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The Magnetization of fcc Co_n (100) and (111) surfaces with GGA and GGA+*U*

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***Abstract*— The Spin polarization of fcc Con (100) and (111) surfaces is investigated with a first-principle calculation of the Density Functional Theory (DFT) ferromagnetic (FM) face-centered cubic (fcc) of Cobalt Con (100) and (111) surfaces for n = 3, 5 and 7 layers. The relaxed ion and and ion + volume, and non-relaxed electronic structures of the both surfaces are determined with generalized gradient approximation (GGA) and generalized gradient approximation + Hubbard (GGA+U). The observed trends can be explained as in earlier studies in terms of the hybridization between d states of Co substrate, also some interesting specific behavior of the magnetization in the fcc Co (100) and (111) surfaces with different layers has been observed.**

Index Terms: **Surface; magnetic moments; relaxation; DOS; Co**

I. INTRODUCTION

Surface magnetism can be very different from the one in the bulk [1], because the electronic structure of the surface is often very different. By studying surface magnetism one can gain insight into certain aspects of the surface electronic structure, especially spin polarization, which is linked to the density of states (DOS) of majority and minority electrons. Ion beams at keV energies and grazing incidence have an extreme sensitivity to the surface region [2]. The surface magneto-optic Kerr effect (SMOKE) was used to investigate the magnetic properties of epitaxial thin films of Co, Ni, and their alloys grown on Cu (100) and Cu (111) [3]. The Curie temperature TC is higher for the same films of a given thickness on Cu (111) than on Cu (100). All the films show a change in the power-law exponent β of the magnetization density M~ (1-T/TC) β with reducing film thickness.

We know that the ferromagnetic properties of transition metals based on an imbalance between the number of spin-up and spin-down electrons. This is reflected in the electronic structure by splitting of their energy bands, which results in more spin-up (majority) and spin-down (minority) occupied states. In Co, for example, this gives rise to a net magnetic moment per atom of 1.595 μB, and 1.785 μB for GGA and

GGA+U calculations respectively [4], the partly occupied, hence truly magnetic.

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The enhancement of magnetic moment at the surfaces of transition metals is a well established fact [5, 6]. Development in experimental techniques along with extremely accurate first-principles, self-consistent local spin-density (LSDA) based calculations have only strengthened this belief. This enhancement is attributed to the reduced symmetry and coordination number at surfaces. This in turn results in band narrowing and hence enhancement of the paramagnetic density of state at EF [7]. Stoner-like arguments then lead to an enhancement of the local magnetic moment. Thought in general it is true that band narrowing leads to enhancement of the surface magnetization.

By combining magnetic circular x-ray dichroism (MCXD) experiments with first principles electronic structure calculations, M. Tischer et al [8], they demonstrate that the orbital contribution to magnetism can be strongly enhanced at surfaces. This effect is illustrated for Co grown on a Cu (100) surface, where the first layer of Co shows an enhancement of the orbital moment (0.26 μB) by a factor of 2 as compared to the bulk. The lowering of the symmetry at the surface, the enhanced spin moment, and the increased value of the density of states at the Fermi level are factors that generally give the observed enhancements.

From a theoretical point of view, a comprehensive first-principles study of the energetic, electronic, and magnetic properties of Co-doped GaN (0001) thin films are presented and the effect of surface structure on the magnetic coupling between Co atoms is demonstrated [9]. It is found that Co atoms prefer to substitute the surface Ga sites in different growth conditions. In particular, a CoN/GaN interface structure with Co atoms replacing the first Ga layer is preferred under N-rich and moderately Ga-rich conditions, while $CoGa_x$/GaN interface is found to be energetically stable under extremely Ga-rich conditions. Also [10], report calculations of electronic structure and magnetic properties of Co clusters (up to 50 atoms) embedded in Cu (001) surfaces, performed using the first-principles linear muffin tin orbital-atomic sphere approximation method, implemented directly in real space. Co agglomerates of different sizes and shapes are considered in order to investigate the influence of the local environment around the Co sites to the magnetism in this class of systems. They found that the magnitude of the Co moments is mainly governed by two factors: the position of the site relative to the Cu (001) surface layer and the number of Cu neighbors. The results show moment enhancement for sites located above the surface and/or placed substitutionally in the surface layer, due to their reduced coordination numbers. For sites with the same coordination number, the moment tends to decrease as the number of Cu neighbors increases. As a consequence, in Co agglomerates, the magnetic moment decreases considerably as one goes from more central sites to those close to the grain boundary at the Co–Cu interface.

