Influence of varying Germanium content on the optical function dispersion of Fe 2MnSi xGe 1-x: An ab initio study

Abstract

The optical dielectric functions of Fe 2MnSi 1-xGe x alloys for selected concentrations (x=0.0, 0.25, 0.5, 0.75 and 1.0) were investigated. The ferromagnetic Fe 2MnSi xGe 1-x is semiconducting with optical band gaps 0.507, 0.531, 0.539, 0.514 and 0.547 eV for the minority spin and is metallic for the majority spin. From the calculated results the half-metallic character and stability of ferromagnetic state for Fe 2MnSi xGe 1-x is determined. The total magnetic moment is found to be 3.0μ B for all alloys with the most contribution from Mn local magnetic moments. Iron atoms however exhibit much smaller spin moments, about 10 of the bulk value, and the sp atoms have induced magnetic moments due to the proximity of Fe first nearest neighbors, which couple antiferromagnetically with Fe and Mn spin moments. We have employed full-potential linearized augmented plane wave method based on spin-polarized density functional theory. The generalized gradient approximation exchange-correlation potential was used. The edge of optical absorption for ε2(ω) of spin-down varies between 0.507 (Fe 2MnGe) and 0.547 eV (Fe 2MnSi). Since the spin-up shows metallic nature, the Drude term was included in the spin-up optical dielectric functions. This confirms our finding that these materials are half-metallic. Furthermore, the reflectivity, refractivity and the absorption coefficient were calculated. These results show that the materials possess half-metallic character.