*IOSR Journal of Applied Physics (IOSR-JAP)*
*e-ISSN: 2278-4861.Volume 11, Issue 6 Ser. I (Nov. −Dec. 2019), PP 53-57*
*www.iosrjournals.org*

# A First-principles Study on the Surface Magnetism of the CsCl Structured CoX (X =Ti, V, Nb) (001) Surface

EunsungJekal, Dao Phuong
*Department of material science, ETH Z¨urich.∗*
*Hefei National Laboratory, University of Science and Technology of China, China.*

Date of Submission: 13-11-2019 Date of Acceptance: 27-11-2019

(Dated: November 10, 2019)

The exchange stiffness constant $A_{ex}$ was linearly propositional to the difference of spin wave resonance field $H_{SWR}$ and ferromagnetic resonance field $H_{FMR}$. In this work, we measured the $H_{SWR}$ and $H_{FMR}$ with in-plane angles in order to analyze the angular dependence of $A_{ex}$ in NiFethin film with thickness of 100 nm. The $A_{ex}$ of NiFe thin film was shown isotropic behavior notdepending on the in-plane angles. The measured value of $A_{ex}$ was $10.9\times10^{-7}$erg/cm and its value should be applied to the spin wave devices.

## I. Introduction

Heterogeneous intermetallic compounds such as CoTi,FeTi, NiTi, etc. have attracted a lot of attention dueto various interesting properties[1–3]. They have highstrength and high melting temperature and exhibit formation memory effects, so they have an x-ray absorption and emission spectrum and x-ray photoelectricity.

The physical properties have been explored using various methods such as self-release, Hall effect and specificheat experiment [4, 5].The basic properties of matter can be understood fromthe density of states and energy bands obtained fromthe calculation of electronic structures. The electronicstructure calculations for these compounds have been followed up since the first time by paconconstantopoulos.Eibler et al calculate the electronic structure of thesecompounds [6]. Rhee et al studied the relationship between the electronic structure and the optical propertiesof these compounds[7].Surface electronic structures of these compounds werealso studied. Canto and de Coss calculated the paramagnetic state of electronic structures using a self-sufficientclose coupling method for the (001) surface of FeTi withCsCl structure. As a result, when Fe atoms appear on thesurface, much of the local density is in a bound state. Thedensity of the state was about 160% of the bulk value,and the Ti surface atoms showed a high degree of antibonding at the local state density and the density of theFermi energy at 350% compared to the bulk. Kotoreevet al. Calculated the state density, charge distributionand work function of the (110) surface in the paramagnetic state of X (X = Fe, Co, Ni) Ti. Mankovsky et al.calculated the electronic structure of the (001) plane forFeTi, which is paramagnetic in bulk, and the magnetic moment of the surface Fe atoms was about 2.27 $\mu_B$, similar to that of bcc iron. The Ti of the layer showed -0.45$\mu_B$ and the middle Ti atom had a magnetic moment of-0.25 $\mu_B$. Kellou et al. describe an electron sphere for thesurface of X (X = Fe, Co, Ni) Ti (001) and the interfacebetween them. As a result, when Ti atoms are on the surface in the XTi (001) system, they are 0.40 $\mu_B$ in FeTi(001), 0.62 $\mu_B$ in CoTi (001), and 0.73 $\mu_B$ in NiTi (001).The magnetic moment was shown to increase. However,they did not present the calculation result when Fe, Co,and Ni atoms came out to the surface.

In this study, we investigate the spin polarization electronic structure of (001) surface in CoTi, CoV and CoNbwhich have magnetic properties in bulk and investigateits surface magnetism.

## II. Method

First, it was calculated whether four compounds of Co,3*d* and 4*d* transition metal alloys, such as CoTi, CoV,CoZr, and CoNb, had a CsCl structure and showed magnetism in bulk. As a result, it was found that only theCoZr paramagnetic state was lower in energy than thespin polarization state and thus did not have magnetism.

Accordingly, surface electronic structure calculations onthe (001) surface of three compounds of CoTi, CoV, andCoNb were performed.When creating (001) surfaces from these three compounds with CsCl structure, there could be a surfaceending with Co and a surface ending with X (X = Ti, V,Nb). Both of these surfaces were considered here. Thinplate model consisting of nine atomic layers each to calculate the electronic structure of two surfaces ending inCo or X atoms. In each system, if Co or X atoms areplaced on the surface, the atoms in the middle layer arealso Co or X atoms. For comparison, the lattice constants of these three compounds were all set to 5.652 a.u. likeCoTi.