From other point of view, Magnetic properties of Co13 and Co55 nanoclusters, passivated by surface ligand shells that exhibit varying electronic interactions with the metal, are studied using density functional theory [11]. The calculations show that the chemical nature of the bond between the ligand and the metal core (X-type or L-type) impacts the total magnetic moment of Co nanoclusters dramatically. Furthermore, the chemical identity of the ligand within each binding motif then provides a fine handle on the exhibited magnetic moment of the cluster. Thus, ligand shell chemistry is predicted to not only stabilize Co nanoclusters, but provide a powerful approach to control their magnetic properties, which combined enable a variety of magnetism-based applications.

In addition to that, Co nanoplatelets with uniform size, height and shape were fabricated by ultrahigh vacuum metal evaporation on the Si (111) - (7 × 7) surface [12], using a two-dimensional identical Al cluster array as the template and spacer. The Al clusters reduce Si dangling bonds significantly and prevent the reaction between Si and the ferromagnetic metal Co. Almost all Co nanoplatelets appear as equilateral triangles with a side length of 5.4 nm and a magic thickness of 2 ML, pointing in the [211] direction. The study demonstrates a promising pathway to directly integrate magnetic nanostructures with Si-based electronic devices.

In discussing surface enhancement the role of d-band is often emphasized. The s and p bands play a significant role, especially in Ni (001) [13], Ni (100) and (111) [6] and hexagonal closed packed (hcp) Co (100) surfaces [14], where the enhancement is feeble. Also [15], they found that the moment enhancement is largest in Fe bcc (100), where the majority band (in bulk) is not saturated and less in Ni and Co where the majority band is almost saturated. In addition to that, the less saturated majority band in bulk leads to the more possibility of enhancement at the surface. For Ni thin films [16], almost the whole of the enhancement at the surface was due to the dx2-y2 orbital, but for this state the majority band was more saturated than the three t2g states in the bulk.

In this work, the results of the systematic theoretical study of the magnetic properties of fcc (100) and (111) surfaces of ferromagnetic metal Con are presented for n = 3, 5, and 7 layers. We have calculated the magnetic moment through the interface region including that of the topmost Co layer. In our calculations the size of the magnetic moment, total energies and the atomic sphere charge for several layers of fcc (100) and (111) Co surfaces have been considered with ion and ion + volume relaxations and without relaxation to carry out a detailed orbital resolved study of magnetic moments and DOS on both Co (100) and (111) surfaces with GGA and GGA+U.

II. COMPUTATIONL METHODS

All calculations have been performed with VASP (Vienna ab initio Simulation Package) [17-21], 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 [22]. 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 [23-25].

The generalized gradient corrections added in form of Perdew-Wang functional PW91 [26] were chosen for the exchange correlation function for the GGA. The spin interpolation of Vosko et a1 was also used [27]. To correct the strong electronic correlation, a simple rotationally invariant DFT+U version proposed by Dudarev et a1 [28,29] and implemented in VASP [30] was used as GGA+U. In this method, the parameters U and J did not enter separately, only the difference U-J was meaningful. Parameters U and J represented on-site Coulomb interaction energy and exchange energy respectively. J was kept to 1 eV, and a value of U-J=1.8 eV [4, 31] was used in our calculations. A detailed description of the DFT+U method can be found in Ref. [32].

All results reported in this work were carried out on a surfaces face-central-cubic ferromagnetic supercell including Con (100) and (111) orientations for n = 3, 5, and 7 layers. 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 [32,33] 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 [34-36].

III. RESULTS AND DISCUSSION

A number of experimental and theoretical calculations based on slab models were reported on the electronic and magnetic properties of Co surfaces [8, 10, 14, 37,38]. In our calculations, 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 order of about 1% and (1-3)% for (100) and of about 1% and (0.4-4)% for (111) slabs respectively. Hence we will show hereafter calculated results for relaxed ion + volume and non-relaxed Con (100) and (111) surfaces for n = 3, 5 and 7 layers.

