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Stability and half-metallicity of the (001) and (111) surfaces of CrTe with rocksalt structure

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We extend the recent study on above-room-temperature half-metallic ferromagnetism in bulk rocksalt CrTe [Y. Liu, S. K. Bose, and J. J. Kudrnovský, Phys. Rev. B **82,** 094435 (2010)] to the (001) and (111) surfaces by using the first-principles calculations. We show that the Te-terminated (111) surface is energetically more stable than both the (001) and the Cr-terminated (111) surfaces over the whole effective Cr chemical potential, and the surface stability of the Te-terminated (111) surface of rocksalt CrTe is comparable with that of the Te-terminated (001) surface of experimental zinc-blende CrTe. In addition, both the (001) and (111) surfaces of rocksalt CrTe retain the bulk half-metallicity. The atomic magnetic moments at the (111) surfaces are greatly different from those in the bulk rocksalt CrTe due to the breakdown of Cr-Te bond at the (111) surface, but the differences are very small for the case of the (001) surface due to the existence of Cr-Te bond at the (001) surface. These results indicate that it is feasible to fabricate the half-metallic CrTe thin films with rocksalt structure other than zinc-blende one. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4767232]

I. INTRODUCTION

Since Akinaga *et al.*[1] predicted theoretically and confirmed experimentally in 2000 the half-metallic (HM) ferromagnetism in zinc-blende (ZB) CrAs, transition-metal pnictides and chalcogenides (TM-PCs) with ZB structure have attracted increasing research interest in the past ten years, because most of this class of compounds were predicted to HM ferromagnets,[2–10] i.e., compounds for which only one spin channel is metallic, resulting in 100% spin polarization at the Fermi level. The half-metallicity and the comparable lattice structure with conventional binary semiconductors make ZB TM-PCs promising candidates of spin-injector materials in spintronic devices. However, for most of the TM-PCs, ZB structure is their metastable phase and their ground-state structure is the NiAs-type (MnP-type for CrAs).[4,9] Therefore, ZB TM-PCs would be experimentally realized mainly in the form of thin films or multilayers.

Remarkably, with the development of new techniques such as the molecular beam epitaxy, several TM-PCs with metastable ZB structure such as CrAs, CrSb, MnAs, MnTe, CrTe, and MnSb have been grown successfully in the form of thin films, multilayers or quantum dots.[1,11–16] Unfortunately, the number of experimental ZB TM-PCs is few due to the instability of the metastable ZB structure, e.g., Etgens *et al.*[17] observed experimentally that CrAs epilayers are orthorhombic for all thickness investigated but show a structural transition from a metastable ZB phase for very thin films, to the usual bulk MnP-type orthorhombic phase at higher thickness. Huang *et al.*[18] proposed theoretically that thick ZB epitaxial films are difficult to obtain by coherent epitaxial growth for vanadium-PCs, because the energy of epitaxial ZB structure is always higher than that of the epitaxial NiAs structure with its optimal match pattern to the substrate.

Therefore, it is necessary to search for new possible phases which are energetically more stable than the ZB phase for TM-PCs in order to realize more HM ferromagnets in them. We note that three of TM-TCs, MnS, MnSe, and MnTe with rocksalt (RS) structure have been synthesized experimentally in the bulk form.[19] In fact, the RS phase is most stable for both MnS and MnSe.[19,20] For MnTe, the most stable phase is the hexagonal NiAs structure,[19,20] but it can also crystallize in a cubic RS phase at $T > 1040\,^{\circ}\mathrm{C}$ or in a cubic ZB phase if grown by molecular-beam epitaxy.[19,21] In addition, HM ferromagnets with RS structure were also found in some alkaline-earth carbides and nitrides.[22,23]

CrTe, as a member of TM-PCs, has also the ground-state structure of NiAs-type.[24] Experimentally, CrTe thin films with metastable ZB structure have been grown on the ZnTe semiconductor substrate, but the measured Curie temperature is only about 100 K.[15] Can CrTe crystallize in the cubic RS phase like MnTe, MnSe, and MnS? Very recently, Liu *et al.*[25] investigated the electronic and magnetic properties of CrTe with RS structure. They found that RS CrTe exhibits HM ferromagnetism with a HM gap of 0.03 eV, and it is feasible to stabilize the RS structure because the RS phase is more stable than the experimental ZB phase with an energy that is about 0.25 eV/atom lower. Importantly, the estimated Curie temperature of RS CrTe is about 600 K, which is considerable higher than that of ZB CrTe.

For the practical applications of HM ferromagnets in spintronic devices, it is necessary to study the surface properties of HM ferromagnets, because the surface usually affects and even destroys the bulk half-metallicity.[6,26–28] In this

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