The method used to calculate the surface electronicstructure is the full-potential liniarized augmented

planewave (FLAPW) method. At this time, the Muffin Tinradius of each atom was set to 2.25 a.u., and the numberof basis functions for constructing the reinforced planarwave was about 150 per atom. The energy eigenvalueswere obtained by solving the Kohn-Sham equation for 36*k*-points distributed evenly in the Brillouin region, whichcannot be reduced two-dimensionally.The general gradient approximation (GGA) of thePW91 type is used to handle exchange-correlation potentials, and the core electrons are treated with the fullrelativity, which solves the Dirac equation. The subrelative treatment was not considered. Self-contained convergence conditions are charge density and spin mill Theplots were set at each time of $2.0 \times 10^{-4}$ e/a.u.$^3$ or less.

## III. Result And Discussion

Tables I, II, and III show the number of spins, thenumber of spin electrons, and the magnetic moment, depending on the angular momentum of each atom in the(001) surface system of CoTi, CoV, and CoNb, each having a CsCl structure in the bulk. For (001) surface endingwith Ti in CoTi surface system, the surface surface of Tishowed that the number of *p* electrons (0.18) decreased significantly (0.24) compared to the middle layer due tothe surface generation.

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**TABLE I.** *l*-decomposed electrons within muffin-tin spheres on the atoms in the Co- and Ti-terminated CoTi(001) surfacesystems. The values of magnetic moments (MMs) calculated for the atoms are also given. S, S-1, and C denote the surface-,subsurface- and center layers.

| Systems | Atom type | s(↑/↓) | p(↑/↓) | d(↑/↓) | Total(↑/↓) | MM |
|---|---|---|---|---|---|---|
| Co-term | Co(S) | 0.40 (0.21/0.19) | 0.18 (0.08/0.10) | 7.15 (4.17/2.98) | 7.73 (4.46/3.27) | 1.19 |
| | Ti(S-1) | 0.21 (0.10/0.11) | 0.22 (0.10/0.12) | 1.73 (-0.72/1.01) | 2.18 (0.94/1.24) | -0.31 |
| | Co(C) | 0.44 (0.23/0.21) | 0.36 (0.18/0.18) | 7.15 (3.98/3.17) | 7.96 (4.40/3.56) | 0.83 |
| Ti-term | Ti(S) | 0.19 (0.10/0.09) | 0.15 (0.08/0.07) | 1.78 (1.24/0.54) | 2.13 (1.42/0.71) | 0.72 |
| | Co(S-1) | 0.44 (0.23/0.21) | 0.36 (0.18/0.18) | 7.13 (4.04/3.09) | 7.93 (4.46/3.47) | 0.98 |
| | Ti(C) | 0.22 (0.11/0.11) | 0.24 (0.12/0.12) | 1.75 (0.88/0.87) | 2.22 (1.11/1.11) | 0.00 |

In this system, the magnetic moment of Ti surface atom was 0.72 $\mu_B$, the middle layer Ti was not magnetic, and the magnetic moment of Coatom of S-1 layer was 0.98 $\mu_B$. The density of states forthese is shown in Fig. 1. When the surface Ti atomsare compared to the center atoms, magnetic momentsare expressed due to some band narrowing and spin separation, which are typical surface effects. Comparing themagnetic moment of each atom obtained in this calculation with the calculation results of Kellou et al. [13],these results indicate that Co atoms of 0.62 $\mu_B$ and subsurface layer were 0.93 $\mu_B$, which had a somewhat largermagnetic moment than the results of this calculation.

