First-principles and Monte Carlo investigations of the magnetic properties of (Co,Ni)CrIn Heusler alloys.

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A wide range of impressive physical effects such as magnetically and thermally induced shape memory effect, large magnetoresistance and giant magnetocaloric effect is a distinguishing feature of ferromagnetic (FM) Heusler alloys [1]. Ones of the most studied and well-investigated Heusler alloys are Ni_2MnZ-based materials [1]. They are ferromagnetic in austenite and martensite. At present, the Co_2CrIn practically is not investigated until now but have attracted a huge interest from both experimental and theoretical points of view due to its complex half-metallic behavior. Besides, the magnetization measurements have shown that Co_2CrIn compound has ferrimagnetic order with a magnetic moment of 1.18 μ_B at 5 K [2].

In this work, we present results of *ab initio* investigations of the ground state and magnetic properties of $Co_{2-x}Ni_xCrIn$ Heusler alloys with the help of density functional theory implemented in VASP [3,4] and the SPR-KKR [5] packages. To perform the crystal structure optimization, we used the 16-atom $L2_1$ supercell with two magnetic configurations. The first one was the ferromagnetic (FM) state, in which all magnetic moments are positive. The second one was the ferromagnetic (FIM) state, where magnetic moments of Ni and Co atoms are positive and ones of Cr have an antiparallel arrangement.

Our results show that ground state of Co_2CrIn alloy is FM. The equilibrium lattice parameter of FM configuration is 5.98 Å. FM configuration of CoNiCrIn alloy is also stable. The equilibrium lattice parameter for CoNiCrIn is 6.03 Å. Ni2CrIn alloys has FIM ground state with pairwise antiparallel Cr magnetic moments and equilibrium lattice parameter 6.05 Å. In order to find a possibility of martensitic transformation for these alloys, we performed the calculations of the total energy relative to the cubic phase as functions of tetragonality c/a. It was found that the tetragonal distortion does not lead to an appearance of a stable martensitic phase of Co_2CrIn and CoNiCrIn alloys. For the case of Ni_2CrIn the stable martensitic phase can realized for FIM magnetic configuration. At the second stage of study, Heisenberg magnetic exchange parameters were calculated for obtained equilibrium lattice parameters. At the final stage, the temperature dependences of magnetization were computed using classical three-dimensional Heisenberg model and Monte Carlo simulations.

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