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$Mn_{3-\delta}X_{\delta}Ga$(X=Fe, Co, Ni)の電子状態に関する第一原理計算

A first-principles study on the electronic structure of $Mn_{3-\delta}X_{\delta}Ga$ (X=Fe, Co, Ni)

一関高専[1]，東北大通研[2]　○谷林 慧[1]，三浦 良雄[2]，白井正文[2]

Ichinoseki Nat. Coll. Tech.[1], RIEC Tohoku Univ.[2]

○Satoru Tanibayashi[1], Yoshio Miura[2], Masafumi Shirai[2]

E-mail: satoru@ichinoseki.ac.jp

Magnetic materials with high perpendicular magneto-crystalline anisotropy (MCA) have great advantage in the reduction of the switching current and the enhancement of the thermal stability of Spin-RAMs. Among the magnetic materials with perpendicular MCA, $D0_{22}$-Mn–Ga alloys have attractive features of experimentally demonstrated the high perpendicular MCA (Ku > 1.0 MJ/m^3), the high Curie temperature (T_C = 730 K) and the small saturation magnetization (M_S = 0.25 μ_B/atom) due to the antiferromagnetic behavior [1,2]. Kubota, *et al*. reported that Mn_3Ga has the totally symmetric Δ_1 band crossing the Fermi level both in the majority- and minority-spin state in contrast to ferromagnetic transition metals such as bcc-Fe, and also that the Fermi level of Mn_3Ga in the minority-spin state is located at the valence band edge of the Δ_1 state [2]. These features show the possibility of the half-metallic electronic structure on the Δ_1 state by increasing valence-electron numbers by substituting transition metals such as Fe, Co, and Ni (denoted as X) for Mn. Although Chadov, *et al.* reported the band structure of $Mn_{3-\delta}Co_{\delta}Ga$ by using the CPA method [3], they did not focus on the Δ_1 state.

In order to study the substitution effects on the Δ_1 state, we investigated the electronic structure of $Mn_{3-\delta}X_{\delta}Ga$ (δ = 0, 0.125, 0.25) by using the first-principles calculations using the VASP code. In our calculations, we used a supercell with the lattice constant a of 7.533 Å, twice the value for the $D0_{22}$-structure of Mn_6Ga_2, including $Mn_{24-\varepsilon}X_{\varepsilon}Ga_8$ (ε = 0, 1, 2). All of the possible substitutions for Mn were examined. In addition, optimization of atomic positions was carried out in all of our calculations, but the changes of the positions were negligible. First, we found that total energies are smaller by 0.3 ~ 0.4 eV in case of substituting X for Mn(I) having negative magnetic moment than for Mn(II) having positive one, and that are independent of X.

Then, we obtained the band structures and the corresponding density of states (DOS) for the most stable atomic structures for ε of 0, 1, and 2, respectively. The total DOS at the Fermi level for the minority-spin states did not show significant decrease whereas the shapes of the DOS slightly changed.

In the presentation, we will report the analysis for the states having $\boldsymbol{k}$ vectors along the [0 0 1] direction.

[1] B. Balke, *et al.*, APL **90**, (2007) 152504.

[2] T. Kubota, *et al.*, APEX **4**, (2011) 043002.

[3] S. Chadov, *et al.*, Adv. Funct. Mater **23**, (2013) 832.