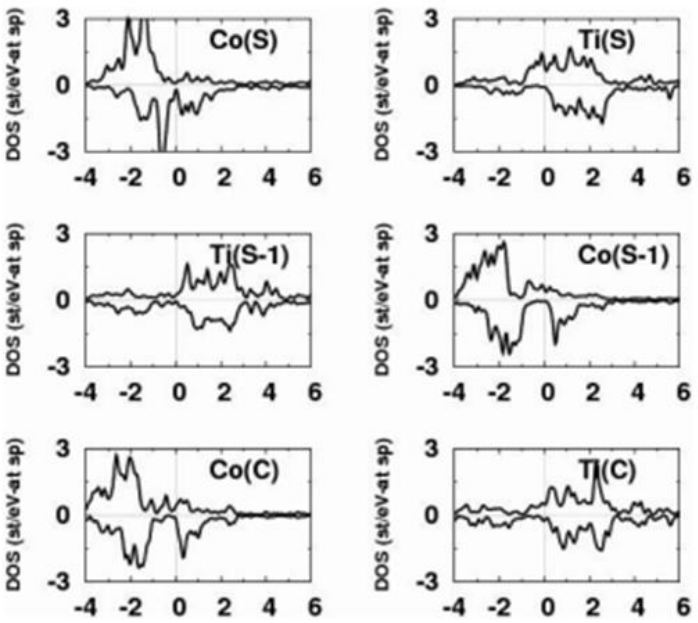


**Fig. 1** Atom-projected spin-polarized density of states (DOS) for thechosen atoms of the Co- (left-pannels) and Ti-terminated (rightpannels) CoTi(001) surface. The spin-down DOS values aremultiplied by a negative number, and the Fermi levels are set to zero.

This seems to be due to the difference in the radius ofthe adopted MT sphere.Surface systems ending with Co atoms have a surfaceCo atom of 1.19 $\mu_B$, which can be considered as a resultof bulking, and is significantly increased from the value oflayer Co atoms of 0.83 $\mu_B$. The magnetic moment of theTi (S-1) layer was negative -0.31 $\mu_B$. However, Kellouet al. do not present the calculation results of surfacesystems ending with Coatoms and cannot be compared.

In the left panel of Fig. 1, the density of surface Coatoms shows a sharp surface state around -0.7 eV forminor spins and an increase in magnetic moment due toincreased spin separation compared to the center layerCo atoms.

**TABLE II.*l*-**decomposed electrons within muffin-tin spheres on the atoms in the Co- and V-terminated CoV(001) surfacesystems. The values of magnetic moments (MMs) calculated for the atoms are also given. S, S-1, and C denote the surface-,subsurface- and center layers

| Systems | Atom type | s(↑/↓) | p(↑/↓) | d(↑/↓) | Total(↑/↓) | MM |
|---|---|---|---|---|---|---|
| Co-term | Co(S) | 0.38 (0.20/0.18) | 0.18 (0.08/0.10) | 7.12 (4.23/2.89) | 7.69 (4.52/3.17) | 1.34 |
| | V(S-1) | 0.21 (0.11/0.12) | 0.22 (0.11/0.12) | 1.73 (1.46/1.27) | 2.18 (1.69/152) | 0.17 |
| | Co(C) | 0.42 (0.22/0.10) | 0.15 (0.08/0.07) | 2.80 (2.21/0.59) | 3.18 (2.41/0.77) | 1.41 |
| V-term | V(S) | 0.22 (0.12/0.10) | 0.20 (0.10/0.10) | 7.22 (3.61/3.61) | 7.82 (3.91/3.91) | 0.00 |
| | Co(S-1) | 0.41 (0.21/0.20) | 0.34 (0.16/0.18) | 7.10 (4.14/2.96) | 7.86 (4.52/3.34) | 1.18 |
| | V(C) | 0.23 (0.11/0.12) | 0.25 (0.12/0.13) | 1.73 (1.69/1.04) | 3.24 (1.94/1.30) | 0.64 |

Table II lists the prime numbers belonging to eachatom in the CoV (001) surface system. The numberof spins and the number of spin electrons and the magnetic moment are given. On the Co-terminated (001)surface, the Co *p*-electron number (0.18) was reduced byhalf compared to the middle Co atomic layer, and thespin moment due to p-electron was -0.02 $\mu_B$. This effect and the magnetic moment due to *d*-electrons werereduced compared to the Co atoms in the middle layer,so that the magnetic moments of the surface Co atomswere decreased by 0.07 $\mu_B$ to 1.34 $\mu_B$ compared to themiddle layer Co atoms. In this system, the magnetic moment of the V atoms in the S-1 layer is 0.17 $\mu_B$, whichis considerably larger than the 0.64 $\mu_B$ of the layer Vatoms, which can be considered bulky in the CoV (001)system ending with V atoms. In the state density of theCoV (001) system ending with the Co atom given in theleft panel of Fig. 2, the surface Co and middle layer Coatoms are compared. As with CoTi (001), a sharp surface condition exists at

