

Magnetic Properties of Cr Substituted SiTe Compounds

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Diluted magnetic semiconductors (DMSs) have stimulated a great deal of interest because of their potential applications in spintronics[1,2]. The intensity of research in this area, both theoretical and experimental, is high. There has been an intense searching for ferromagnetic ordering in doped DMSs focusing on possible spin-transport properties, which has many potentially interesting device applications. Spintronics devices such as spin-valve transistors spin light-emitting diodes, non-volatile memory, logic devices, optical isolators and ultra-fast optical switches are some of the areas of interest for introducing the ferromagnetic properties at room temperature in a semiconductor[3-5]. Recently, it was shown that transition metal (TM) compounds based on the rock-salt GeTe are half-metallic ferromagnets[6]. It is then of interest to study related compounds, such as SiTe doped with TM atoms, so their electronic and magnetic properties are revealed.

We report systematic full-potential linearized augmented plane wave calculations of ternary TM compounds based on rock salt SiTe structure. All the calculations were carried out with the use of a first-principle full potential linearized augmented plane wave (FLAPW) method as implemented in QMD-FLAPW code[7] with the generalized gradient approximation[8] to the exchange-correlation potential. Lattice harmonics with $l \leq 8$ were employed to expand the charge density, potential, and wave functions inside the muffin-tin radii of 2.20, 2.50, and 2.60 a.u. for Cr, Si, and Te atoms, respectively. The number of basis functions was about 200 per atom. All core electrons were treated fully relativistically, while valence states were treated scalar relativistically. The self-consistent calculations were considered to be converged only when the integrated charge difference per formula unit between the input and the output charge densities was less than 1×10^{-4} .

The conventional unit cell of the hypothetical rock salt SiTe consists of one anion fcc lattice of Te and one cation fcc lattice of Si. In the case of 25 % substitution by Cr atoms, one transition metal atom is placed at one of the four sites of the Si fcc lattice, which result in the space group Pm-3m. The 50% substitution is realized by replacing two of the four Si atoms in the Si fcc lattice by the transition metal atom. In this way one obtains a tetragonal structure (P4/mmm). Since the investigated compounds are hypothetical, their exact lattice constant is not determined. Therefore, the calculations were carried out for different values of the lattice constants, so the total energy curve as dependent on the value of lattice constant could be drawn. From a function fitting to the curve we found the equilibrium lattice constant for the two investigated systems. In the case of the cubic CrSi_3Te_4 it was 11.64 a.u. and for the tetragonal CrSiTe_2 it was 7.89 a.u.

The obtained results confirm the magnetic properties of the both compounds. The presence of Cr atoms causes that the other atoms become slightly magnetized in both the cubic CrSi_3Te_4 and the tetragonal the presence CrSiTe_2 . In the equilibrium 25% substituted SiTe, i.e. in the CrSi_3Te_4 , the values of magnetic moment (MM) on the Cr atoms is 3.615 μB . The Si atoms are positively spin-polarized and the calculated MM on the atom is 0.183 μB . As for the Te atoms, there are two types: Te1 and Te2 with different surrounding. Both types of the Te atoms are negatively spin-polarized: the MMs are -0.013 and -0.065 on Te1 and Te2, respectively. Similar trends are observed in the other, CrSiTe_2 , compound with 50% substitution of Si atoms: the values of magnetic moments are 3.626, 0.032, -0.074, and -0.119 μB on Cr, Si, Te1, and Te2 atoms, respectively.

The results of our calculation suggest that the not yet synthesized materials such as CrSi_3Te_4 and CrSiTe_2 , can be considered for potential applications as magnetic materials.

References

- [1] Y. D. Park, A. T. Hanbicki, S. C. Erwin, C. S. Hellberg, J. M. Sullivan, J. E. Mattson, T. F. Ambrose, A. Wilson, G. Spanos, and B. T. Jonker, *Science* 295, 651 (2002).
- [2] S. Cho, S. Choi, S. C. Hong, Y. Kim, J. B. Ketterson, B.J. Kim, Y. C. Kim, and J.H. Jung, *Phys. Rev. B* 66, 033303 (2002).
- [3] A. Punnoose, K.M. Reddy, J. Hays *et al.*, *Appl. Phys. Lett.* 89 112509 (2006).
- [4] S.A. Chambers, *Mater. Today* 5, 34 (2002).
- [5] D.Chiba, M.Yamanouchi, F.Matsukara, H.Ohno, *Science* 301, 943 (2003).
- [6] Y. H. Zhao, W. H. Xie, L. F. Zhu, and B. G. Liu, *J. Phys.:Condens. Matter* 18, 10259 (2006).
- [7] P. Hohenberg and W. Kohn, *Phys. Rev.* 136, B864 (1964); W. Kohn and L. J. Sham, *Phys. Rev.* 140, A1133 (1965).
- [8] J. P. Perdew, K. Burke, and M. Ernzerhof, *Phys. Rev. Lett.* 77, 3865 (1996).