected in Fig. 4. The figure show that the GGA and GGA+U_{Ni} results have lower energy, so they are more stable than other cases and are quite similar. While the relaxed cases are more stable than non-relaxed cases for all of our calculations for different numbers of Co overlayers. In Fig. 5 we reflected the total DOS of Co_n/Ni (111) orientation for n = 1-3 overlayers, for non-relaxed and relaxed GGA calculations respectively. From the figure we found that the total DOS at Fermi level increase with increasing the number of layers for relaxed and non-relaxed GGA calculations. Also for GGA+*U* calculations we found the same behavior for all of our study cases. While Fig. 6 shows the layer projected total density of states (Total DOS) for three layers of Co_n/Ni (111) orientation for n=3 overlayers for relaxed and non-relaxed GGA and GGA+U calculations respectively. The three overlayers shows the characteristic narrowing and higher DOS for GGA+U_{Co} and GGA+U_{Co}+U_{Ni}, while for GGA and GGA+U_{Ni} the characteristic wider and lower DOS. Also the figure show that the values of Total DOS at Fermi level is higher for relaxed cases than non-relaxed one for all of our study cases.

CONCLUSION

In this work, the magnetic order is studied for F Co_n/Ni (111) orientation for n=1-3 overlayers. The main results can be summarized as follows:

- The magnetic moment of Co overlayers in Co_n/Ni (111) orientation is found to be larger than that of the Co surface layer in pure semi-infinite surfaces (Mohammed *et al*., 2016) due to the presence of Ni interfacial layer.
- Systems of Co_n/Ni (111) orientation show interesting magnetic properties associated with interlayer AF coupling in the Co-rich region and F coupling in the Ni-rich region for GGA and GGA+U_{Ni} calculations.
- The relaxed and non-relaxed local magnetic moments in Co_n/Ni (111) orientation oscillatory decreases from the surface layer (S) to the interface layer (I) toward the bulk value.
- When strong correlation is included, the magnetic moments and the total charge density of Co_n/Ni (111) orientation increased.
- Total DOS at Fermi level increase with increasing the number of layers for relaxed and non-relaxed GGA calculations of Co_n/Ni (111) orientation.

- Total DOS at Fermi level is higher for relaxed cases than non-relaxed one for all of our study cases.

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