-0.7 eV. In the CoV (001) surfacesystem ending with V atoms, the magnetic moment ofthe surface V atoms is 1.64 $\mu_B$, which is an increase of2.5 times compared to 0.64 $\mu_B$ in the middle layer V.This is due to the significant increase in spin separationat the surface V atoms, as shown in the right panel of2. Table III summarizes the data for the CoNb (001)surface system.

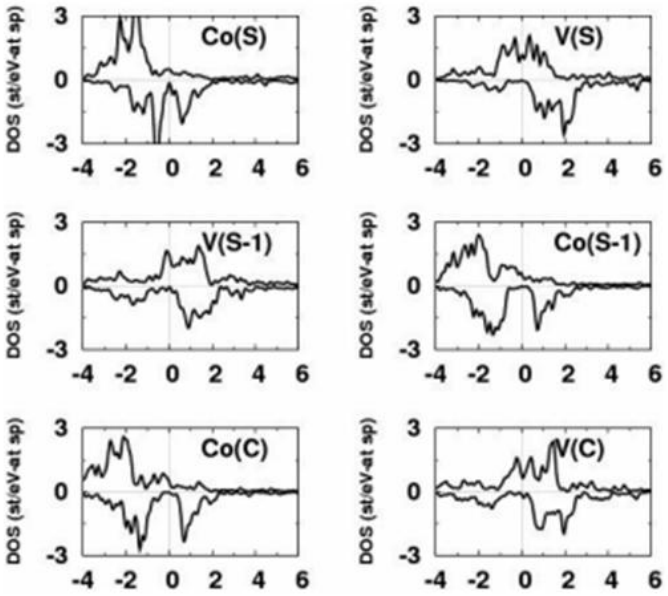


**Fig. 2** Atom-projected spin-polarized density of states (DOS) for the chosen atoms of the Co- (left-pannels) and V-terminated (rightphannels) CoV(001) surface. The spin-down DOS values are multiplied by a negative number, and the Fermi levels are set to zero.

**TABLE III.*l*-**decomposed electrons within muffin-tin spheres on the atoms in the Co- and Nb-terminated Co(001) surfacesystems. The values of magnetic moments (MMs) calculated for the atoms are also given. S, S-1, and C denote the surface-,subsurface- and center layers

| Systems | Atom type | s(↑/↓) | p(↑/↓) | d(↑/↓) | Total(↑/↓) | MM |
|---|---|---|---|---|---|---|
| Co-term | Co(S) | 0.40 (0.20/0.20) | 0.20 (0.1/0.10) | 7.22 (3.61/3.91) | 7.82 (3.91/3.91) | 0.00 |
| | Nb(S-1) | 0.18 (0.09/0.09) | 0.20 (0.10/0.10) | 2.14 (1.07/1.07) | 2.56 (1.28/1.28) | 0.00 |
| | Co(C) | 0.46 (0.23/0.23) | 0.28 (0.19/0.19) | 7.23 (3.62/3.61) | 8.10 (4.06/4.04) | 0.02 |
| Nb-term | Nb(S) | 0.16 (0.08/0.08) | 0.13 (0.07/0.06) | 2.23 (1.24/0.99) | 2.54 (1.40/1.14) | 0.26 |
| | Co(S-1) | 0.46 (0.24/0.22) | 0.39 (0.20/0.19) | 7.15 (4.22/2.93) | 8.03 (4.48/3.35) | 1.33 |
| | Nb(C) | 0.18 (0.09/0.09) | 0.22 (0.11/0.11) | 2.19 (1.24/0.95) | 2.63 (1.46/1.17) | 0.29 |

As shown in this table, in CoNb (001) systems ending with Nb atoms, the magnetic moment of the surfaceNb atoms was 0.26 $\mu_B$, which was slightly reduced compared to 0.29 $\mu_B$ of the middle layer Nb atoms, but themagnetic moment of the Co atoms in the S-1 layer hada size of 1.33 $\mu_B$. This can also be seen in the panel'sstate density in the middle right. One interesting thingis that the CoNb (001) surface system, which ends withCo atoms, shows in Table III that the magnetism dies because the magnetic moment of all atoms is close to zero.Comparing the case of surface Co atom and middle layerCo atom at the state density given in the left panel of 3,both surface spin atoms and surface spin atoms appearto be near -1.0 eV in the case of majority spin or minorspin electrons. Spin separation for both atoms have nomagnetic moment.