In this work we used the lattice constants of our previous DFT bulk Co calculations [4], which produce a ferromagnetic solution with lattice constant, magnetic moment, and bulk modulus of 3.52 Å, 1.595 μB and 187.1 GPa for GGA, while for GGA+U (U-J = 1.8 eV) the obtained values are 3.55 Å, 1.785 μB, and 175.9 GPa respectively. Tables 1, show us the charge profile of the relaxed and non-relaxed orbital in various layers for a seven-layer slab Co (100) with GGA and GGA+U respectively. The GGA+U calculations show the enhancement of the charge due the strong correlations. Other crystallographic orientation is also considered. The charge profile of the relaxed and non-relaxed orbital for seven-layer slab Co (111) with GGA and GGA+U are given in Tables 2 respectively. Similar behaviors of slab Co (100) are obtained.

Table 1: The GGA and GGA+U (U-J = 1.8 eV) atomic sphere charge of seven-layer slab Co (100) with and without relaxation. Surface (S) atoms. S-1 and S-2 denote the first and second atomic layers below the surface atoms, and C labels to the atom in the Center of the film.

Layer			s	p	d	Total
GGA	Relaxed	S	0.432	0.342	7.228	8.003
		S-1	0.456	0.493	7.270	8.219
		S-2	0.459	0.498	7.264	8.221
		C	0.459	0.496	7.265	8.221
	Non-relaxed	S	0.417	0.315	7.215	7.946
		S-1	0.439	0.457	7.246	8.142
		S-2	0.441	0.462	7.241	8.144
		C	0.442	0.460	7.246	8.148
GGA+*U* (*U-J* = 1.8 eV)	Relaxed	S	0.430	0.340	7.212	7.983
		S-1	0.451	0.478	7.265	8.194
		S-2	0.454	0.482	7.261	8.198
		C	0.454	0.479	7.251	8.184
	Non-relaxed	S	0.415	0.313	7.296	7.924
		S-1	0.433	0.441	7.231	8.105
		S-2	0.435	0.445	7.226	8.106
		C	0.437	0.443	7.227	8.107

Table 2: The GGA and GGA+U atomic sphere of seven-layer slab Co (111) with and without relaxation.

Layer			s	p	d	Total
GGA	Relaxed	S	0.451	0.380	7.225	8.055
		S-1	0.453	0.488	7.258	8.199
		S-2	0.458	0.490	7.259	8.208
		C	0.456	0.491	7.258	8.205
	Non-relaxed	S	0.437	0.355	7.237	8.029
		S-1	0.439	0.459	7.230	8.128
		S-2	0.444	0.461	7.226	8.131
		C	0.442	0.463	7.227	8.132
GGA+*U* (*U-J* = 1.8 eV)	Relaxed	S	0.440	0.363	7.242	8.045
		S-1	0.449	0.474	7.268	8.191
		S-2	0.456	0.480	7.259	8.194
		C	0.452	0.480	7.264	8.195
	Non-Relaxed	S	0.422	0.333	7.219	7.874
		S-1	0.429	0.435	7.246	8.111
		S-2	0.435	0.440	7.228	8.104
		C	0.432	0.441	7.241	8.114

Table 1 and 2, also, shows that the charge-density oscillates with order of the layers. While Fig 1, show that the Total Charge Density increase with increasing the number of layers for both GGA and GGA+U calculations, in addition to that, the total Charge Density for the relaxed cases are greater than that of the non-relaxed cases for both (100) and (111) slabs of about order of 1% for GGA and GGA+U respectively.

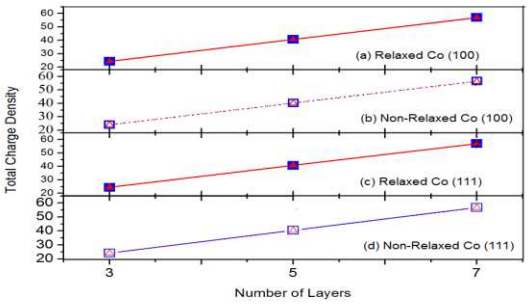

Fig. 1: Calculated total charge density for different layers of Co (100) and (111) slabs. Square for GGA and triangle for GGA+U respectively. Solid and doted lines for relaxed and non-relaxed respectively.

