High Spin Polarization and Mechanic Stability of Half-Heusler Compounds: CrFeSn and CrFeGe as a Candidate in the Spin-FETs for Spintronic Applications

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ABSTRACT

In this work, we have performed self-consistent ab-initio calculation using the full-potential muffin-tin orbital method based on density functional theory (DFT), to study the electronic, magnetic and elastic properties of the half-Heusler compounds CrFeSn and CrFeGe with generalized gradient approximation (GGA+U) and mBJ- GGA+U. The magnetic proprieties of CrFeSn and CrFeGe are well defined within mBJ with an exact integer value of magnetic moment, using this approach for the total energy as a function of the strain. We calculate the elastic constants of the compounds studied in their structure which are not yet reported in the *C1b* structure, and can therefore be realized under ideal experimental circumstances. These alloys seem to be a potential candidate in the spin-FETs for spintronic applications.

Keywords: Half-Heusler, Magnetic, ab initio, Spin-FET, Spintronic.

Introduction

Several research groups have worked on the spin-field effect transistors (spin-FETs) device using semi-Heusler metals are considered to be optimal electrodes have also been employed in the spin-FETs where the spin polarized current injectors to lateral spin valves for spintronic applications [1]. The compounds (CrFeSn and CrFeGe) prove to be potential topological insulators and are promising candidates for improving the performance of microelectronics and optoelectronics [2]. A further investigation on the electronic and magnetic properties still required. In this letter, we present a computational study on the two CrFeSn and CrFeGe half-Heusler compounds using the full-potential muffin-tin orbital (FP-LMTO) method based on DFT.

Method Description

All electron full-potential linear muffin-tin orbital methodas implemented in the LMTART code is used for the calculation of the physical properties of the XYZ compounds and the density of state (DOS) [4], within the DFT in the generalized gradient approximation GGA + U approach for the optoelectronic properties. The half- Heusler compounds XYZ crystallizes in the face centered cubic (fcc) (Figure 1) structure with the space group F43m (No.216). The electronic configurations with core level correction are Cr (3d44s2), Fe (3d64s2) and Ge (4s24p2) [5], respectively. The self-consistent calculations are considered to converge only when the calculated total energy of the crystal

DOI: 10.21467/abstracts.122 ISBN: 978-81-954993-3-5

converges too less than 0.0001Ry. The convergence was obtained using k points in the first Brillouin zone where 1500 special k points were used for CrFeSn and CrFeGe compounds. For the Hubbard parameter U employed in the GGA+U, we have used U=4 eV for Fe and U=3.5 eV for Cr [9, 10].The exchange interaction J is set to J=0.

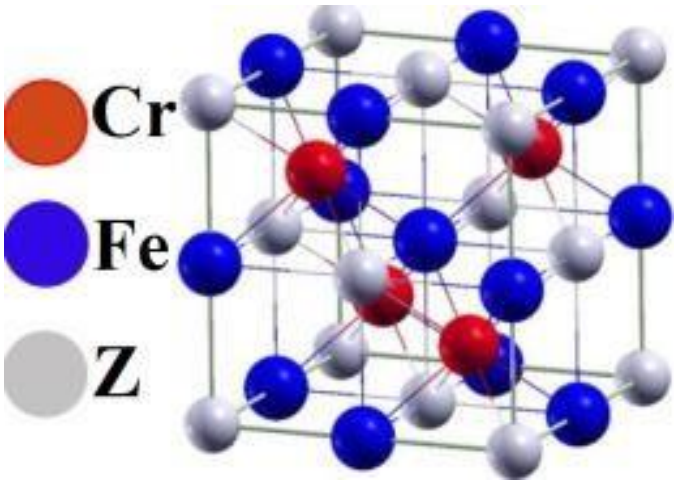

Fig.1 XYZ half-Heusler crystal structure

Results and Discussion

The two half-Heusler compounds (CrFeSn and CrFeGe) in *C1b* phases at zero temperature. Therefore, it is possible to say that this half-Heusler compound is a metallic ferromagnetic material when GGA method is used. However, when the mBJ method was used, the band gap was seen around the Fermi energy level in spin up electrons. This showed that spin-up electrons had semiconductor properties and spin-down electrons had metallic nature. Thus, in the mBJ method, the half- Heusler compound showed half-metal ferromagnetic nature.

Conclusion

Our calculation showed that the dependence of the magnetic properties on the Sn and Ge element in the investigated half-Heusler systems using DFT based on the full-potential muffin-tin orbital (FP-LMTO) method. The half-metallicity of the two families have also been confirmed. Furthermore, the studied of CrFeSn and CrFeGe compounds have demonstrated a certain mechanical stability performance against compression. These compounds can be considered as an ideal electrode material to achieve the ohmic contacts of spin-FET devices for spintronic applications.

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ISBN: 978-81-954993-3-5
DOI: 10.21467/abstracts.122
Series: AIJR Abstracts