Effect of Co substitution on Ni_2MnGe Heusler alloy: first principles study

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Many studies of Ni_2MnGe and Co_2MnGe indicated several intriguing properties of these alloys. Both Ni_2MnGe and Co_2MnGe are known as Heusler alloys with the $L2_1$ crystallographic structure. The study is focused on the effect on the magnetic properties induced by substitution of Ni by Co. The unit cell of the studied $Ni_{2-x}Co_xMnGe$ ($0 \leq x \leq 1.0$) system is the cubic $L2_1$, which contains four *fcc* sublattices at A(0 0 0), B($\frac{1}{4}$ $\frac{1}{4}$ $\frac{1}{4}$), C($\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$) and D($\frac{3}{4}$ $\frac{3}{4}$ $\frac{3}{4}$) sites. These sites are occupied by Ni, Mn, Ni and Ge atoms, respectively. Due to the Co substitution the chemical disorder between A and C sites is assumed, and the studied system is treated in band calculations within the CPA as implemented in FPLO. It follows that, the Co substitution instead of Ni may lead to a decrease of the lattice constant and an increase of the total magnetic moment of compound. The Mn(B) has the largest local moment (above 3 μ_B) coupled parallel to moments on the Ni(A,C) and Co(A,C), which are found in the ranges of $0.19 \div 0.26$ μ_B for Ni(A,C) and $1.03 \div 0.97$ μ_B for Co(A,C). Since Co_2MnGe has been previously predicted to be half-metallicity, it is interesting to track the spin-polarization at changing Co content and disorder rate.