Effect of local environment on the magnetic properties of the $(Cu_{1-x}Co_x)_2MnSn$ alloy

M. Pugaczowa-Michalska
Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland

9.7 cm

The electronic structure and the ground state properties of the quaternary Heusler alloy $(Cu_{1-x}Co_x)_2MnSn$ has been studied using the self-consistent the spin-polarized tight-binding linear muffin-tin orbital (TB-LMTO) method. The self-consistent band calculations were performed for the experimental lattice constant [1]. The $(Ni_{1-x}Co_x)_2MnSn$ compound has been calculated for the supercell structure and for the following values of the parameter x: 0; 0.125; 0.25; 0.375; 0.5; 0.625; 0.75; 0.875; 1.0. The supercell structure with 16 atoms in the cell can be divided into 16 simple cubic sublattices. Eight of them are occupied by Mn and Sn atoms ordered in a L21 structure, whereas Ni and Co randomly occupy the remaining eight sublattices. The magnetic properties are in good agreement with experimental data presented in [1]. In particular the observed linear change of total magnetic moment with concentration of Co is reproduced by our calculations. We present the values of local magnetic moments of the Co and Cu atoms for various possible configurations. The dependence of magnetic moments on the local environment is studied for all concentrations.

[1] E.Uhl, J. Magn. Magn. Magn. 25 (1981) 221-227.

13.4 cm

Subject category :

7. Computations of Electronic Band Structures

Presentation mode :
poster

Corresponding author :
M. Pugaczowa-Michalska

Address for correspondence :
Institute of Molecular Physics,
Polish Academy of Sciences,
Smoluchowskiego 17,
60-179 Poznan, Poland

Email address :
maria@ifmpan.poznan.pl