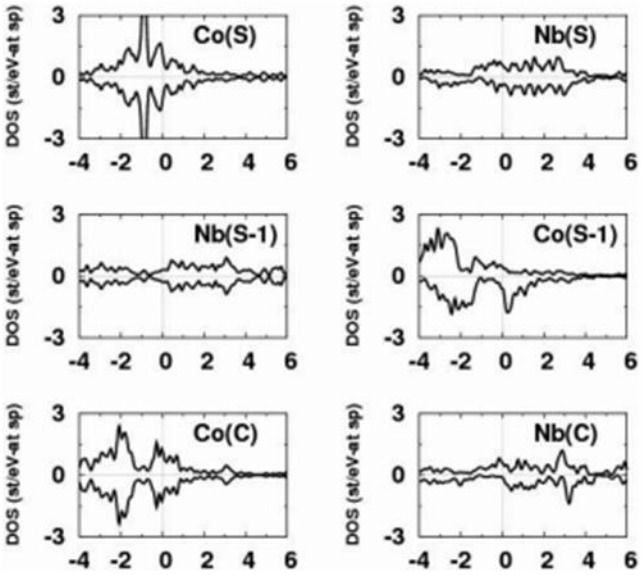


**Fig. 3** Atom-projected spin-polarized density of states (DOS) for the chosen atoms of the Co- (left-pannels) and Nb-terminated (rightpannels) CoNb(001) surface. The spin-down DOS values are multiplied by a negative number, and the Fermi levels are set to zero.

In this study, the electronic structure of the surfacesystem was not calculated because CoZr showed paramagnetism in the bulk, but it is necessary to check whetherthe magnetic surface is expressed on the surface as inFeTi (001) system in near future.

## IV. Conclusion

The electronic structure of the (001) surface systemin Co and X (X = Ti, V, Nb) binary compounds withCsCl structure in bulk state was calculated by using the fullpotential liniarized augmented plane wave (FLAPW)method and its surface magnetism was investigated. Todo this, we adopted a single-plate model consisting ofnine layers, each terminated with Co or X atoms. In

CoTi (001) systems ending with Co atoms, the surfacestate at -0.7 eV and their magnetic moments were 1.19$\mu_B$, a significant increase over 0.83 μB of the middle layerCo atom. In the CoV (001) surface system ending withV atoms, the magnetic moment of the surface V atomswas 1.64 $\mu_B$, which is 2.5 times larger than that of themiddle layer. The magnetic moment of the surface Coatoms was 1.34 $\mu_B$, which decreased slightly comparedto the center Co atoms. In the CoNb (001) system, themagnetism disappeared in the surface system

ending withCo atoms, and in the system ending with Nb atoms, the magnetic moment of the surface Nb atoms was 0.26 $\mu_B$,0.03 $\mu_B$ less than that of the middle layer Nb atoms.

TABLE II.l-decomposed electrons within muffin-tin spheres on the atoms in the Co- and V-terminated CoV(001) surfacesystems. The values of magnetic moments (MMs) calculated for the atoms are also given. S, S-1, and C denote the surface-,subsurface- and center layers

| Systems | Atom type | s(↑/↓) | p(↑/↓) | d(↑/↓) | Total(↑/↓) | MM |
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| | V(C) | 0.23 (0.11/0.12) | 0.25 (0.12/0.13) | 1.73 (1.69/1.04) | 3.24 (1.94/1.30) | 0.64 |

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IOSR Journal of Applied Physics (IOSR-JAP) is UGC approved Journal with Sl. No. 5010, Journal no. 49054.

EunsungJekal " A First-principles Study on the Surface Magnetism of the CsCl Structured CoX (X =Ti, V, Nb) (001) Surface." IOSR Journal of Applied Physics (IOSR-JAP) , vol. 11, no. 6, 2019, pp. 53-57.