Calculation of electronic, structural, optical and elastic properties of Heusler compounds (Co_2CrAl and Co_2CrGa)

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Abstract

In this paper, the structural, electronic, optical and elastic properties of Heusler compounds Co_2CrZ(Z=Al,Ga) have been studied. Calculations were performed using the Full-Potential-Linearized Argumented Plane Wave(FP-LAPW) method in the framework of density functional theory with GGA approximations by Wien2k computational code. The structural properties of Co_2CrZ(Z=Al,Ga) such as lattice constants, bulk modulus and its derivative properties are investigated during structural calculations. The lattice constants used in the calculations are 5.6787 (Å) and 5.7235(Å) for Co_2CrAl and Co_2CrGa compounds respectively. Moreover, electronic properties such as bandstructure and density of states were investigated. Co_2CrAl and Co_2CrGa compounds do not have any band gap at majority spin channel, but in minority channel there is a small band gap by an amount of 0.4 (eV) and 0.2 (eV) respectively, so these compounds are half-metals. We also studied the elastic properties of these compounds and the results showed that Co_2CrAl has more elastic resistivity than Co_2CrGa. Moreover, optical properties revealed good agreement between density of states and the imaginary part of dielectric function and the investigated static refractive index from real part of dielectric constants is about 10.

Keywords: Heusleralloys, density functional theory, bulk modul, elastic constants, youngmodul, optical properties

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