First Principles Calculations on Magnetism of $(CrAs)_1(GaAs)_1$ Superlattice

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Recently intensive studies have being carried out on magnetic semiconductors and ferromagnet-semiconductor hetrostructure s due to their possibility of application to spintronic industry in future. Thanks to hard works on this field ferromagnetic semiconductors with T_c above room temperature have been found out.[1,2] Recently CrAs, which has a NiAs structure, can be grown epitaxially in a zinc blende structure on a GaAs substrate and was proved to be a ferromagnetic half-metal with Curie temperature over 400 K.[3]

In this study, we investigated zinc-blend bulk CrAs and $(CrAs)_1(GaAs)_1$ superlattice by using the full-potential linearized augmented plane-wave (FLAPW)[4] method based on local spin density approximation(LSDA). The GaAs lattice constant was adopted and no relaxation was allowed. The ferromagnetic state is more stable compared to an antiferromagnetic state by about 270 meV for both of the bulk and the superlattice. The magnetism and electronic structure of the CrAs in the superlattice were not changed significantly from the those of the bulk zinc blende CrAs. The both systems were calculated to be half-metallic. The calculated total mangentic moments per Cr are $3.0\mu_B$/Cr for the both systems. The As atoms are coupled antiferromagetically to the Cr atoms and has appreciable magnetic moment of $-0.18\ \mu_B$.

References

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