Tables 3 and 4, shows us the magnetic moments for different numbers of layers for relaxed and non-relaxed of Co (100) and (111) slabs with GGA and GGA+U respectively. From these tables we see that the surface magnetic moment of layer oscillatory increases with increasing the number of layers. In one hand, the magnetic moments of the atoms in the center of the films for GGA oscillatory decreases with increasing the number of layers towards the bulk value for both (100) and (111) slabs. In the other hand, the magnetic moments of the atoms in the center of the films for GGA+U oscillatory increase with increasing the number of layers from the bulk value for both (100) and (111) slabs. However, it is the manner in which the charge redistribution takes place

among the five d orbital, which makes surface magnetization Our estimate of the enhancement of the surface magnetic moments agrees closely with the result of Alden [39]. Fig. 2 reflected the calculation of the total energies for different different from bulk. Also, we found that the magnetic moments for both (100) and (111) surfaces decries from the surface layer toward the bulk value (Center layer) for relaxed for relaxed and non-relaxed cases.

number of layers for Co (100) and (111) slabs. The figure show that the GGA results are more stable than that of the GGA+U relaxed and non-relaxed cases.

Table 4: The GGA and GGA+U Magnetic moments of fcc Con (100) for n = 3, 5, and 7 layers with and without relaxation.

		relaxed				non-relaxed			
	n	C	S	S-1	S-2	C	S	S-1	S-2
GGA	3	1.595	1.821			1.651	1.857		
	5	1.589	1.838	1.587		1.623	1.853	1.625	
	7	1.570	1.815	1.573	1.576	1.577	1.818	1.589	1.588
GGA+*U*	3	1.789	1.950			1.826	1.966		
	5	1.811	1.948	1.804		1.843	1.970	1.839	
	7	1.830	1.959	1.820	1.831	1.883	1.989	1.872	1.888

Table 5: The GGA and GGA+U Magnetic moments of fcc Con (111) for n = 3, 5, and 7 layers with and without relaxation.

		relaxed				non-relaxed			
	n	C	S	S-1	S-2	C	S	S-1	S-2
GGA	3	1.662	1.712			1.671	1.716		
	5	1.532	1.691	1.628		1.558	1.709	1.646	
	7	1.614	1.723	1.648	1.591	1.646	1.707	1.678	1.634
GGA+*U*	3	1.790	1.839			1.889	1.915		
	5	1.857	1.825	1.812		1.893	1.914	1.884	
	7	1.805	1.817	1.812	1.830	1.827	1.843	1.832	1.851

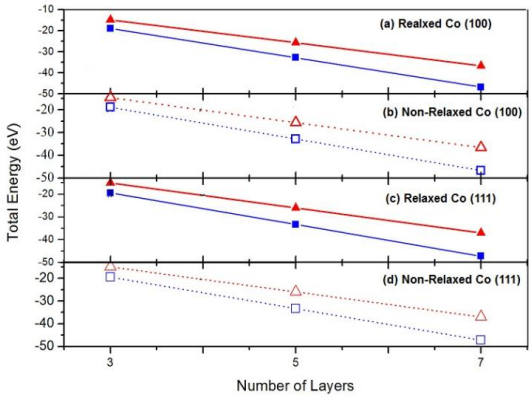

Fig. 2: Calculated total energy for different number of layers for Co (100) and (111) slabs. Square for GGA and triangle for GGA+U respectively. Solid and doted lines for relaxed and non-relaxed respectively.

The magnetic moments of seven-layers of Co (100) and (111) slabs are reflected in Fig. 3, which shows that the magnetic moments oscillatory decreases from the surface layer (S) to the central layer (C) toward the bulk value for both GGA and GGA+U calculations respectively. The figure also shows that the magnetic moments of GGA+U greater than that of the GGA calculations due to the strong correlations of Hubbard in good agreemet with Ni (100) and (111) slabs [6].

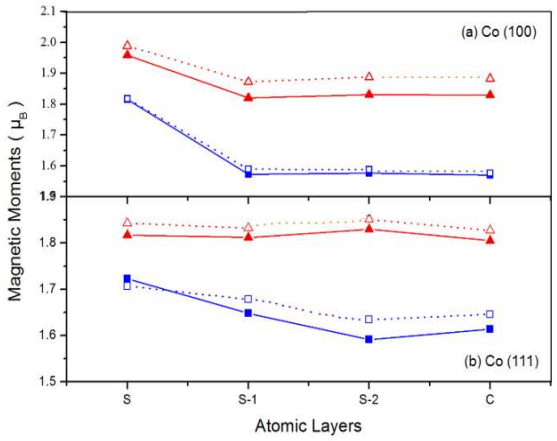

Fig. 3: Oscillatory magnetic moments of seven-layers for (a) Co (100) (b) Co (111) slabs. Solid symbols straight lines for relaxed and open symbols doted lines for non-relaxed. Square for GGA and triangle for GGA+U respectively.

