A First-principles Study on the Electronic Structures and Magnetism of Antiperovskite $MnCo_3N$ (001) surfaces

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Ferromagnetic transition metal nitrides are very interesting materials for future applications in spintronics [1] whose electronic properties have been extensively investigated. The crystal structure of the nitrides richest in transition metal is said to be fcc with a nitrogen atom in the center of the cube. If the atoms at the face centers are substituted by another element, a simple cubic antiperovskite structure is obtained.

We report the study of the electronic structures and the magnetic properties of manganese substituted cobalt nitride ($MnCo_3N$) (001) surface carried out with the use of all-electron full potential linearized augmented plane-wave (FLAPW) method [2] as embodied in the QMD-FLAPW code, within the generalized gradient approximation to the exchange correlation potential. In $MnCo_3N$ there are two possible terminations of (001) surface: one contains Mn and Co atoms only, and the other is composed of Co and N atoms, as shown in Fig.1.

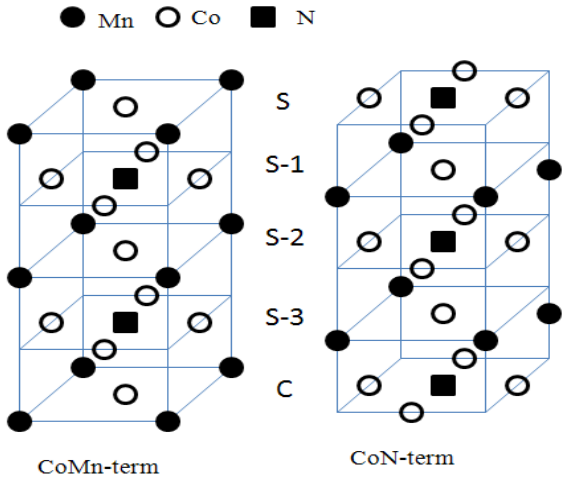

Figure 1. Schematic view of the $MnCo_3N$ (001) surface with CoMn-term and CoN-term.

In Table I, l-decomposed majority and minority spin electrons inside the muffin-tin sphere of the atoms in S, S-1, and C layers of $MnCo_3N$ (001) surface with CoMn-term and CoN-term and the values of the magnetic moments (MMs) calculated for the atom are collected. The values obtained for the atoms in the S-2 and S-3 layers are not shown since they were very close to those calculated for the atoms in the C layer.

TABLE I. l-decomposed majority and minority spin electrons inside the muffin-tin sphere of atoms in the S, S-1, and C layers of $MnCo_3N$ (001) surface with CoMn-term and CoN-term together with the values of the magnetic moments (MMs) calculated for the atoms.

CoMn-term					
Atom	s (↑ ↓)	p(↑ ↓)	d(↑ ↓)	total(↑ ↓)	MM [B]
Co(S)	0.09/0.08	0.06/0.06	3.99/2.72	4.14/2.87	1.270
Mn(S)	0.08/0.06	0.04/0.04	4.05/0.45	4.17/0.56	3.607
Co(S-1)	0.09/0.09	0.09/0.10	3.98/2.70	4.17/2.89	1.282
N(S-1)	0.66/0.65	1.38/1.28	0.03/0.03	2.07/1.96	0.109
Co(C)	0.09/0.09	0.09/0.10	4.03/2.65	4.22/2.84	1.373
Mn(C)	0.07/0.06	0.06/0.06	3.97/0.53	4.10/0.65	3.450
CoN-term					
Co(S)	0.09/0.09	0.08/0.08	4.07/2.59	4.25/2.76	1.488
N(S)	0.66/0.66	1. 36/1.26	0.02/0.02	2.04/1.94	0.105
Co(S-1)	0.09/0.09	0.09/0.10	4.00/2.67	4.20/2.86	1.342
Mn(S-1)	0.07/0.06	0.06/0.06	3.97/0.53	4.10/0.65	3.447
Co(C)	0.09/0.09	0.09/0.09	4.03/2.66	4.22/2.85	1.370
N(C)	0.66/0.65	0.40/1.27	0.03/0.03	2.09/1.95	0.144

Co atoms in the CoN-terminated surface have enhanced magnetic properties, as compared with the CoMn-terminated surface, which is confirmed by the calculated values of magnetic moments (MM) on these atoms (1.49 and 1.27 μB, respectively). In contrary, the magnetic properties of Mn atoms are manifested stronger at CoMn-terminated surface. The Mn atom at the topmost layer has MM of 3.61 μB while the MM on Mn subsurface atom in CoN-terminated surface is 3.45 μB. The surface Mn atoms are dominant for the magnetic properties of the systems. Since the calculated MMs on the atoms in the deeper layers of the both systems are considerably smaller than those at the surface, we conclude that the existence of the surface enhances the magnetic properties of $MnCo_3N$.

참고문헌

[1] S. Ishida and K. Kitawatase, J. Magn. Magn. Mater. **130**, 353 (1994).

[2] E. Wimmer, H. Krakauer, M. Weinert, and A. J. Freeman, Phys. Rev. B **24**, 6864 (1981) M. Weinert, E. Wimmer, and A. J. Freeman, Phys. Rev. B **26**, 4571 (1982).