Abstract

The thesis shows that the cobalt based Heusler alloys can be potential materials for spintronics research and it tries to investigate on the structural, electronic and magnetic properties of the same in detail. It addresses different approaches to study structural, electronic and magnetic properties of cobalt based Heusler alloys. Density functional theory based calculations were carried out after experimentally measuring the structural and magnetic parameters of the alloys. At the end, machine learning model was used, based on the databases of different types of Heusler alloys, to predict some of the structural and magnetic parameters studied above. We observed very close agreement of the results found using these three approaches.

We have experimentally measured the lattice constant (5.74 Å), saturation magnetization (6.1 μ B /f.u.), Curie temperature (1073 K) and spin wave stiffness constant (10.4 nm 2 -meV) of Co_2FeGe full Heusler alloy. All these parameters are found to be one of the highest reported values in Heusler alloys domain, indicating the presence of strong exchange interactions between the constituent magnetic elements. Detailed theoretical calculations were carried out simulating the effect of the lattice stress, electron-electron correlations and atomic site disorder on the magnetic moment and half-metallicity of the alloy. From the phase stability analysis, ferromagnetic phase was found as the most stable one and from the ground state energy differences between the ferromagnetic and antiferromagnetic configurations, Curie temperature was calculated which shows very close agreement with the experimentally measured counterpart. Study of the phonon dispersion curves revealed that the alloy was dynamically stable.

Next, the effect of doping Ti atoms in place of Fe atoms in Co_2FeGe Heusler alloy in the $Co_2Fe_{1-x}Ti_xGe$ phase with x = 0, 0.5 and 0.75 was studied. The lattice constant gradually increased and the saturation magnetization decreased gradually with increasing Ti concentrations due to the larger atomic radius and ferrimagnetic coupling of Ti atoms. The measured spin wave stiffness constant was decreased to 2.56 nm^2-meV and 4.56 nm^2-meV for Ti concentration (x) equal to 0.5 and 0.75 respectively. The effect of the electron-electron correlations on the band structure, electronic density of states and phonon dispersion curve was calculated in detail. We measured the lattice constant (5.74 Å), the saturation magnetization (1.24 μ B /f.u.), Curie temperature (583 K) and the spin wave stiffness constant (3.259 nm 2 -meV) of the CoFeTiSi quaternary Heusler alloy. The calculated lattice constant and saturation magnetization closely followed the experimental results. Electron density of states calculation showed that the alloy is perfectly half-metallic in nature. Effect of lattice stress and atomic site disorder on the electronic density of states was calculated. Dynamical stability of the alloy was also confirmed from the phonon dispersion curve.

At last, a cost effective alternative way to predict the lattice constant, formation energy and saturation magnetization of full, half, inverse and quaternary Heusler alloys was formulated based on the Random forest supervised machine learning approach. The model prediction was sufficiently accurate which was further compared with the previously theoretically calculated and experimentally measured lattice constants and saturation magnetizations of the Co^2FeGe and CoFeTiSi Heusler alloys, indicating the potential prediction ability of the technique.