First principles study of the new half-metallicferromagnetic full-Heusler alloysCo2CrSi1_xGex: An ab-initio study

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Abstract : We have studied the structural, electronic, elastic,magnetic, thermal and thermodynamic property of thequaternary Heusler alloys Co2CrSi1-xGe(x = 0, 0.25, 0.5, 0.75, 1)with the linearized augmented plane wave method based ondensity functional theory (DFT)and implemented in wien2kcode. For exchange correlation potential we have used thegeneralized gradient approximation (GGA) of Perdew et al. Ourresults provide a theoretical study for the mixed HeuslerCo2CrSi1-xGexx(0 <x <1) in which no experimental or theoreticaldata are currently available. In their equilibrium L2structure,all concentrations are magnetic and metallic. However, there islinear variation of the lattice parameter. The bulk modulus, theelastic constants and the Debye temperature was studied withvariation of composition x of Ge. A regular solution model is usedto investigate the thermodynamic stability of the alloy which isessentially shows a miscibility gap phase by calculating thecritical temperatures of the alloys. In addition, the quasiharmonicDebye model is applied to determine the thermalproperties of the alloy.

Keywords : DFT, wien2k, GGA, Heusler, Debye