Fig. 4 shows the layer projected total density of states (Total DOS) for a different layer 3, 5 and 7 slabs for Co (100) relaxed and non-relaxed GGA and GGA+U calculations respectively. The 7 layer shows the characteristic narrowing and higher DOS, while the values of Total DOS at Fermi

level oscillatory increase from 3 layers and have the highest value for 5 layers then again decrease at 7 layers for GGA and GGA+U relaxed and non-relaxed calculations respectively. Other crystallographic layer projected Total DOS are also considered for slab Co (111) with relaxed and non-relaxed GGA and GGA+U calculations respectively, the result is reflected in Fig. 5. Similar behaviors of slab Co (100) are obtained. Our measurements of the Total DOS show that in slab Co (100) and (111) the 5 layers have a higher density of states at the Fermi energy than 3 and 7 layers for relaxed and non-relaxed cases (see Figs. 4 and 5) in a good agreement with WC (100) surface works [40] predicted. An interesting facet of this study is the steep suppression of the magnetic moment for the atoms below the surface layer (see Fig. 3).

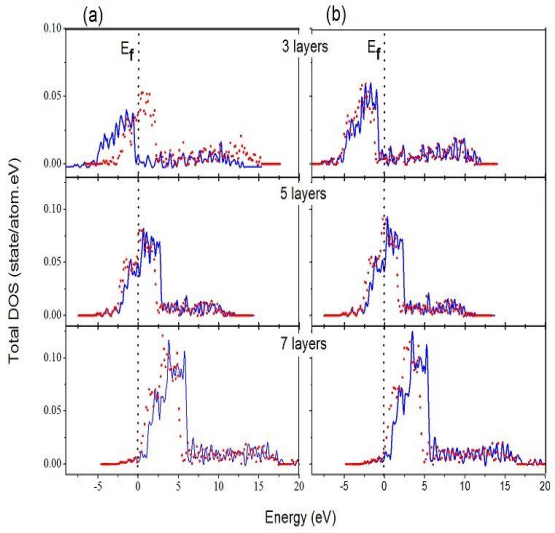

Fig. 4: Total DOS of 3, 5 and 7 layers for Co (100) slabs. (a) Relaxed and (b) Non-relaxed. Solid and dotted lines for GGA and GGA+U respectively. (Ef) is Fermi

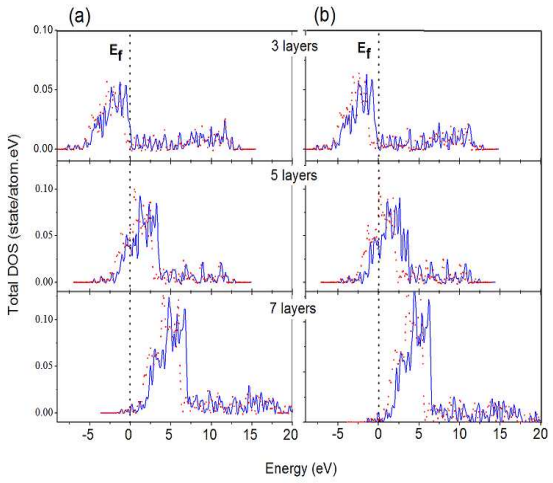

Fig. 5: Total DOS of 3, 5 and 7 layers for Co (111) slabs. (a) Relaxed and (b) Non-relaxed. Solid and dotted lines for GGA and GGA+U respectively. (Ef) is Fermi energy.

VI. CONCLUSION

The main points of our study can be summarized as following:

- Oscillatory magnetic moments and charges in all cases studied were observed.
- Co (100) and (111) surfaces magnetic moments enhancement attributed to the reduced symmetry and coordination number at surfaces.
- The relaxed and non-relaxed surface local magnetic moments of Co (100) and (111) oscillatory increase with increasing the number of layers, and the local magnetic moments of the atom in the center of the films oscillates decrease towards the bulk value.
- When strong correlation is included, the magnetic moments and the total charge density of Co (100) and (111) surfaces increased.
- Total DOS at Fermi level oscillatory change with increasing the number of layers for for relaxed and non-relaxed GGA and GGA+U calculations of Co (100) and (111) surfaces.

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