First-principles calculations on magnetism of $CrAu_3$ nano film

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Magnetism of a nano film has been attracting considerable attention because it is significantly modified as compared to that of the relevant bulk material.[1,2] A magnetic phase transition of ferromagnetic (FM) to antiferromagnetic (AFM) structure takes a places at $MnPt_3$(001) surface[2] whereas the reverse transition was observed at $MnAu_3$ (001) surface.[1] Films of $Au_{1-x}Cr_x$ fcc alloy formed at the interface when Cr was deposited on Au(001) and the magnetic moment of the Cr atom was significantly enhanced (~4 μ_B).[3] It was found from *ab initio* calculations[4] that it is energetically favorable for 3*d* transition metal impurities on Au(001) surface to exchange their site for Au atoms. In this study, we investigated magnetism of $CrAu_3$ nano films using the FLAPW method[5] in GGA for exchange correlation potential.

Before investigating the magnetism of the alloy ultrathin films, for the reference, calculations on bulk $CrAu_3$ have been done for plausible magnetic structures (PM, FM, and A-, C-, and G-type AFM states for $L1_2$ and PM, FM, and A-type AFM states for $D0_{22}$ crystal structures).

Magnetism of some $CrAu_3$ nano films (free standing CrAu(001) monolayer, 1(CrAu)/1Au/1(CrAu)(001), 1(CrAu)/3Au/1(CrAu)(001), and 1Au/1(CrAu)/1Au) was investigated. The nano films were calculated to be stable in a in-plane antiferromagnetic state. The calculated magnetic moments of Cr are 4.06, 3.86, 3.87, and 3.69 μ_B, respectively.

References

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